RESEARCH CENTER
Saclay - Île-de-France

FIELD

Activity Report 2019

Section New Results

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AVIZ Project-Team

7. New Results

7.1. A Model of Spatial Directness in Interactive Visualization

Participants: Stefan Bruckner [University of Bergen], Tobias Isenberg [correspondant], Timo Ropinski [University of Ulm], Alexander Wiebel [Hochschule Worms University of Applied Sciences].

$$\begin{tikzcd}
 & \mathscr{V} \arrow[r, "o"] \arrow[dd, dashed, "vi"] & \mathscr{O} \arrow[dr, "u_p"] \arrow[dd, dashed, "om"] & \\
\mathscr{D} \arrow[ur, "v"] & & & \mathscr{U} \arrow[dl, "u_a"] \\
 & \mathscr{I} \arrow[ul, "i"] & \mathscr{M} \arrow[l, "m"] &
\end{tikzcd}$$

Figure 4. Illustration of the model of interaction directness.

We discuss the concept of directness in the context of spatial interaction with visualization [2] . In particular, we propose a model that allows practitioners to analyze and describe the spatial directness of interaction techniques, ultimately to be able to better understand interaction issues that may affect usability. To reach these goals, we distinguish between different types of directness (Figure 4). Each type of directness depends on a particular mapping between different spaces, for which we consider the data space, the visualization space, the output space, the user space, the manipulation space, and the interaction space. In addition to the introduction of the model itself, we also show how to apply it to several real-world interaction scenarios in visualization, and thus discuss the resulting types of spatial directness, without recommending either more direct or more indirect interaction techniques. In particular, we will demonstrate descriptive and evaluative usage of the proposed model, and also briefly discuss its generative usage.

More on the project Web page: https://tobias.isenberg.cc/VideosAndDemos/Bruckner2019MSD.

7.2. Increasing the Transparency of Research Papers with Explorable Multiverse Analyses

Participants: Pierre Dragicevic [correspondant], Yvonne Jansen [CNRS], Abhraneel Sarma [University of Michigan], Matthew Kay [University of Michigan], Fanny Chevalier [University of Toronto].

We presented explorable multiverse analysis reports, a new approach to statistical reporting where readers of research papers can explore alternative analysis options by interacting with the paper itself [34]. This approach draws from two recent ideas: i) multiverse analysis, a philosophy of statistical reporting where paper authors report the outcomes of many different statistical analyses in order to show how fragile or robust their findings are; and ii) explorable explanations, narratives that can be read as normal explanations but where the reader can also become active by dynamically changing some elements of the explanation. Based on five examples and a design space analysis, we showed how combining those two ideas can complement existing reporting approaches and constitute a step towards more transparent research papers. This work received a best paper award at ACM CHI.

More on the project Web page, including interactive demos: https://explorablemultiverse.github.io/.

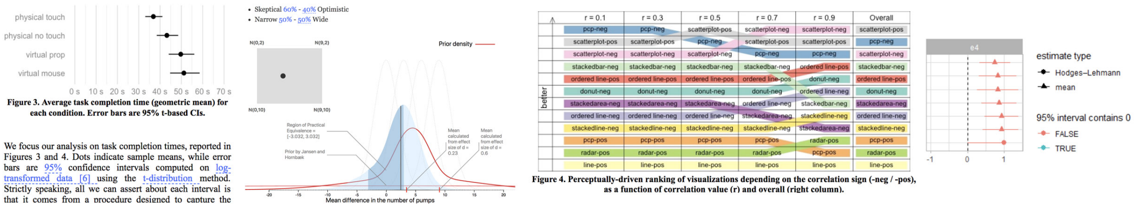


Figure 5. Examples of explorable multiverse analyses.

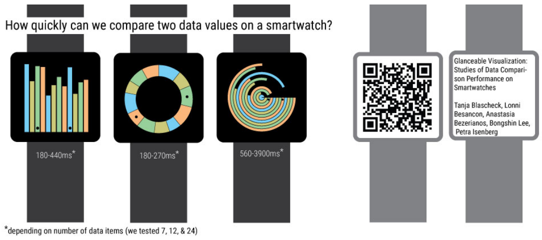


Figure 6. Comparison of bar, donut, and radial bar charts on a smartwatch.

7.3. Glanceable Visualizations for Smartwatches

Participants: Tanja Blascheck [correspondant], Lonni Besançon [Linköpping University], Anastasia Bezerianos, Bongshin Lee [Microsoft Research], Petra Isenberg.

The goal of this project is to study very small data visualizations, micro visualizations, in display contexts that can only dedicate minimal rendering space for data representations. Specifically, we define micro visualizations as small-scale visualizations that lack or have a limited set of reference structures such as labels, data axes, or grid lines and have a small physical footprint of a few square centimeters. Micro visualizations can be as simple as small unit-based visualizations such as a battery indicator but also include multi-dimensional visualizations such as star glyphs, small geographic visualizations or even small network visualizations. Although micro visualizations are essential to mobile visualization contexts, we know surprisingly little about their general visual and interaction design space or people's ability in interpreting micro visualizations. We will address this gap by proposing a common framework, conducting empirical studies to understand people's abilities to interpret these visualizations while in motion, and by developing a software toolkit to aid practitioners in developing micro visualizations for emerging mobile and wearable displays.

In summary, we aim at paving the way for a pervasive use of visualizations and thus a better and broader understanding of the complex world around us.

More information in related publications ([1],[48]) and on the project Web page: https://www.aviz.fr/smartwatchperception.

7.4. Hybrid Touch/Tangible Spatial 3D Data Selection

Participants: Lonni Besançon [Linköpping University], Mickael Sereno [correspondant], Lingyun Yu [Hangzhou Dianzi University], Mehdi Ammi [University of Paris 8], Tobias Isenberg.

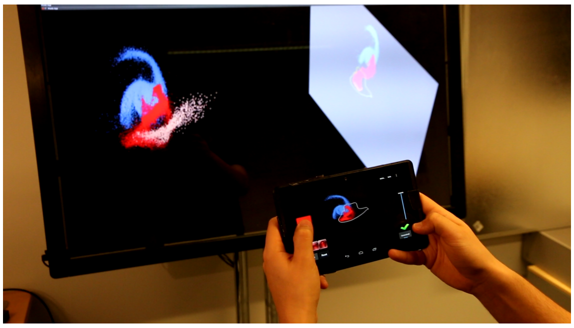


Figure 7. Illustration of Tangible Brush application which combines a spatial-aware multi-touch tablet and a remote large screen which shows different perspectives of the view shared with the tablet.

We discussed spatial selection techniques for three-dimensional datasets. Such 3D spatial selection is fundamental to exploratory data analysis. While 2D selection is efficient for datasets with explicit shapes and structures, it is less efficient for data without such properties.

We first proposed a new taxonomy of 3D selection techniques [12], focusing on the amount of control the user has to define the selection volume. We then described the 3D spatial selection technique Tangible Brush (Figure 7), which gives manual control over the final selection volume. It combines 2D touch with 6-DOF 3D tangible input to allow users to perform 3D selections in volumetric data. We use touch input to draw a 2D lasso, extruding it to a 3D selection volume based on the motion of a tangible, spatially-aware tablet. We described our approach and presented its quantitative and qualitative comparison to state-of-the-art structure-dependent selection. Our results show that, in addition to being dataset-independent, Tangible Brush is more accurate than existing dataset-dependent techniques, thus providing a trade-off between precision and effort.

7.5. Is there a reproducibility crisis around here? Maybe not, but we still need to change

Participants: Alex Holcombe [The University of Sydney], Charles Ludowici [The University of Sydney], Steve Haroz.

Those of us who study large effects may believe ourselves to be unaffected by the reproducibility problems that plague other areas [39]. However, we will argue that initiatives to address the reproducibility crisis, such as preregistration and data sharing, are worth adopting even under optimistic scenarios of high rates of replication success. We searched the text of articles published in the Journal of Vision from January through October of 2018 for URLs (our code is here: https://osf.io/cv6ed/) and examined them for raw data, experiment code, analysis code, and preregistrations. We also reviewed the articles' supplemental material. Of the 165 articles, approximately 12% provide raw data, 4% provide experiment code, and 5% provide analysis code. Only one article contained a preregistration. When feasible, preregistration is important because p-values are not interpretable unless the number of comparisons performed is known, and selective reporting appears to be common across fields. In the absence of preregistration, then, and in the context of the low rates of successful replication found across multiple fields, many claims in vision science are shrouded by uncertain credence. Sharing de-identified data, experiment code, and data analysis code not only increases credibility and ameliorates the negative impact of errors, it also accelerates science. Open practices allow researchers to build on others' work more quickly and with more confidence. Given our results and the broader context of concern by funders, evident in the recent NSF statement that "transparency is a necessary condition when designing scientifically valid research" and "pre-registration..." can help ensure the integrity and transparency of the proposed research", there is much to discuss.

CEDAR Project-Team

7. New Results

7.1. Quotient summaries of RDF graphs

We have continued and finalized our work on the question of efficiently computing informative summaries of large, heterogeneous RDF graphs. Such summaries simplify the users' efforts to understand and grasp the content of an RDF graph with which they are not familiar. For instance, Figure 1 shows the summary constructed fully automatically out of a benchmark graph of a bit more than 100 million triples.

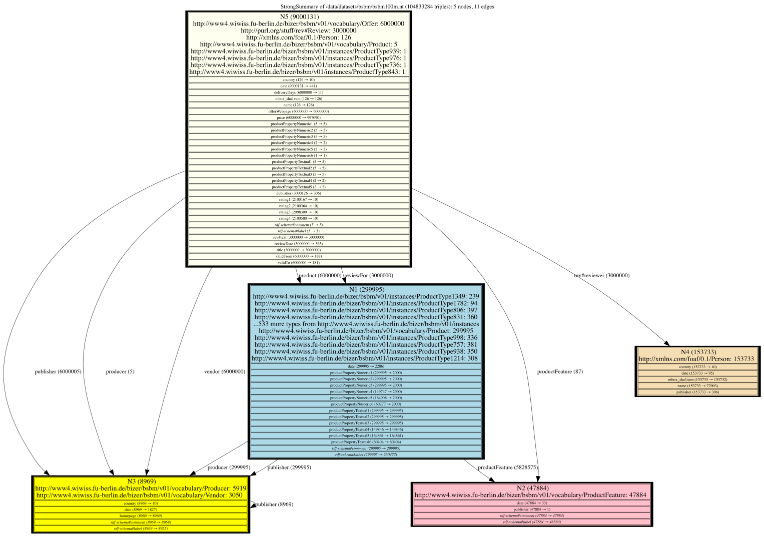


Figure 1. RDFQuotient summary of a 100 million triples graph.

We have presented, together with co-authors, a tutorial on the problem of summarizing RDF graphs, at the EDBT 2019 conference [21].

We have demonstrated new algorithms for efficiently building RDF quotient summaries out of large RDF graphs, in an incremental fashion, in [19].

Last but not least, a VLDB Journal submitted article systematizing most of our contributions in this area has been accepted (pending a minor, strictly cosmetic revision which will be sent out in January 2020).

7.2. Efficient query answering over semantic graphs

Query answering in RDF knowledge bases has traditionally been performed either through graph saturation, that is, adding all implicit triples to the graph, or through query reformulation, i.e. modifying the query to look for the explicit triples entailing precisely what the original query asks for. The most expressive fragment of RDF for which reformulation-based quey answering exists is the so-called database fragment of RDF (Goasdoué et al., EDBT 2013), in which implicit triples are restricted to those entailed using an RDFS ontology. Within this fragment, query answering was so far limited to the interrogation of data triples (non-RDFS ones); however, a powerful feature specific to RDF is the ability to query data and schema triples together. In [12], we address the general query answering problem by reducing it, through a pre-query reformulation step, to that solved by the query reformulation technique mentioned above (EDBR 2013). Our experiments also demonstrate the very modest cost (performance overhead) of this more powerful (more expressive) reformulation algorithm.

7.3. Scalable storage for polystores

Big data applications routinely involve diverse datasets: relations flat or nested, complex-structure graphs, documents, poorly structured logs, or even text data. To handle the data, application designers usually rely on several data stores used side-by-side, each capable of handling one or a few data models (e.g., many relational stores can also handle JSON data), and each very efficient for some, but not all, kinds of processing on the data.

A current limitation is that applications are written taking into account which part of the data is stored in which store and how. This fails to take advantage of (i) possible redundancy, when the same data may be accessible (with different performance) from distinct data stores; (ii) partial query results (in the style of materialized views) which may be available in the stores. If data migrates to another store, to take advantage of its performance for a specific task, applications must be re-written; this is tedious and error-prone.

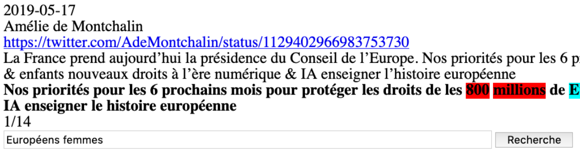
In [11], we present ESTOCADA, a novel approach connecting applications to the potentially heterogeneous systems where their input data resides. ESTOCADA can be used in a polystore setting to transparently enable each query to benefit from the best combination of stored data and available processing capabilities. ESTOCADA leverages recent advances in the area of view-based query rewriting under constraints, which we use to describe the various data models and stored data. Our experiments illustrate the significant performance gains achieved by ESTOCADA.

7.4. Novel fact-checking architectures and algorithms

A frequent journalistic fact-checking scenario is concerned with the **analysis of statements** made by individuals, whether in public or in private contexts, and the propagation of information and hearsay (“who said/knew what when”), mostly in the public sphere (e.g., in discourses, statements to the media, or on public social networks such as Twitter), but also in private contexts (these become accessible to journalists through their sources). Inspired by our collaboration with fact-checking journalists from Le Monde, France’s leading newspaper, we have described in [17] a Linked Data (RDF) model, endowed with formal foundations and semantics, for describing *facts, statements*, and *beliefs*. Our model combines temporal and belief dimensions to trace propagation of knowledge between agents along time, and can answer a large variety of interesting questions through RDF query evaluation. A preliminary feasibility study of our model incarnated in a corpus of tweets demonstrates its practical interest.

Based on the above model, we implemented and demonstrated BELINK [13], a prototype capable of storing such interconnected corpora, and answer powerful queries over them relying on SPARQL 1.1. The demo showcased the exploration of a rich real-data corpus built from Twitter and mainstream media, and interconnected through extraction of statements with their sources, time, and topics.

Statistic (numerical) data, e.g., on unemployment rates or immigrant populations, are hot fact-checking topics. In prior work, we have transformed a corpus of high-quality statistics from INSEE, the French national statistics institute, into an RDF dataset (Cao et al., Semantic Big Data Workshop, 2017, https://hal.inria.fr/hal-01583975), and shown how to locate inside the information most relevant to (thus, most likely to be useful to fact-check) a given keyword query (Cao et al., Web and Databases Workshop, 2018, https://hal.inria.fr/hal-01745768). Following on the above work, in [16], we present a novel approach to extract from text documents, e.g., online media articles, mentions of statistic entities from a reference source. A claim states that an entity has certain value, at a certain time. This completes a fact-checking pipeline from text, to the reference data closest to the claim. Using it, fact-checking journalists only have to interpret the difference between the claimed and the reference value. We evaluated our method on the INSEE reference dataset and show that it is efficient and effective. Further, this algorithm was adapted also to the (more challenging) context of content published on Twitter. This has lead to a semi-automatic interface for detecting statistic claims made in tweets and starting a semi-automatic fact-check of those claims, based on INSEE data. Figure 2 depicts the interface of this Twitter fact-checking system, which was shared with our Le Monde journalist partners.



2019-05-17
Amélie de Montchalin
https://twitter.com/AdeMontchalin/status/1129402966983753730
La France prend aujourd'hui la présidence du Conseil de l'Europe. Nos priorités pour les 6 prochains mois pour protéger les droits des 800 millions d'Européens : droits des femmes & enfants nouveaux droits à l'ère numérique & IA enseigner l'histoire européenne
Nos priorités pour les 6 prochains mois pour protéger les droits de les 800 millions de Européens : droits de les femmes & enfants nouveaux droits à le ère numérique & IA enseigner le histoire européenne
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Européens femmes

Figure 2. Screen capture of our Twitter fact-checking module.

7.5. Semantic graph exploration through interesting aggregates

RDF graphs can be large and complex; finding out interesting information within them is challenging. One easy method for users to discover such graphs is to be shown *interesting aggregates* (under the form of two-dimensional graphs, i.e., bar charts), where interestingness is evaluated through statistics criteria. While well understood for relational data, such exploration raises multiple challenges for RDF: facts, dimensions and measures have to be *identified* (as opposed to known beforehand); as there are more candidate aggregates, assessing their interestingness can be very costly; finally, *ontologies* bring novel specific challenges through the presence of *implicit* data, but also novel opportunities, enabling *ontology-driven exploration* from an aggregate initially proposed by the system.

The system DAGGER we had previously proposed (2017) pioneered this approach, however its is quite inefficient, in particular due to the need to evaluate numerous, expensive aggregation queries.

In 2019, we have built upon DAGGER to develop more efficient and more expressive versions thereof. Thus:

- In [22], we describe DAGGER$^+$, which builds upon DAGGER and leverages *sampling* to speed up the evaluation of potentially interesting agregates. We show that DAGGER$^+$ achieves very significant execution time reductions, while reaching results very close to those of the original, less efficient system.
- Going beyond the expressive power of (candidate aggregates enumerated by) DAGGER, we have developed and demonstrated [15] SPADE, a *generic, extensible framework*, which we instantiated with: (i) novel methods for enumerating candidate measures and dimensions in the vast space of possibilities provided by an RDF graph; (ii) a set of aggregate interestingness functions; (iii) ontology-based interactive exploration, and (iv) efficient early-stop techniques for estimating the interestingness of an aggregate query. A multi-dimensional aggregate automatically identified by SPADE appears in Figure 3 .

7.6. A Next-Generation Unified Data Analytics Optimizer

Big data analytics systems today still lack the ability to take user performance goals and budgetary constraints, collectively referred to as "objectives", and automatically configure an analytic job to achieve the objectives.

In [10], we present a unified data analytics optimizer that can automatically determine the parameters of the runtime system, collectively called a job configuration, for general dataflow programs based on user objectives. UDAO embodies key techniques including in-situ modeling, which learns a model for each user objective in the same computing environment as the job is run, and multi-objective optimization, which computes a Pareto optimal set of job configurations to reveal tradeoffs between different objectives.

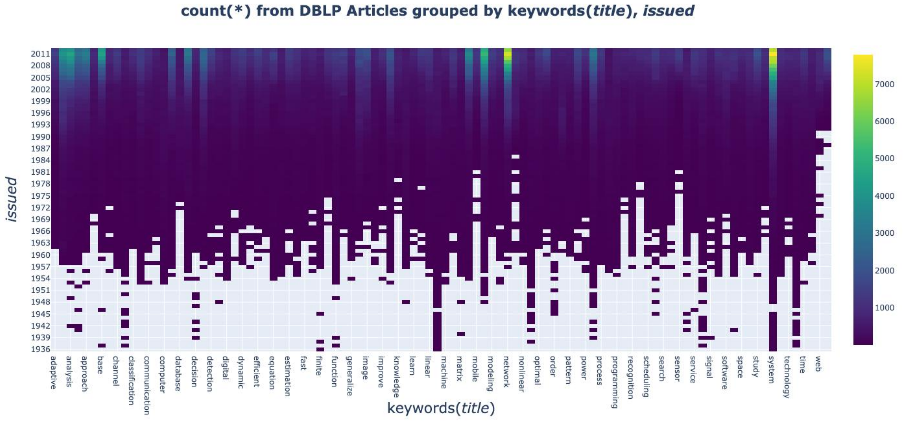

Figure 3. Interesting multi-dimensional aggregate automatically identified by DAGGER.

Using benchmarks developed based on industry needs, our demonstration will allow the user to explore (1) learned models to gain insights into how various parameters affect user objectives; (2) Pareto frontiers to understand interesting tradeoffs between different objectives and how a configuration recommended by the optimizer explores these tradeoffs; (3) end- to-end benefits that UDAO can provide over default configurations or those manually tuned by engineers.

We demonstrated this work at the VLDB 2019 conference.

7.7. A factorized version space algorithm for interactive database exploration

One challenge in building an interactive database exploration system is that existing active learning (AL) techniques experience slow convergence when learning the user interest on large datasets. To address this slow convergence problem, we augmented version space-based AL algorithms, which have strong theoretical results on convergence but are very costly to run, with additional insights obtained in the user labeling process. These insights lead to a novel algorithm that factorizes the version space to perform active learning in a set of subspaces, with provable results on optimality, as well as optimizations for better performance. Evaluation results using real world datasets show that our algorithm significantly outperforms state-of-the-art version space algorithms, as well as our previous data exploration algorithm DSM (Huang et al., PVLDB 2018), for large database exploration.

The above work was accepted as a conference paper at ICDM 2019 [14]. In addition, we have presented a demonstration of our software at NeurIPS 2019 [26], where people could interact with our system over two real-world datasets, and also observe how our system compares against traditional AL algorithms.

CELESTE Project-Team

6. New Results

6.1. Minimal penalty algorithms for model selection

Birgé and Massart proposed in 2001 the slope heuristics as a way to choose optimally from data an unknown multiplicative constant in front of a penalty. It is built upon the notion of minimal penalty, and it has been generalized since to some "minimal-penalty algorithms". The survey [3] by S. Arlot reviews the theoretical results obtained for such algorithms, with a self-contained proof in the simplest framework, precise proof ideas for further generalizations, and a few new results. Explicit connections are made with residual-variance estimators —with an original contribution on this topic, showing that for this task the slope heuristics performs almost as well as a residual-based estimator with the best model choice— and some classical algorithms such as L-curve or elbow heuristics, Mallows' C_p, and Akaike's FPE. Practical issues are also addressed, including two new practical definitions of minimal-penalty algorithms that are compared on synthetic data to previously-proposed definitions. Finally, several conjectures and open problems are suggested as future research directions. This extensive survey is followed by a discussion by 13 authors, and a rejoinder in which another original result is proved (theoretical validation of the slope heuristics when all models in the collection are biased).

6.2. Kernel change-point detection

In collaboration with A. Celisse and Z. Harchaoui, S. Arlot worked on the change-point problem with data belonging to a general set. They built a penalty for choosing the number of change-points in the kernel-based method of Harchaoui and Cappé (2007). This penalty generalizes the one proposed by Lebarbier (2005) for one-dimensional signals. They prove in [4] a non-asymptotic oracle inequality for the proposed method, thanks to a new concentration result for some function of Hilbert-space valued random variables. Experiments on synthetic and real data illustrate the accuracy of our method, showing that it can detect changes in the whole distribution of data, even when the mean and variance are constant. This method has since been used successfully by several authors in various applied contexts.

6.3. A probabilistic method to characterize genomic alterations of tumors

Characterizing the genomic copy number alterations (CNA) in cancer is of major importance in order to develop personalized medicine. Single nucleotide polymorphism (SNP) arrays are still in use to measure CNA profiles. Among the methods for SNP-array analysis, the Genome Alteration Print (GAP) by Popova et al, based on a preliminary segmentation of SNP-array profiles, uses a deterministic approach to infer the absolute copy numbers profile. C. Keribin with Y. Liu, Y. Rozenholch and T. Popova developed a probabilistic model in [9] for GAP and define a Gaussian mixture model where centers are constrained to belong to a frame depending on unknown parameters such as the proportion of normal tissue. The estimation is performed using an expectation-maximization (EM) algorithm to recover the parameters characterizing the genomic alterations as well as the most probable copy number change of each segment and the unknown proportion of normal tissue. The tumor ploidy can be deduced from penalized model selection criterion. The model is tested on simulated and real data.

Surprisingly, the BIC selection criterion cannot recover the actual ploidy in the real data sets as slope heuristics do, even though all models are wrong. C. Keribin, in a discussion of S. Arlot's survey, gave some arguments to explain these behaviors [8].

6.4. New results for stochastic bandits

M. Brégère and G. Stoltz, in collaboration with P. Gaillard (Sierra team) and Y. Goude (EDF), provided a methodology in [5] based on a modeling by linear bandits, for managing (influencing) electricity consumption by sending tariff incentives. The main result is the very modeling of the problem: consumption is modeled as a generalized additive model based on the probabilistic allocation of tariffs picked and on the context (given by the type of day, hour of the day, weather conditions, etc.). Mathematical results are, on the other hand, direct extensions of earlier results for the LinUCB algorithm (see Li et al., 2010; Chu et al., 2011; Abbasi-Yadkori et al., 2011). Simulations on realistic data are provided: for bandit algorithms, one needs a data simulator, which we created based on an open data set consisting of households in London.

A second important result was obtained by H. Hadiji: he characterized the cost of adaptation to the unknown (Höderian) smoothness payoff functions in continuum-armed bandits [14]. He first rewrote and slightly extended the regret lower bounds exhibited by Locatelli and Carpentier (2018), and then exhibited an algorithm with matching regret upper bounds. This algorithm, unlike virtually all previous algorithms in X-armed bandits, which zoomed in as time passes, zooms out as time passes. This solves a problem that had been open for several years.

Also, H. Hadiji and G. Stoltz, in collaboration with P. Ménard (SequeL team) and A. Garivier, submitted a revised version of their results of simultaneous optimality (from both a distribution-dependent and a distribution-free viewpoints) for a variant of the KL-UCB algorithm in the case of vanilla K-armed stochastic bandits [22].

6.5. Robust risk minimization for machine learning

In collaboration with S. Minsker (USC), T. Mathieu worked on obtaining new excess risk bounds in robust empirical risk minimization. The method proposed in [29] is inspired from the robust risk minimization procedure using median-of-means estimators in Lecué, Lerasle and Mathieu (2018). The obtained excess risk are faster than the so-called "slow rate of convergence" obtained for the minimization procedure in Lecué, Lerasle and Mathieu (2018) and a slightly modified procedure achieves a minimax rate of convergence under low moment assumptions. Experiments on synthetic corrupted data and real dataset illustrate the accuracy of the method showing high performance in classification and regression tasks in a corrupted setting.

6.6. Optimal pair-matching

The sequential pair-matching problem appears in many applications (in particular for the internet) where one wants to discover, sequentially, good matches between pairs of individuals, for a given budget. C. Giraud, Y. Issartel, L. Lehéricy and M. Lerasle propose a formulation of this problem as a special bandit problem on graphs [23]. Formally, the set of individuals is represented by the nodes of a graph where the edges, unobserved at first, represent the potential good matches. The algorithm queries pairs of nodes and observes the presence/absence of edges. Its goal is to discover as many edges as possible with a fixed budget of queries. Pair-matching is a particular instance of multi-armed bandit problem in which the arms are pairs of individuals and the rewards are edges linking these pairs. This bandit problem is non-standard though, as each arm can only be played once.

Given this last constraint, sublinear regret can be expected only if the graph has some underlying structure. C. Giraud, Y. Issartel, L. Lehéricy and M. Lerasle show in [23] that sublinear regret is achievable in the case where the graph is generated according to a Stochastic Block Model (SBM) with two communities. Optimal regret bounds are computed for this pair-matching problem. They exhibit a phase transition related to the Kesten-Stigund threshold for community detection in SBMs. In practice, it is meaningful to constrain each node to be sampled less than a given amount of times, in order to avoid concentration of queries on a set of individuals. This setting is more challenging both on the statistical side and the algorithmic side. Optimal rates are also derived in this context, exhibiting how the regret deteriorates with this constraint.

6.7. Minimax estimation of network complexity in graphon model

In network analysis, the graphon model has attracted a lot of attention as a non-parametric model with some universal properties. However, this approach suffers from interpretability and identifiability issues in practice. A first solution to this problem was obtained by Y. Issartel: he introduces an identifiable and interpretable functional of the graphon, which measures the complexity of network [25]. It has simple interpretations on popular examples of random graphs: it matches the number of communities in stochastic block models; the dimension of the Euclidean space in random geometric graphs; the regularity of the link function in Hölder graphons. He also provides an estimation procedure of this complexity that is minimax optimal.

COMETE Project-Team

7. New Results

7.1. Foundations of privacy and quantitative information flow

Privacy and information flow have the common goal of trying to protect sensitive information. Comete focuses in particular on the potential leaks due to inference from data that are public, or anyway available to the adversary. We consider the probabilistic aspects, and we use concepts and tools from information theory.

7.1.1. Black-box Leakage Estimation

In [16] we have considered the problem of measuring how much a system reveals about its secret inputs under the black-box setting. Black-box means that we assume no prior knowledge of the system's internals: the idea is to run the system for choices of secrets and measure its leakage from the respective outputs. Our goal was to estimate the Bayes risk, from which one can derive some of the most popular leakage measures (e.g., min-entropy, additive, and multiplicative leakage). The state-of-the-art method for estimating these leakage measures is the frequentist paradigm, which approximates the system's internals by looking at the frequencies of its inputs and outputs. Unfortunately, this does not scale for systems with large output spaces, where it would require too many input-output examples. Consequently, it also cannot be applied to systems with continuous outputs (e.g., time side channels, network traffic). In [16] we have exploited an analogy between Machine Learning (ML) and black-box leakage estimation to show that the Bayes risk of a system can be estimated by using a class of ML methods: the universally consistent learning rules; these rules can exploit patterns in the input-output examples to improve the estimates' convergence, while retaining formal optimality guarantees. We have focused on a set of them, the nearest neighbor rules; we show that they significantly reduce the number of black-box queries required for a precise estimation whenever nearby outputs tend to be produced by the same secret; furthermore, some of them can tackle systems with continuous outputs. We have illustrated the applicability of these techniques on both synthetic and real-world data, and we compared them with the state-of-the-art tool, leakiEst, which is based on the frequentist approach.

7.1.2. An Axiomatization of Information Flow Measures

Quantitative information flow aims to assess and control the leakage of sensitive information by computer systems. A key insight in this area is that no single leakage measure is appropriate in all operational scenarios; as a result, many leakage measures have been proposed, with many different properties. To clarify this complex situation, in [11] we have studied information leakage axiomatically, showing important dependencies among different axioms. We have also established a completeness result about the g-leakage family, showing that any leakage measure satisfying certain intuitively-reasonable properties can be expressed as a g-leakage.

7.1.3. Comparing systems: max-case refinement orders and application to differential privacy

Quantitative Information Flow (QIF) and Differential Privacy (DP) are both concerned with the protection of sensitive information, but they are rather different approaches. In particular, QIF considers the expected probability of a successful attack, while DP (in both its standard and local versions) is a max-case measure, in the sense that it is compromised by the existence of a possible attack, regardless of its probability. Comparing systems is a fundamental task in these areas: one wishes to guarantee that replacing a system A by a system B is a safe operation, that is the privacy of B is no-worse than that of A. In QIF, a refinement order provides strong such guarantees, while in DP mechanisms are typically compared (wrt privacy) based on the ε privacy parameter that they provide.

In [15] we have explored a variety of refinement orders, inspired by the one of QIF, providing precise guarantees for max-case leakage. We have studied simple structural ways of characterizing them, the relation between them, efficient methods for verifying them and their lattice properties. Moreover, we have applied these orders in the task of comparing DP mechanisms, raising the question of whether the order based on ε provides strong privacy guarantees. We have shown that, while it is often the case for mechanisms of the same "family" (geometric, randomised response, etc.), it rarely holds across different families.

7.1.4. A Logical Characterization of Differential Privacy

Differential privacy (DP) is a formal definition of privacy ensuring that sensitive information relative to individuals cannot be inferred by querying a database. In [12], we have exploited a modeling of this framework via labeled Markov Chains (LMCs) to provide a logical characterization of differential privacy: we have considered a probabilistic variant of the Hennessy-Milner logic and we have defined a syntactical distance on formulae in it measuring their syntactic disparities. Then, we have defined a trace distance on LMCs in terms of the syntactic distance between the sets of formulae satisfied by them. We have proved that such distance corresponds to the level of privacy of the LMCs. Moreover, we have used the distance on formulae to define a real-valued semantics for them, from which we have obtained a logical characterization of weak anonymity: the level of anonymity is measured in terms of the smallest formula distinguishing the considered LMCs. Then, we have focused on bisimulation semantics on nondeterministic probabilistic processes and we have provided a logical characterization of generalized bisimulation metrics, namely those defined via the generalized Kantorovich lifting. Our characterization is based on the notion of mimicking formula of a process and the syntactic distance on formulae, where the former captures the observable behavior of the corresponding process and allows us to characterize bisimilarity. We have shown that the generalized bisimulation distance on processes is equal to the syntactic distance on their mimicking formulae. Moreover, we have used the distance on mimicking formulae to obtain bounds on differential privacy.

7.1.5. Geo-indistinguishability vs Utility in Mobility-based Geographic Datasets

In [17] we have explored the trade-offs between privacy and utility in mobility-based geographic datasets. Our aim was to find out whether it is possible to protect the privacy of the users in a dataset while, at the same time, maintaining intact the utility of the information that it contains. In particular, we have focused on geo-indistinguishability as a privacy-preserving sanitization methodology, and we have evaluated its effects on the utility of the Geolife dataset. We have tested the sanitized dataset in two real world scenarios: 1. Deploying an infrastructure of WiFi hotspots to offload the mobile traffic of users living, working, or commuting in a wide geographic area; 2. Simulating the spreading of a gossip-based epidemic as the outcome of a device-to-device communication protocol. We have shown the extent to which the current geo-indistinguishability techniques trade privacy for utility in real world applications and we focus on their effects at the levels of the population as a whole and of single individuals.

7.1.6. Utility-Preserving Privacy Mechanisms for Counting Queries

Differential privacy(DP) and local differential privacy(LPD) are frameworks to protect sensitive information in data collections. They are both based on obfuscation. In DP the noise is added to the result of queries on the dataset, whereas in LPD the noise is added directly on the individual records, before being collected. The main advantage of LPD with respect to DP is that it does not need to assume a trusted third party. The main disadvantage is that the trade-off between privacy and utility is usually worse than in DP, and typically to retrieve reasonably good statistics from the locally sanitized data it is necessary to have a huge collection of them. In [25], we focus on the problem of estimating counting queries from collections of noisy answers, and we propose a variant of LDP based on the addition of geometric noise. Our main result is that the geometric noise has a better statistical utility than other LPD mechanisms from the literature.

7.1.7. Differential Inference Testing: A Practical Approach to Evaluate Sanitizations of Datasets

In order to protect individuals' privacy, data have to be "well-sanitized" before sharing them, i.e. one has to remove any personal information before sharing data. However, it is not always clear when data shall be deemed well-sanitized. In this paper, we argue that the evaluation of sanitized data should be based on whether the data allows the inference of sensitive information that is specific to an individual, instead of being centered around the concept of re-identification. In [20] we have proposed a framework to evaluate the effectiveness of different sanitization techniques on a given dataset by measuring how much an individual's record from the sanitized dataset influences the inference of his/her own sensitive attribute. Our intent was not to accurately predict any sensitive attribute but rather to measure the impact of a single record on the inference of sensitive information. We have demonstrated our approach by sanitizing two real datasets in different privacy models and evaluate/compare each sanitized dataset in our framework.

7.2. Foundations of Process Calculi

7.2.1. Group Distributed Knowledge.

We introduced spatial constraint systems (scs) as semantic structures for reasoning about spatial and epistemic information in concurrent systems. They have been used to reason about beliefs, lies, and group epistemic behaviour inspired by social networks. They have also been used for proving new results about modal logics and giving semantics to process calculi. In [19] we developed the theory of scs to reason about the distributed information of potentially infinite groups. We characterized the notion of distributed information of a group of agents as the infimum of the set of join-preserving functions that represent the spaces of the agents in the group. We provided an alternative characterization of this notion as the greatest family of join-preserving functions that satisfy certain basic properties. We showed compositionality results for these characterizations and conditions under which information that can be obtained by an infinite group can also be obtained by a finite group. Finally, we provided algorithms that compute the distributive group information of finite groups. Furthermore, in [14] we summarized all the main results we have obtained about scs.

7.2.2. Group Polarization.

Social networks can make their users become more radical and isolated in their own ideological circle causing dangerous splits in society in a phenomenon known as group polarization. In [22] we developed a preliminary model for social networks, and a measure of the level of polarization in these social networks, based on Esteban and Ray's classic measure of polarization for economic situations. Our model includes information about each agent's quantitative strength of belief in a proposition of interest and a representation of the strength of each agent's influence on every other agent. We considered how the model changes over time as agents interact and communicate, and included several different options for belief update, including rational belief update and update taking into account irrational responses such as confirmation bias and the backfire effect. Under various scenarios, we considered the evolution of polarization over time, and the implications of these results for real world social networks.

7.2.3. Lattice Theory.

Structures involving a lattice and join-endomorphisms on it are ubiquitous in computer science. In [28] we studied the cardinality of the set $J(L)$ of all join-endomorphisms of a given finite lattice L. We showed that the cardinality of $J(L)$ is sub-exponential, exponential and super-exponential in the size of the lattice for boolean algebras, linear-orders, and arbitrary lattices, respectively. We also studied the following problem: Given a lattice L of size n and a subset S of $J(L)$ of size m, find the greatest lower bound in $J(L)$ of S. This join-endomorphism has meaningful interpretations in epistemic logic, distributed systems, and Aumann structures. We showed that this problem can be solved with worst-case time complexity in $O(n + mlogn)$ for powerset lattices, $O(mn^2)$ for lattices of sets, and $O(mn + n^3)$ for arbitrary lattices. The complexity is expressed in terms of the basic binary lattice operations performed by the algorithm.

7.2.4. Festschrift Contribution.

In a Festschrift dedicated to Catuscia Palamidessi [26], we presented an article with original solutions to four challenging mathematical puzzles [23]. The first two are concerned with random processes. The first problem can be reduced to computing, for arbitrary large values of n, the expected number of iterations of a program that increases a variable at random between 1 and n until exceeds n. The second problem can be reduced to determining the probability of reaching a given point after visiting all the others in a circular random walk. The other two problems involve finding optimal winning group strategies in guessing games.

COMMANDS Project-Team

7. New Results

7.1. Stochastic control and HJB equations

7.1.1. Monotone and second order consistent schemes for the Pucci and Monge-Ampere equations

In [9] we introduce a new strategy for the design of second-order accurate discretiza-tions of non-linear second order operators of Bellman type, which preserves degenerate ellipticity. The approach relies on Selling's formula, a tool from lattice geometry, and is applied to the Pucci and Monge-Ampere equations, discretized on a two dimensional cartesian grid. In the case of the Monge-Ampere equation, our work is related to both the stable formulation and the second order accurate scheme. Numerical experiments illustrate the robustness and the accuracy of the method.

7.1.2. Mean-field games of control

In [3], an existence result for a class of mean field games of controls is provided. In the considered model, the cost functional to be minimized by each agent involves a price depending at a given time on the controls of all agents and a congestion term. The existence of a classical solution is demonstrated with the Leray–Schauder theorem; the proof relies in particular on a priori bounds for the solution, which are obtained with the help of a potential formulation of the problem.

7.2. Optimal control of PDEs

7.2.1. Optimal Control of an Age-Structured System with State Constraints

In [10] we study an optimal control problem with state constraints where the state is given by an age-structured, abstract parabolic differential equation. We prove the existence and uniqueness of solution for the state equation and provide first and second parabolic estimates. We analyze the differentiability of the cost function and, based on the general theory of Lagrange multipliers, we give a first order optimality condition. We also define and analyze the regularity of the costate. Finally, we present a pregnancy model, where two coupled age-structured equations are involved, and we apply the obtained results to this case.

7.2.2. Feedback laws

The articles [4], [5], [6], co-written by L. Pfeiffer in the framework of his former position at the University of Graz, deal with the computation of feedback laws for stabilization problems of PDE systems. These problems are formulated as infinite-horizon optimal control problems.

In [5], we prove that the value function associated with bilinear stabilization problems (including some control problems of the Fokker-Planck equation) can be expanded as a Taylor expansion, where the second-order term is the solution to an algebraic Riccati equation and where the terms of order three and more are solutions to well-posed linear equations. These equations are obtained by successive differentiation of the HJB equation. A polynomial feedback law can be deduced from the Taylor approximation and its efficiency is analyzed. This approach generalizes the classical LQR-stabilization method.

In [4], we apply the methodology previously described to a stabilization problem of the 2D Navier-Stokes equation. Numerical results are provided.

In [6], we analyze an implementation of the Receding-Horizon Control method utilizing the Taylor expansion of the value function as a terminal cost. More precisely, we show that the method converges at an exponential rate with respect to the prediction horizon and the degree of the Taylor approximation.

7.3. Energy management for hybrid vehicles

7.3.1. A stochastic data-based traffic model applied to vehicles energy consumption estimation

In [7], a new approach to estimate traffic energy consumption via traffic data aggregation in (speed,acceleration) probability distributions is proposed. The aggregation is done on each segment composing the road network. In order to reduce data occupancy, clustering techniques are used to obtain meaningful classes of traffic conditions. Different times of the day with similar speed patterns and traffic behavior are thus grouped together in a single cluster. Different energy consumption models based on the aggregated data are proposed to estimate the energy consumption of the vehicles in the road network. For validation purposes, a microscopic traffic simulator is used to generate the data and compare the estimated energy consumption to the reference one. A thorough sensitivity analysis with respect to the parameters of the proposed method (i.e. number of clusters, size of the distributions support, etc.) is also conducted in simulation. Finally, a real-life scenario using floating car data is analyzed to evaluate the applicability and the robustness of the proposed method.

7.3.2. A bi-level energy management strategy for HEVs under probabilistic traffic conditions

In [11], we propose a new approach to optimize the consumption of a hybrid electric vehicle taking into account the traffic conditions. The method is based on a bi-level decomposition in order to make the implementation suitable for online use. The offline lower level computes cost maps thanks to a stochastic optimization that considers the influence of traffic, in terms of speed/acceleration probability distributions. At the online upper level, a deterministic optimization computes the ideal state of charge at the end of each road segment, using the computed cost maps. Since the high computational cost due to the uncertainty of traffic conditions has been managed at the lower level, the upper level is fast enough to be used online in the vehicle. Errors due to discretization and computation in the proposed algorithm have been studied. Finally, we present numerical simulations using actual traffic data, and compare the proposed bi-level method to a deterministic optimization with perfect information about traffic conditions. The solutions show a reasonable over-consumption compared with deterministic optimization, and manageable computational times for both the offline and online parts.

7.3.3. An Eco-routing algorithm for HEVs under traffic conditions

In [12], an extension of the bi-level optimization for the energy management of hybrid electric vehicles (HEVs) proposed above to the eco-routing problem is presented. Using the knowledge of traffic conditions over the entire road network, we search both the optimal path and state of charge trajectory. This problem results in finding the shortest path on a weighted graph whose nodes are (position, state of charge) pairs for the vehicle, the edge cost being evaluated thanks to the cost maps from optimization at the 'micro' level of a bi-level decomposition. The error due to the discretization of the state of charge is proven to be linear if the cost maps are Lipschitz. The classical $A*$ algorithm is used to solve the problem, with a heuristic based on a lower bound of the energy needed to complete the travel. The eco-routing method is validated by numerical simulations and compared to the fastest path on a synthetic road network.

DATASHAPE Project-Team

5. New Results

5.1. Algorithmic aspects of topological and geometric data analysis

5.1.1. Sampling and Meshing Submanifolds

Participants: Jean-Daniel Boissonnat, Siargey Kachanovich.

In collaboration with Mathijs Wintraecken (IST Autria).

This work [41], [11] presents a rather simple tracing algorithm to sample and mesh an m-dimensional submanifold of $\mathbb{R}^d$ for arbitrary m and d. We extend the work of Dobkin et al. to submanifolds of arbitrary dimension and codimension. The algorithm is practical and has been thoroughly investigated from both theoretical and experimental perspectives. The paper provides a full description and analysis of the data structure and of the tracing algorithm. The main contributions are : 1. We unify and complement the knowledge about Coxeter and Freudenthal-Kuhn triangulations. 2. We introduce an elegant and compact data structure to store Coxeter or Freudenthal-Kuhn triangulations and describe output sensitive algorithms to compute faces and cofaces or any simplex in the triangulation. 3. We present a manifold tracing algorithm based on the above data structure. We provide a detailled complexity analysis along with experimental results that show that the algorithm can handle cases that are far ahead of the state-of-the-art.

5.1.2. Topological correctness of PL-approximations of isomanifolds

Participant: Jean-Daniel Boissonnat.

In collaboration with Mathijs Wintraecken (IST Autria).

Isomanifolds are the generalization of isosurfaces to arbitrary dimension and codimension, i.e. manifolds defined as the zero set of some multivariate multivalued function $f : \mathbb{R}^d \to \mathbb{R}^{d-n}$. A natural (and efficient) way to approximate an isomanifold is to consider its Piecewise-Linear (PL) approximation based on a triangulation $\mathcal{T}$ of the ambient space $\mathbb{R}^d$. In this paper [43], we give conditions under which the PL-approximation of an isomanifold is topologically equivalent to the isomanifold. The conditions are easy to satisfy in the sense that they can always be met by taking a sufficiently fine triangulation $\mathcal{T}$. This contrasts with previous results on the triangulation of manifolds where, in arbitrary dimensions, delicate perturbations are needed to guarantee topological correctness, which leads to strong limitations in practice. We further give a bound on the Fréchet distance between the original isomanifold and its PL-approximation. Finally we show analogous results for the PL-approximation of an isomanifold with boundary.

5.1.3. Dimensionality Reduction for k-Distance Applied to Persistent Homology

Participants: Jean-Daniel Boissonnat, Kunal Dutta.

In collaboration with Shreya Arya (Duke University)

Given a set P of n points and a constant k, we are interested in computing the persistent homology of the Čech filtration of P for the k-distance, and investigate the effectiveness of dimensionality reduction for this problem, answering an open question of Sheehy [*Proc. SoCG, 2014*] [38]. We first show using the Johnson-Lindenstrauss lemma, that the persistent homology can be preserved up to a $(1 \pm \epsilon)$ factor while reducing dimensionality to $O(k \log n/\varepsilon^2)$. Our main result shows that the target dimension can be improved to $O(\log n/\varepsilon^2)$ under a reasonable and naturally occuring condition. The proof involves a multi-dimensional variant of the Hanson-Wright inequality for subgaussian quadratic forms and works when the random matrices are used for the Johnson-Lindenstrauss mapping are subgaussian. This includes the Gaussian matrices of Indyk-Motwani, the sparse random matrices of Achlioptas and the Ailon-Chazelle fast Johnson-Lindenstrauss transform. To provide evidence that our condition encompasses quite general situations, we show that it is satisfied when the points are independently distributed (i) in $\mathbb{R}^D$ under a subgaussian distribution, or (ii) on a spherical shell in $\mathbb{R}^D$ with a minimum angular separation, using Gershgorin's theorem. Our results also show that the JL-mapping preserves up to a $(1 \pm \epsilon)$ factor, the Rips and Delaunay filtrations for the k-distance, as well as the Čech filtration for the approximate k-distance of Buchet et al.

5.1.4. Edge Collapse and Persistence of Flag Complexes

Participants: Jean-Daniel Boissonnat, Siddharth Pritam.

In this article [42], we extend the notions of dominated vertex and strong collapse of a simplicial complex as introduced by J. Barmak and E. Miniam adn build on the initial success of [30]. We say that a simplex (of any dimension) is dominated if its link is a simplicial cone. Domination of edges appear to be very powerful and we study it in the case of flag complexes in more detail. We show that edge collapse (removal of dominated edges) in a flag complex can be performed using only the 1-skeleton of the complex. Furthermore, the residual complex is a flag complex as well. Next we show that, similar to the case of strong collapses, we can use edge collapses to reduce a flag filtration $\mathcal{F}$ to a smaller flag filtration $\mathcal{F}^c$ with the same persistence. Here again, we only use the 1-skeletons of the complexes. The resulting method to compute $\mathcal{F}^c$ is simple and extremely efficient and, when used as a preprocessing for Persistence Computation, leads to gains of several orders of magnitude wrt the state-of-the-art methods (including our previous approach using strong collapse). The method is exact, irrespective of dimension, and improves performance of Persistence Computation even in low dimensions. This is demonstrated by numerous experiments on publicly available data.

5.1.5. DTM-based Filtrations

Participants: Frédéric Chazal, Marc Glisse, Raphael Tinarrage.

In collaboration with Anai, Hirokazu and Ike, Yuichi and Inakoshi, Hiroya and Umeda, Yuhei (Fujitsu Labs).

Despite strong stability properties, the persistent homology of filtrations classically used in Topological Data Analysis, such as, e.g. the Čech or Vietoris-Rips filtrations, are very sensitive to the presence of outliers in the data from which they are computed. In [15], we introduce and study a new family of filtrations, the DTM-filtrations, built on top of point clouds in the Euclidean space which are more robust to noise and outliers. The approach adopted in this work relies on the notion of distance-to-measure functions, and extends some previous work on the approximation of such functions.

5.1.6. Recovering the homology of immersed manifolds

Participant: Raphael Tinarrage.

Given a sample of an abstract manifold immersed in some Euclidean space, in [57], we describe a way to recover the singular homology of the original manifold. It consists in estimating its tangent bundle -seen as subset of another Euclidean space- in a measure theoretic point of view, and in applying measure-based filtrations for persistent homology. The construction we propose is consistent and stable, and does not involve the knowledge of the dimension of the manifold.

5.1.7. Regular triangulations as lexicographic optimal chains

Participant: David Cohen-Steiner.

In collaboration with André Lieutier and Julien Vuillamy (Dassault Systèmes).

We introduce [46] a total order on n-simplices in the n-Euclidean space for which the support of the lexicographic-minimal chain with the convex hull boundary as boundary constraint is precisely the n-dimensional Delaunay triangulation, or in a more general setting, the regular triangulation of a set of weighted points. This new characterization of regular and Delaunay triangulations is motivated by its possible generalization to submanifold triangulations as well as the recent development of polynomial-time triangulation algorithms taking advantage of this order.

5.1.8. Discrete Morse Theory for Computing Zigzag Persistence

Participant: Clément Maria.

In collaboration with Hannah Schreiber (Graz University of Technology, Austria)

We introduce a framework to simplify zigzag filtrations of general complexes using discrete Morse theory, in order to accelerate the computation of zigzag persistence. Zigzag persistence is a powerful algebraic generalization of persistent homology. However, its computation is much slower in practice, and the usual optimization techniques cannot be used to compute it. Our approach is different in that it preprocesses the filtration before computation. Using discrete Morse theory, we get a much smaller zigzag filtration with same persistence. The new filtration contains general complexes. We introduce new update procedures to modify on the fly the algebraic data (the zigzag persistence matrix) under the new combinatorial changes induced by the Morse reduction. Our approach is significantly faster in practice [35].

5.1.9. Computing Persistent Homology with Various Coefficient Fields in a Single Pass

Participants: Jean-Daniel Boissonnat, Clément Maria.

This article [18] introduces an algorithm to compute the persistent homology of a filtered complex with various coefficient fields in a single matrix reduction. The algorithm is output-sensitive in the total number of distinct persistent homological features in the diagrams for the different coefficient fields. This computation allows us to infer the prime divisors of the torsion coefficients of the integral homology groups of the topological space at any scale, hence furnishing a more informative description of topology than persistence in a single coefficient field. We provide theoretical complexity analysis as well as detailed experimental results. The code is part of the Gudhi software library.

5.1.10. Exact computation of the matching distance on 2-parameter persistence modules

Participant: Steve Oudot.

In collaboration with Michael Kerber (T.U. Graz) and Michael Lesnick (SUNY).

The matching distance is a pseudometric on multi-parameter persistence modules, defined in terms of the weighted bottleneck distance on the restriction of the modules to affine lines. It is known that this distance is stable in a reasonable sense, and can be efficiently approximated, which makes it a promising tool for practical applications. In [31] we show that in the 2-parameter setting, the matching distance can be computed exactly in polynomial time. Our approach subdivides the space of affine lines into regions, via a line arrangement. In each region, the matching distance restricts to a simple analytic function, whose maximum is easily computed. As a byproduct, our analysis establishes that the matching distance is a rational number, if the bigrades of the input modules are rational.

5.1.11. Decomposition of exact pfd persistence bimodules

Participant: Steve Oudot.

In collaboration with Jérémy Cochoy (Symphonia).

In [24] we identify a certain class of persistence modules indexed over $\mathbb{R}^2$ that are decomposable into direct sums of indecomposable summands called blocks. The conditions on the modules are that they are both pointwise finite-dimensional (pfd) and exact. Our proof follows the same scheme as the one for pfd persistence modules indexed over $\mathbb{R}$, yet it departs from it at key stages due to the product order not being a total order on $\mathbb{R}^2$, which leaves some important gaps open. These gaps are filled in using more direct arguments. Our work is motivated primarily by the study of interlevel-sets persistence, although the proposed results reach beyond that setting.

5.1.12. Level-sets persistence and sheaf theory

Participants: Nicolas Berkouk, Steve Oudot.

In collaboration with Grégory Ginot (Paris 13).

In [39] we provide an explicit connection between level-sets persistence and derived sheaf theory over the real line. In particular we construct a functor from 2-parameter persistence modules to sheaves over R, as well as a functor in the other direction. We also observe that the 2-parameter persistence modules arising from the level sets of Morse functions carry extra structure that we call a Mayer-Vietoris system. We prove classification, barcode decomposition, and stability theorems for these Mayer-Vietoris systems, and we show that the aforementioned functors establish a pseudo-isometric equivalence of categories between derived constructible sheaves with the convolution or (derived) bottleneck distance and the interleaving distance of strictly pointwise finite-dimensional Mayer-Vietoris systems. Ultimately, our results provide a functorial equivalence between level-sets persistence and derived pushforward for continuous real-valued functions.

5.1.13. Intrinsic Interleaving Distance for Merge Trees

Participant: Steve Oudot.

In collaboration with Ellen Gasparovic (Union College), Elizabeth Munch (Michigan State), Katharine Turner (Australian National University), Bei Wang (Utah), and Yusu Wang (Ohio-State).

Merge trees are a type of graph-based topological summary that tracks the evolution of connected components in the sublevel sets of scalar functions. They enjoy widespread applications in data analysis and scientific visualization. In [49] we consider the problem of comparing two merge trees via the notion of interleaving distance in the metric space setting. We investigate various theoretical properties of such a metric. In particular, we show that the interleaving distance is intrinsic on the space of labeled merge trees and provide an algorithm to construct metric 1-centers for collections of labeled merge trees. We further prove that the intrinsic property of the interleaving distance also holds for the space of unlabeled merge trees. Our results are a first step toward performing statistics on graph-based topological summaries.

5.2. Statistical aspects of topological and geometric data analysis

5.2.1. Estimating the Reach of a Manifold

Participants: Frédéric Chazal, Jisu Kim, Bertrand Michel.

In collaboration with E. Aamari (Univ. Paris-Diderot), A. Rinaldo, L. Wasserman (Carnegie Mellon University).

In [13], various problems in manifold estimation make use of a quantity called the reach, denoted by τ_M, which is a measure of the regularity of the manifold. This paper is the first investigation into the problem of how to estimate the reach. First, we study the geometry of the reach through an approximation perspective. We derive new geometric results on the reach for submanifolds without boundary. An estimator $\widehat{\tau}$ of τ_M is proposed in an oracle framework where tangent spaces are known, and bounds assessing its efficiency are derived. In the case of i.i.d. random point cloud X_n, $\widehat{\tau}(X_n)$ is showed to achieve uniform expected loss bounds over a C^3-like model. Finally, we obtain upper and lower bounds on the minimax rate for estimating the reach.

5.2.2. A statistical test of isomorphism between metric-measure spaces using the distance-to-a-measure signature

Participant: Claire Brecheteau.

In [20], we introduce the notion of DTM-signature, a measure on $\mathbb{R}$ that can be associated to any metric-measure space. This signature is based on the function distance to a measure (DTM) introduced in 2009 by Chazal, Cohen-Steiner and Mérigot. It leads to a pseudo-metric between metric-measure spaces, that is bounded above by the Gromov-Wasserstein distance. This pseudo-metric is used to build a statistical test of isomorphism between two metric-measure spaces, from the observation of two N-samples.

The test is based on subsampling methods and comes with theoretical guarantees. It is proven to be of the correct level asymptotically. Also, when the measures are supported on compact subsets of $\mathbb{R}^d$, rates of convergence are derived for the $L1$-Wasserstein distance between the distribution of the test statistic and its subsampling approximation. These rates depend on some parameter $\rho > 1$. In addition, we prove that the power is bounded above by $\exp(-CN1/\rho)$, with C proportional to the square of the aforementioned pseudo-metric between the metric-measure spaces. Under some geometrical assumptions, we also derive lower bounds for this pseudo-metric.

An algorithm is proposed for the implementation of this statistical test, and its performance is compared to the performance of other methods through numerical experiments.

5.2.3. *On the choice of weight functions for linear representations of persistence diagrams*

Participant: Vincent Divol.

In collaboration with Wolfgang Polonik (UC Davis).

Persistence diagrams are efficient descriptors of the topology of a point cloud. As they do not naturally belong to a Hilbert space, standard statistical methods cannot be directly applied to them. Instead, feature maps (or representations) are commonly used for the analysis. A large class of feature maps, which we call linear, depends on some weight functions, the choice of which is a critical issue. An important criterion to choose a weight function is to ensure stability of the feature maps with respect to Wasserstein distances on diagrams. In [21], we improve known results on the stability of such maps, and extend it to general weight functions. We also address the choice of the weight function by considering an asymptotic setting; assume that $\mathbb{X}_n$ is an i.i.d. sample from a density on $[0,1]^d$. For the Č ech and Rips filtrations, we characterize the weight functions for which the corresponding feature maps converge as n approaches infinity, and by doing so, we prove laws of large numbers for the total persistences of such diagrams. Those two approaches (stability and convergence) lead to the same simple heuristic for tuning weight functions: if the data lies near a d-dimensional manifold, then a sensible choice of weight function is the persistence to the power α with $\alpha \geq d$.

5.2.4. *Understanding the Topology and the Geometry of the Persistence Diagram Space via Optimal Partial Transport*

Participants: Vincent Divol, Théo Lacombe.

Despite the obvious similarities between the metrics used in topological data analysis and those of optimal transport, an optimal-transport based formalism to study persistence diagrams and similar topological descriptors has yet to come. In [48], by considering the space of persistence diagrams as a measure space, and by observing that its metrics can be expressed as solutions of optimal partial transport problems, we introduce a generalization of persistence diagrams, namely Radon measures supported on the upper half plane. Such measures naturally appear in topological data analysis when considering continuous representations of persistence diagrams (e.g. persistence surfaces) but also as limits for laws of large numbers on persistence diagrams or as expectations of probability distributions on the persistence diagrams space. We study the topological properties of this new space, which will also hold for the closed subspace of persistence diagrams. New results include a characterization of convergence with respect to transport metrics, the existence of Fréchet means for any distribution of diagrams, and an exhaustive description of continuous linear representations of persistence diagrams. We also showcase the usefulness of this framework to study random persistence diagrams by providing several statistical results made meaningful thanks to this new formalism.

5.3. Topological approach for multimodal data processing

5.3.1. *A General Neural Network Architecture for Persistence Diagrams and Graph Classification*

Participants: Frédéric Chazal, Théo Lacombe, Martin Royer.

In collaboration with Mathieu Carrière (Colombia Univ.) and Umeda Yuhei and Ike Yiuchi (Fujitsu Labs).

Persistence diagrams, the most common descriptors of Topological Data Analysis, encode topological properties of data and have already proved pivotal in many different applications of data science. However, since the (metric) space of persistence diagrams is not Hilbert, they end up being difficult inputs for most Machine Learning techniques. To address this concern, several vectorization methods have been put forward that embed persistence diagrams into either finite-dimensional Euclidean space or (implicit) infinite dimensional Hilbert space with kernels. In [44], we focus on persistence diagrams built on top of graphs. Relying on extended persistence theory and the so-called heat kernel signature, we show how graphs can be encoded by (extended) persistence diagrams in a provably stable way. We then propose a general and versatile framework for learning vectorizations of persistence diagrams, which encompasses most of the vectorization techniques used in the literature. We finally showcase the experimental strength of our setup by achieving competitive scores on classification tasks on real-life graph datasets.

5.3.2. Topological Data Analysis for Arrhythmia Detection through Modular Neural Networks

Participant: Frédéric Chazal.

In collaboration with Umeda Yuhei and Meryll Dindin (Fujitsu Labs).

In [47], we present an innovative and generic deep learning approach to monitor heart conditions from ECG signals.We focus our attention on both the detection and classification of abnormal heartbeats, known as arrhythmia. We strongly insist on generalization throughout the construction of a deep-learning model that turns out to be effective for new unseen patient. The novelty of our approach relies on the use of topological data analysis as basis of our multichannel architecture, to diminish the bias due to individual differences. We show that our structure reaches the performances of the state-of-the-art methods regarding arrhythmia detection and classification.

5.3.3. ATOL: Automatic Topologically-Oriented Learning

Participants: Frédéric Chazal, Martin Royer.

In collaboration with Umeda Yuhei and Ike Yiuchi (Fujitsu Labs).

There are abundant cases for using Topological Data Analysis (TDA) in a learning context, but robust topological information commonly comes in the form of a set of persistence diagrams, objects that by nature are uneasy to affix to a generic machine learning framework. In [56], we introduce a vectorisation method for diagrams that allows to collect information from topological descriptors into a format fit for machine learning tools. Based on a few observations, the method is learned and tailored to discriminate the various important plane regions a diagram is set into. With this tool one can automatically augment any sort of machine learning problem with access to a TDA method, enhance performances, construct features reflecting underlying changes in topological behaviour. The proposed methodology comes with only high level tuning parameters such as the encoding budget for topological features. We provide an open-access, ready-to-use implementation and notebook. We showcase the strengths and versatility of our approach on a number of applications. From emulous and modern graph collections to a highly topological synthetic dynamical orbits data, we prove that the method matches or beats the state-of-the-art in encoding persistence diagrams to solve hard problems. We then apply our method in the context of an industrial, difficult time-series regression problem and show the approach to be relevant.

5.3.4. Inverse Problems in Topological Persistence: a Survey

Participant: Steve Oudot.

In collaboration with Elchanan Solomon (Duke).

In [27] we review the literature on inverse problems in topological persistence theory.The first half of the survey is concerned with the question of surjectivity, i.e. the existence of rightinverses, and the second half focuses on injectivity, i.e. left inverses. Throughout, we highlightthe tools and theorems that underlie these advances, and direct the reader’s attention to openproblems, both theoretical and applied.

5.3.5. *Intrinsic Topological Transforms via the Distance Kernel Embedding*

Participants: Clément Maria, Steve Oudot.

In collaboration with Elchanan Solomon (Duke).

Topological transforms are parametrized families of topological invariants, which, by analogy with transforms in signal processing, are much more discriminative than single measurements. The first two topological transforms to be defined were the Persistent Homology Transform and Euler Characteristic Transform, both of which apply to shapes embedded in Euclidean space. The contribution of this work [54] is to define topological transforms that depend only on the intrinsic geometry of a shape, and hence are invariant to the choice of embedding. To that end, given an abstract metric measure space, we define an integral operator whose eigenfunctions are used to compute sublevel set persistent homology. We demonstrate that this operator, which we call the distance kernel operator, enjoys desirable stability properties, and that its spectrum and eigenfunctions concisely encode the large-scale geometry of our metric measure space. We then define a number of topological transforms using the eigenfunctions of this operator, and observe that these transforms inherit many of the stability and injectivity properties of the distance kernel operator.

5.3.6. *A Framework for Differential Calculus on Persistence Barcodes*

Participant: Steve Oudot.

In collaboration with Jacob Leygonie and Ulrike Tillmann (Oxford).

In [52], we define notions of differentiability for maps from and to the space of persistence barcodes. Inspired by the theory of diffeological spaces, the proposed framework uses lifts to the space of ordered barcodes, from which derivatives can be computed. The two derived notions of differentiability (respectively from and to the space of barcodes) combine together naturally to produce a chain rule that enables the use of gradient descent for objective functions factoring through the space of barcodes. We illustrate the versatility of this framework by showing how it can be used to analyze the smoothness of various parametrized families of filtrations arising in topological data analysis.

5.4. Experimental research and software development

5.4.1. *Robust Stride Detector from Ankle-Mounted Inertial Sensors for Pedestrian Navigation and Activity Recognition with Machine Learning Approaches*

Participants: Bertrand Beaufils, Frédéric Chazal, Bertrand Michel.

In collaboration with Marc Grelet (Sysnav).

In [16], a stride detector algorithm combined with a technique inspired by zero velocity update (ZUPT) is proposed to reconstruct the trajectory of a pedestrian from an ankle-mounted inertial device. This innovative approach is based on sensor alignment and machine learning. It is able to detect 100% of both normal walking strides and more than 97% of atypical strides such as small steps, side steps, and backward walking that existing methods can hardly detect. This approach is also more robust in critical situations, when for example the wearer is sitting and moving the ankle or when the wearer is bicycling (less than two false detected strides per hour on average). As a consequence, the algorithm proposed for trajectory reconstruction achieves much better performances than existing methods for daily life contexts, in particular in narrow areas such as in a house. The computed stride trajectory contains essential information for recognizing the activity (atypical stride, walking, running, and stairs). For this task, we adopt a machine learning approach based on descriptors of these trajectories, which is shown to be robust to a large of variety of gaits. We tested our algorithm on recordings of healthy adults and children, achieving more than 99% success. The algorithm also achieved more than 97by children suffering from movement disorders. Compared to most algorithms in the literature, this original method does not use a fixed-size sliding window but infers this last in an adaptive way

5.4.2. *Robust pedestrian trajectory reconstruction from inertial sensor*

Participants: Bertrand Beaufils, Frédéric Chazal, Bertrand Michel.

In collaboration with Marc Grelet (Sysnav).

In [28], a strides detection algorithm combined with a technique inspired by Zero Velocity Update (ZUPT) is proposed using inertial sensors worn on the ankle. This innovative approach based on a sensors alignment and machine learning can detect both normal walking strides and atypical strides such as small steps, side steps and backward walking that existing methods struggle to detect. As a consequence, the trajectory reconstruction achieves better performances in daily life contexts for example, where a lot of these kinds of strides are performed in narrow areas such as in a house. It is also robust in critical situations, when for example the wearer is sitting and moving the ankle or bicycling, while most algorithms in the literature would wrongly detect strides and produce error in the trajectory reconstruction by generating movements.Our algorithm is evaluated on more than 7800 strides from seven different subjects performing several activities. We validated the trajectory reconstruction during motion capture sessions by analyzing the stride length. Finally, we tested the algorithm in a challenging situation by plotting the computed trajectory on the building map of an 5 hours and 30 minutes office worker recording.

5.5. Algorithmic and Combinatorial Aspects of Low Dimensional Topology

5.5.1. Treewidth, crushing and hyperbolic volume

Participant: Clément Maria.

In collaboration with Jessica S. Purcell (Monash University, Australia)

The treewidth of a 3-manifold triangulation plays an important role in algorithmic 3-manifold theory, and so it is useful to find bounds on the tree-width in terms of other properties of the manifold. In [26], we prove that there exists a universal constant c such that any closed hyperbolic 3-manifold admits a triangulation of tree-width at most the product of c and the volume. The converse is not true: we show there exists a sequence of hyperbolic 3-manifolds of bounded tree-width but volume approaching infinity. Along the way, we prove that crushing a normal surface in a triangulation does not increase the carving-width, and hence crushing any number of normal surfaces in a triangulation affects tree-width by at most a constant multiple.

5.5.2. Parameterized complexity of quantum knot invariants

Participant: Clément Maria.

In [53], we give a general fixed parameter tractable algorithm to compute quantum invariants of links presented by diagrams, whose complexity is singly exponential in the carving-width (or the tree-width) of the diagram. In particular, we get a $O(N^{3/2\mathrm{cw}}\mathrm{poly}(n))$ time algorithm to compute any Reshetikhin-Turaev invariant-derived from a simple Lie algebra g of a link presented by a planar diagram with n crossings and carving-width cw, and whose components are coloured with g-modules of dimension at most N. For example, this includes the Nth-coloured Jones polynomial and the Nth-coloured HOMFLYPT polynomial.

5.6. Miscellaneous

5.6.1. Material Coherence from Trajectories via Burau Eigenanalysis of Braids

Participant: David Cohen-Steiner.

In collaboration with Melissa Yeung and Mathieu Desbrun (Caltech).

In this paper [58], we provide a numerical tool to study material coherence from a set of 2D Lagrangian trajectories sampling a dynamical system, i.e., from the motion of passive tracers. We show that eigenvectors of the Burau representation of a topological braid derived from the trajectories have levelsets corresponding to components of the Nielsen-Thurston decomposition of the dynamical system. One can thus detect and identify clusters of space-time trajectories corresponding to coherent regions of the dynamical system by solving an eigenvalue problem. Unlike previous methods, the scalable computational complexity of our braid-based approach allows the analysis of large amounts of trajectories. Studying two-dimensional flows and their induced transport and mixing properties is key to geophysical studies of atmospheric and oceanic processes.

However, one often has only sparse tracer trajectories (e.g., positions of buoys in time) to infer the overall flow geometry. Fortunately, topological methods based on the theory of braid groups have recently been proposed to extract structures from such a sparse set of trajectories by measuring their entan-glement. This braid viewpoint offers sound foundations for the definition of coherent structures. Yet, there has been only limited efforts in developing practical tools that can leverage topological properties for the efficient analysis of flow structures: handling a larger number of tra-jectories remains computationally challenging. We contribute a new and simple computational tool to extract Lagrangian structures from sparse trajectories by noting that the eigenstructure of the Burau matrix representation of a braid of particle trajectories can be used to reveal coherent regions of the flows. Detection of clusters of space-time trajectories corresponding to coherent regions of the dynamical system can thus be achieved by solving a simple eigenvalue problem. This paper establishes the theoretical foundations behind this braid eigenanalysis approach, along with numerical validations on various flows.

5.6.2. Quantitative stability of optimal transport maps and linearization of the 2-Wasserstein space

Participants: Alex Delalande, Frédéric Chazal.

In collaboration with Quentin Mérigot (Institut de Mathématiques d'Orsay).

In [55], we study an explicit embedding of the set of probability measures into a Hilbert space, defined using optimal transport maps from a reference probability density. This embedding linearizes to some extent the 2-Wasserstein space, and enables the direct use of generic supervised and unsupervised learning algorithms on measure data. Our main result is that the embedding is (bi-)Holder continuous, when the reference density is uniform over a convex set, and can be equivalently phrased as a dimension-independent Hölder-stability results for optimal transport maps.

DEDUCTEAM Project-Team

6. New Results

6.1. Implementation of Dedukti

During his master internship with Frédéric Blanqui and Bruno Barras, Gabriel Hondet developed a new rewrite engine for Dedukti [22]. The algorithm used in the new rewriting engine is formalised and a correctness proof is provided. This algorithm is based on the pattern matching algorithm by Maranget and used in OCaml. It is extended to rewriting rules, λ terms and non linear patterns. Some interesting implementation details are evinced and then we compare the efficiency of the new engine to a naive matching algorithm and to the rewriting engine of Dedukti. The results show that our implementation handles large rewrite systems better that the naive algorithm, and is always better than Dedukti's.

During her internship with Frédéric Blanqui and Emilio Gallego, Houda Mouzoun developed a Dedukti plugin for the VSCode editor.

During his internship with Frédéric Blanqui and Valentin Blot, Jui-Hsuan Wu implemented a prototype algorithm for deciding whether a function defined by rewriting rules is injective or not [23], and also a new algorithm proposed by Frédéric Blanqui for checking that user-defined rewrite rules preserve typing.

Bruno Barras has developed a reduction machine implementing a strong call-by-need strategy for β-reduction and pattern-matching. Higher-order pattern-matching is not yet fully implemented. Regarding efficiency, an exponential speed-up can be observed compared to the current call-by-name implementation on a large class of examples, but a constant slow-down shows on examples where call-by-name is the optimal strategy. With Beniamino Accattoli, he has started studying the correctness of this machine, without pattern-matching. They proved that the machine correctly implements β-reduction, but have no result yet regarding the strategy or the time complexity.

6.2. Theory of $\lambda\Pi$-calculus modulo rewriting

Dependency pairs are a key concept at the core of modern automated termination provers for first-order term rewriting systems. In [14][15], Frédéric Blanqui, Guillaume Genestier and Olivier Hermant introduced an extension of this technique for a large class of dependently-typed higher-order rewriting systems. This improves previous results by Wahlstedt on the one hand and the first author on the other hand to strong normalization and non-orthogonal rewriting systems. This new result has been implemented in the termination-checker SizeChangeTool [17], which participated in the Termination Competition and is used by Dedukti.

During his internship with Frédéric Blanqui and Valentin Blot, Jui-Hsuan Wu designed an algorithm for deciding whether a function defined by rewriting rules is injective or not [23]. This allows to improve the unification algorithm used in Dedukti for inferring types and missing arguments.

The expressiveness of dependent type theory can be extended by identifying types modulo some additional computation rules. But, for preserving the decidability of type-checking or the logical consistency of the system, one must make sure that those user-defined rewriting rules preserve typing. Frédéric Blanqui has developed a new method to check that property using Knuth-Bendix completion. A prototype implementation by Jui-Hsuan Wu is available in Dedukti.

Confluence is a crucial property of rewriting. Gaspard Férey and Jean-Pierre Jouannaud formalized the higher-order rewriting relation on untyped terms implemented in Dedukti and studied various criteria to obtain confluence of higher-order rewrite systems considered together with beta. In particular Von Oostrom's decreasing diagrams technique is applied to multi-steps extensions of simple term rewriting to achieve confluence criteria based on the decidable computation of (orthogonal) higher-order critical pairs. This work assumes left-linearity of rules for now but current work aims at extending these techniques to prove confluence of non-left-linear rule restricted to subsets of terms [20].

Fran cois Thiré has worked on a criterion that would help proving metatheoretical results on Cumulative Type Systems, such as expansion postponment and the equivalence between typed and untyped presentations of conversion. This has been published andpresented at LFMTP'19 [19]

Frédéric Gilbert has written a preprint about the definition of proof certificates for predicative subtyping [21].

6.3. Proof reconstruction

Proof assistants often call automated theorem provers to prove subgoals. However, each prover has its own proof calculus and the proof traces that it produces often lack many details to build a complete proof. Hence these traces are hard to check and reuse in proof assistants. Dedukti is a proof checker whose proofs can be translated to various proof assistants: Coq, HOL, Lean, Matita, PVS. Yacine El Haddad, Guillaume Burel and Frédéric Blanqui implemented a tool Ektraskto [16] that extracts TPTP subproblems from a TSTP file and reconstructs complete proofs in Dedukti using automated provers able to generate Dedukti proofs like ZenonModulo or ArchSAT. This tool is generic: it assumes nothing about the proof calculus of the prover producing the trace, and it can use different provers to produce the Dedukti proof. We applied our tool on traces produced by automated theorem provers on the CNF problems of the TPTP library and we were able to reconstruct a proof for a large proportion of them, significantly increasing the number of Dedukti proofs that could be obtained for those problems.

Zenon Modulo and iProverModulo, two automated theorem provers that can produce Dedukti proofs, have been presented in an article accepted in the Journal of Automated Reasoning [12].

6.4. Translating proofs to Dedukti

Agda is a dependently-typed programming language developed at Chalmers University, Gothenburg, Sweden, for 20 years. Thanks to the propositions-as-types correspondence of Curry-Howard, Agda is often used as a proof-assistant. Guillaume Genestier developed with Jesper Cockx a prototypical translator from Agda to Dedukti, which supports well some of the mainly used features of Agda and translates hundreds of definitions of the standard libraries. This implementation led to new encodings of theories in Dedukti, regarding: Universe Polymorphism, Inductive and Record Types, Dependent Pattern Matching, eta convertibility. The implementation of this translator permits to improve both Agda and Dedukti. Indeed, we discovered some bugged (almost not used) functions in Agda and had to extend some existing functions to our purpose. On the Dedukti side, this implementation was the first usage of the newly implemented feature of rewriting modulo associativity and commutativity, which required some minor improvements. Furthermore, our translation of eta-expansion using a defined function led to an improvement in the verification of type preservation of rewriting rules in Dedukti.

Isabelle is a logical framework developed at Technical University of Munich and Cambridge University since the 90s. It implements several logics such as HOL and ZF and is used as part of large verification projects such as seL4 and Flyspeck. Gabriel Hondet developed with Makarius Wenzel (from Augsburg) an export from Isabelle propositions to Dedukti, which was later extended by Michael Färber and Makarius Wenzel to export proofs. This required substantial work on the Isabelle kernel to extend the reconstruction of proof terms based on the work of Stefan Berghofer. Our newly developed proof export allows for an independent verification of a substantial portion of the Isabelle/HOL standard library as well as for the integration of results proved in Isabelle into Logipedia.

6.5. Models of cubical type theory

Bruno Barras and Rehan Malak have developed further their Dedukti library of presheaves. Using this library, they have built a semi-simplicial model of System F.

6.6. A proof system for PCTL and CTL*

Gilles Dowek, Ying Jiang, and Wu Peng, have proposed a proof system for the probabilistic modal logic PCTL. A paper is in preparation.

Gilles Dowek, Ying Jiang, Wu Peng, and Wenhui Zhang have started to study a proof system for CTL*, that mixes constructive and classical aspects.

The article Towards Combining Model Checking and Proof Checking, of Ying Jiang, Jian Liu, Gilles Dowek, and Kailiang Ji, has been published in The Computer Journal [13].

6.7. System I

Gilles Dowek and Alejandro Díaz-Caro have defined a lambda-calculus, the system I, to represent the proofs of a variant minimal propositional logic where isomorphic propositions are identified. Their paper Proof Normalisation in a Logic Identifying Isomorphic Propositions, has been presented at the International Conference on Formal Structures for Computation and Deduction. A second paper The virtues of eta-expansion in System I, showing that the addition of eta-expansion to system I actually simplies the system has been submitted to publication.

6.8. Computing with global environments

The call-by-need evaluation strategy for the λ-calculus is an evaluation strategy that lazily evaluates arguments only if needed, and if so, shares computations across all places where it is needed. To implement this evaluation strategy, abstract machines require some form of global environment. While abstract machines usually lead to a better understanding of the flow of control during the execution, easing in particular the definition of continuation-passing style translations, the case of machines with global environments turns out to be much more subtle.

In collaboration with Hugo Herbelin, Étienne Miquey introduced F_Υ, a calculus featuring a data type for typed stores and a mechanism of explicit coercions witnessing store extensions. This calculus defines a generic target of typed continuationand-environment-passing style translations for several calculi with global environment: it is compatible with different evaluation strategy (call-by-need, call-by-name, call-by-value) and different type systems (simple types, system F). On the logical side, these translations broadly amounts to a Kripke forcing-like translation mixed with a negative translation (for the continuation-passing part).

6.9. Computional interpretation of the axiom scheme of comprehension

The axiom scheme of comprehension is the cornerstone of second-order arithmetic, a logical theory in which most of mathematics can be formalized. Historically, comprehension was obtained from the negative translation of the axiom of choice, this axiom being interpreted by bar recursion. This led to cluttered and inefficient interpretations of second-order arithmetic.

Valentin Blot simplified this interpretation by proving that the axiom scheme of comprehension has a direct computational interpretation through a variant of bar recursion called update recursion. This new interpretation leads to a more efficient computational interpretation of proofs in second-order arithmetic, and paves the way for a convergence of the two existing interpretations: bar recursion and System F.

6.10. Alignment of logical connectives

Émilie Grienenberger and Gilles Dowek have studied in practice the alignment of logical connectives between proofs systems, a first step towards concept alignement, by the export of the HOL Light standard library using axiomatized connectives to Dedukti. More theoretically, an ecumenical system–where classical and intuitionistic logics coexist–was introduced to act as an exchange platform between proof systems.

6.11. Quantum Computing

The article Two linearities for quantum computing in the lambda calculus, of Alejandro Díaz-Caro, Gilles Dowek, and Juan Pablo Rinaldi, first published in the proceedings of Theory and Practice of Natural Computing 2017, has been published in the journal Biosystems.

DEFI Project-Team

5. New Results

5.1. Qualitative and quantitative methods for inverse problems

5.1.1. Differential tomography of micromechanical evolution in elastic materials of unknown micro/macrostructure

H. haddar and F. Pourahmadian

Differential evolution indicators are introduced for 3D spatiotemporal imaging of micromechanical processes in complex materials where progressive variations due to manufacturing and/or aging are housed in a highly scattering background of a-priori unknown or uncertain structure. In this vein, a three-tier imaging platform is established where: (1) the domain is periodically (or continuously) subject to illumination and sensing in an arbitrary configuration; (2) sequential sets of measured data are deployed to distill segment-wise scattering signatures of the domain's internal structure through carefully constructed, non-iterative solutions to the scattering equation; and (3) the resulting solution sequence is then used to rigorously construct an imaging functional carrying appropriate invariance with respect to the unknown stationary components of the background e.g., pre-existing interstitial boundaries and bubbles. This gives birth to differential indicators that specifically recover the 3D support of micromechanical evolution within a network of unknown scatterers. The direct scattering problem is formulated in the frequency domain where the background is comprised of a random distribution of monolithic fragments. The constituents are connected via highly heterogeneous interfaces of unknown elasticity and dissipation which are subject to spatiotemporal evolution. The support of internal boundaries are sequentially illuminated by a set of incident waves and thusinduced scattered fields are captured over a generic observation surface. The performance of the proposed imaging indicator is illustrated through a set of numerical experiments for spatiotemporal reconstruction of progressive damage zones featuring randomly distributed cracks and bubbles [35].

5.1.2. Microwave tomographic imaging of cerebrovascular accidents by using high-performance computing

P.-H. Tournier, I. Aliferis, M. Bonazzoli, M. De Buhan, M. Darbas, V. Dolean, F. Hecht, P. Jolivet, I. El Kanfoud, C. Migliaccio, F. Nataf, C. Pichot, S. Semenov

The motivation of this work is the detection of cerebrovascular accidents by microwave tomographic imaging. This requires the solution of an inverse problem relying on a minimization algorithm (for example, gradient-based), where successive iterations consist in repeated solutions of a direct problem. The reconstruction algorithm is extremely computationally intensive and makes use of efficient parallel algorithms and high-performance computing. The feasibility of this type of imaging is conditioned on one hand by an accurate reconstruction of the material properties of the propagation medium and on the other hand by a considerable reduction in simulation time. Fulfilling these two requirements will enable a very rapid and accurate diagnosis. From the mathematical and numerical point of view, this means solving Maxwell's equations in time-harmonic regime by appropriate domain decomposition methods, which are naturally adapted to parallel architectures [20].

5.1.3. A Factorization Method for Inverse Time Domain Obstacles with Impedance Boundary Conditions

H. Haddar and X. Liu

We develop a factorization method to obtain explicit characterization of a (possibly non-convex) impedance scattering object from measurements of time-dependent causal scattered waves in the far field regime. In particular, we prove that far fields of solutions to the wave equation due to particularly modified incident waves, characterize the obstacle by a range criterion involving the square root of the time derivative of the corresponding far field operator. Our analysis makes essential use of a coercivity property of the solution of the initial boundary value problem for the wave equation in the Laplace domain. This forces us to consider this particular modification of the far field operator. The latter in fact, can be chosen arbitrarily close to the true far field operator given in terms of physical measurements. We provide validating numerical examples in 2D on synthetic data. The latter is generated using a FDTD solver with PML. An article on this topic is under preparation.

5.1.4. A robust Expectation-Maximization method for the interpretation of small angle scattering data on dense nanoparticle samples

M. Bakry, H. Haddar and O. Bunau

The Local Monodisperse Approximation (LMA) is a two-parameters model commonly employed for the retrieval of size distributions from the small angle scattering (SAS) patterns obtained on dense nanoparticle samples (e.g. dry powders and concentrated solutions). This work features an original, beyond state-of-the-art implementation of the LMA model resolution for the inverse scattering problem. Our method is based on the Expectation Maximization iterative algorithm and is free from any fine tuning of model parameters. The application of our method on SAS data acquired in laboratory conditions on dense nanoparticle samples is shown to provide very good results [2].

5.1.5. Factorization Method for Imaging a Local Perturbation in Inhomogeneous Periodic Layers from Far Field Measurements

H. Haddar and A. Konschin

We analyze the Factorization method to reconstruct the geometry of a local defect in a periodic absorbing layer using almost only incident plane waves at a fixed frequency. A crucial part of our analysis relies on the consideration of the range of a carefully designed far field operator, which characterizes the geometry of the defect. We further provide some validating numerical results in a two dimensional setting [9].

5.1.6. Shape reconstruction of deposits inside a steam generator using eddy current measurements

L. Audibert, H. Girardon and H. Haddar

Non-destructive testing is an essential tool to assess the safety of the facilities within nuclear plants. In particular, conductive deposits on U-tubes in steam generators constitute a major danger as they may block the cooling loop. To detect these deposits, eddy-current probes are introduced inside the U-tubes to generate currents and measuring back an impedance signal. Based on earlier work on this subject, we develop a shape optimization technique with regularized gradient descent to invert these measurements and recover the deposit shape. To deal with the unknown, and possibly complex, topological nature of the latter, we propose to model it using a level set function. The methodology is first validated on synthetic axisymmetric configurations and fast convergence in ensured by careful adaptation of the gradient steps and regularization parameters. We then consider a more realistic modeling that incorporates the support plate and the presence of imperfections on the tube interior section. We employ in particular an asymptotic model to take into account these imperfections and treat them as additional unknowns in our inverse problem. A multi-objective optimization strategy, based on the use of different operating frequencies, is then developed to solve this problem. Various numerical experimentation with synthetic data demonstrated the viability of our approach. The approach is also successfully validated against experimental data. An article on this topic is under preparation.

5.1.7. *On quasi-reversibility solutions to the Cauchy problem for the Laplace equation: regularity and error estimates*

L. Bourgeois, L. Chesnel

We are interested in the classical ill-posed Cauchy problem for the Laplace equation. One method to approximate the solution associated with compatible data consists in considering a family of regularized well-posed problems depending on a small parameter $\varepsilon > 0$. In this context, in order to prove convergence of finite elements methods, it is necessary to get regularity results of the solutions to these regularized problems which hold uniformly in ε. In the present work, we obtain these results in smooth domains and in 2D polygonal geometries. In presence of corners, due the particular structure of the regularized problems, classical techniques *à la* Grisvard do not work and instead, we apply the Kondratiev approach. We describe the procedure in detail to keep track of the dependence in ε in all the estimates. The main originality of this study lies in the fact that the limit problem is ill-posed in any framework [4].

5.1.8. *Data Completion Method For the Helmholtz Equation Via Surface Potentials for Partial Cauchy Data*

M. Aussal, Y. Boukari and H. Haddar

We propose and study a data completion algorithm for recovering missing data from the knowledge of Cauchy data on parts of the same boundary. The algorithm is based on surface representation of the solution and is presented for the Helmholtz equation. This work is an extension of the data completion algorithm proposed by the two last authors where the case of data available of a closed boundary was studied. The proposed method is a direct inversion method robust with respect to noisy incompatible data. Classical regularization methods with discrepancy selection principles can be employed and automatically lead to a convergent schemes as the noise level goes to zero. We conduct 3D numerical investigations to validate our method on various synthetic examples [31].

5.2. Invisiblity and transmission eigenvalues

5.2.1. *Inside-outside duality with artificial backgrounds*

L. Audibert, L. Chesnel, H. Haddar

We use the inside-outside duality approach proposed by Kirsch-Lechleiter to identify transmission eigenvalues associated with artificial backgrounds. We prove that for well chosen artificial backgrounds, in particular for the ones with zero index of refraction at the inclusion location, one obtains a necessary and sufficient condition characterizing transmission eigenvalues via the spectrum of the modified far field operator. We also complement the existing literature with a convergence result for the invisible generalized incident field associated with the transmission eigenvalues [1].

5.2.2. *Surface waves in a channel with thin tunnels and wells at the bottom: non-reflecting underwater topography*

L. Chesnel, S.A. Nazarov, J. Taskinen

We consider the propagation of surface water waves in a straight planar channel perturbed at the bottom by several thin curved tunnels and wells. We propose a method to construct non reflecting underwater topographies of this type at an arbitrary prescribed wave number. To proceed, we compute asymptotic expansions of the diffraction solutions with respect to the small parameter of the geometry taking into account the existence of boundary layer phenomena. We establish error estimates to validate the expansions using advances techniques of weighted spaces with detached asymptotics. In the process, we show the absence of trapped surface waves for perturbations small enough. This analysis furnishes asymptotic formulas for the scattering matrix and we use them to determine underwater topographies which are non-reflecting. Theoretical and numerical examples are given [6]

5.2.3. *Exact zero transmission during the Fano resonance phenomenon in non symmetric waveguides*

L. Chesnel, S.A. Nazarov

We investigate a time-harmonic wave problem in a waveguide. We work at low frequency so that only one mode can propagate. It is known that the scattering matrix exhibits a rapid variation for real frequencies in a vicinity of a complex resonance located close to the real axis. This is the so-called Fano resonance phenomenon. And when the geometry presents certain properties of symmetry, there are two different real frequencies such that we have either $R = 0$ or $T = 0$, where R and T denote the reflection and transmission coefficients. In this work, we prove that without the assumption of symmetry of the geometry, quite surprisingly, there is always one real frequency for which we have $T = 0$. In this situation, all the energy sent in the waveguide is backscattered. However in general, we do not have $R = 0$ in the process. We provide numerical results to illustrate our theorems [33].

5.2.4. *Homogenization of Maxwell's equations and related scalar problems with sign-changing coefficients*

R. Bunoiu, L. Chesnel, K. Ramdani, M. Rihani

In this work, we are interested in the homogenization of time-harmonic Maxwell's equations in a composite medium with periodically distributed small inclusions of a negative material. Here a negative material is a material modelled by negative permittivity and permeability. Due to the sign-changing coefficients in the equations, it is not straightforward to obtain uniform energy estimates to apply the usual homogenization techniques. The goal of this work is to explain how to proceed in this context. The analysis of Maxwell's equations is based on a precise study of two associated scalar problems: one involving the sign-changing permittivity with Dirichlet boundary conditions, another involving the sign-changing permeability with Neumann boundary conditions. For both problems, we obtain a criterion on the physical parameters ensuring uniform invertibility of the corresponding operators as the size of the inclusions tends to zero. In the process, we explain the link existing with the so-called Neumann-Poincaré operator, complementing the existing literature on this topic. Then we use the results obtained for the scalar problems to derive uniform energy estimates for Maxwell's system. At this stage, an additional difficulty comes from the fact that Maxwell's equations are also sign-indefinite due to the term involving the frequency. To cope with it, we establish some sort of uniform compactness result [32].

5.3. Shape and topology optimization

5.3.1. *Null space gradient flows for constrained optimization with applications to shape optimization*

G. Allaire, F. Feppon and C. Dapogny

The purpose of this article is to introduce a gradient-flow algorithm for solving equality and inequality constrained optimization problems, which is particularly suited for shape optimization applications. We rely on a variant of the Ordinary Differential Equation (ODE) approach proposed by Yamashita for equality constrained problems: the search direction is a combination of a null space step and a range space step, aiming to decrease the value of the minimized objective function and the violation of the constraints, respectively. Our first contribution is to propose an extension of this ODE approach to optimization problems featuring both equality and inequality constraints. In the literature, a common practice consists in reducing inequality constraints to equality constraints by the introduction of additional slack variables. Here, we rather solve their local combinatorial character by computing the projection of the gradient of the objective function onto the cone of feasible directions. This is achieved by solving a dual quadratic programming subproblem whose size equals the number of active or violated constraints. The solution to this problem allows to identify the inequality constraints to which the optimization trajectory should remain tangent. Our second contribution is a formulation of our gradient flow in the context of—infinite-dimensional—Hilbert spaces, and of even more general optimization sets such as sets of shapes, as it occurs in shape optimization within the framework of Hadamard's boundary variation method. The cornerstone of this formulation is the classical operation of extension and regularization of shape derivatives. The numerical efficiency and ease of implementation of our algorithm are demonstrated on realistic shape optimization problems. An article on this topic is under preparation.

5.3.2. *A variational formulation for computing shape derivatives of geometric constraints along rays*

G. Allaire, F. Feppon and C. Dapogny

In the formulation of shape optimization problems, multiple geometric constraint functionals involve the signed distance function to the optimized shape Ω. The numerical evaluation of their shape derivatives requires to integrate some quantities along the normal rays to Ω, a task that is usually achieved thanks to the method of characteristics. The goal of the present paper is to propose an alternative, variational approach for this purpose. Our method amounts, in full generality, to compute integral quantities along the characteristic curves of a given velocity field without requiring the explicit knowledge of these curves on the spatial discretization; it rather relies on a variational problem which can be solved conveniently by the finite element method. The well-posedness of this problem is established thanks to a detailed analysis of weighted graph spaces of the advection operator $\beta \cdot \nabla$ associated to a $\mathcal{C}^1$ velocity fields β. One novelty of our approach is the ability to handle velocity fields with possibly unbounded divergence: we do not assume $\div(\beta) \in L^{\infty}$. Our working assumptions are fulfilled in the context of shape optimization of $\mathcal{C}^2$ domains Ω, where the velocity field $\beta = \nabla d_{\Omega}$ is an extension of the unit outward normal vector to the optimized shape. The efficiency of our variational method with respect to the direct integration of numerical quantities along rays is evaluated on several numerical examples. Classical albeit important implementation issues such as the calculation of a shape's curvature and the detection of its skeleton are discussed. Finally, we demonstrate the convenience and potential of our method when it comes to enforcing maximum and minimum thickness constraints in structural shape optimization. An article on this topic is under preparation.

5.3.3. *3-d topology optimization of modulated and oriented periodic microstructures by the homogenization method*

G. Allaire, P. Geoffroy-Donders and O. Pantz

This paper is motivated by the optimization of so-called lattice materials which are becoming increasingly popular in the context of additive manufacturing. Generalizing our previous work in 2-d we propose a method for topology optimization of structures made of periodically perforated material, where the microscopic periodic cell can be macroscopically modulated and oriented. This method is made of three steps. The first step amounts to compute the homogenized properties of an adequately chosen parametrized microstructure (here, a cubic lattice with varying bar thicknesses). The second step optimizes the homogenized formulation of the problem, which is a classical problem of parametric optimization. The third, and most delicate, step projects the optimal oriented microstructure at a desired length scale. Compared to the 2-d case where rotations are parametrized by a single angle, to which a conformality constraint can be applied, the 3-d case is more involved and requires new ingredients. In particular, the full rotation matrix is regularized (instead of just one angle in 2-d) and the projection map which deforms the square periodic lattice is computed component by component. Several numerical examples are presented for compliance minimization in 3-d. An article on this topic is under preparation.

5.4. Analysis of some wave problems

5.4.1. *On well-posedness of time-harmonic problems in an unbounded strip for a thin plate model*

L. Bourgeois, L. Chesnel, S. Fliss

We study the propagation of elastic waves in the time-harmonic regime in a waveguide which is unbounded in one direction and bounded in the two other (transverse) directions. We assume that the waveguide is thin in one of these transverse directions, which leads us to consider a Kirchhoff-Love plate model in a locally perturbed 2D strip. For time harmonic scattering problems in unbounded domains, well-posedness does not hold in a classical setting and it is necessary to prescribe the behaviour of the solution at infinity. This is challenging for the model that we consider and constitutes our main contribution. Two types of boundary conditions are considered: either the strip is simply supported or the strip is clamped. The two boundary conditions are treated with two different methods. For the simply supported problem, the analysis is based on a result of Hilbert basis in the transverse section. For the clamped problem, this property does not hold. Instead we adopt the Kondratiev's approach, based on the use of the Fourier transform in the unbounded direction, together with techniques of weighted Sobolev spaces with detached asymptotics. After introducing radiation conditions, the corresponding scattering problems are shown to be well-posed in the Fredholm sense. We also show that the solutions are the physical (outgoing) solutions in the sense of the limiting absorption principle. [5]

5.4.2. *Domain decomposition preconditioning for the high-frequency time-harmonic Maxwell equations with absorption*

M. Bonazzoli, V. Dolean, I. G. Graham, E. A. Spence and P.-H. Tournier

In this work we rigorously analyse preconditioners for the time-harmonic Maxwell equations with absorption, where the PDE is discretised using curl-conforming finite-element methods of fixed, arbitrary order and the preconditioner is constructed using additive Schwarz domain decomposition methods. The theory we developed shows that if the absorption is large enough, and if the subdomain and coarse mesh diameters and overlap are chosen appropriately, then the classical two-level overlapping additive Schwarz preconditioner (with PEC boundary conditions on the subdomains) performs optimally–in the sense that GMRES converges in a wavenumber-independent number of iterations–for the problem with absorption. An important feature of the theory is that it allows the coarse space to be built from low-order elements even if the PDE is discretised using high-order elements. It also shows that additive methods with minimal overlap can be robust. Several numerical experiments illustrate the theory and its dependence on various parameters. These experiments motivate some extensions of the preconditioners which have better robustness for problems with less absorption, including the propagative case. Finally, we illustrate the performance of these on two substantial applications; the first (a problem with absorption arising from medical imaging) shows the empirical robustness of the preconditioner against heterogeneity, and the second (scattering by a COBRA cavity) shows good scalability of the preconditioner with up to 3,000 processors [3].

5.4.3. *Multi-Trace FEM-BEM formulation for acoustic scattering by composite objects*

M. Bonazzoli, X. Claeys

This work is about the scattering of an acoustic wave by an object composed of piecewise homogenous parts and an arbitrarily heterogeneous part. We propose and analyze a formulation that couples, adopting a Costabel-type approach, boundary integral equations for the homogeneous subdomains with domain variational formulations for the heterogenous subdomain. This is an extension of Costabel FEM-BEM coupling to a multi-domain configuration, with junctions points allowed, i.e. points where three or more subdomains abut. Usually just the exterior unbounded subdomain is treated with the BEM; here we wish to exploit the BEM whenever it is applicable, that is for all the homogenous parts of the scattering object, since it yields a reduction in the number of unknowns compared to the FEM. Our formulation is based on the multi-trace formalism for acoustic scattering by piecewise homogeneous objects; here we allow the wavenumber to vary arbitrarily in a part of the domain. We prove that the bilinear form associated with the proposed formulation satisfies a Gårding coercivity inequality, which ensures stability of the variational problem if it is uniquely solvable. We identify conditions for injectivity and construct modified versions immune to spurious resonances. An article on this topic is under preparation.

5.4.4. *Domain decomposition preconditioners for non-self-adjoint or indefinite problems*

M. Bonazzoli, X. Claeys, F. Nataf, P.-H. Tournier

The matrices arising from the finite element discretization of problems such as high-frequency Helmholtz, time-harmonic Maxwell or convection-diffusion equations are not self-adjoint or positive definite. For this reason, it is difficult to analyze the convergence of Schwarz domain decomposition preconditioners applied to these problems. Note also that the conjugate gradient method cannot be used, and the analysis of the spectrum of the preconditioned matrix is not sufficient for methods suited for general matrices such as GMRES. In order to apply Elman-type estimates for the convergence of GMRES we need to prove an upper bound on the norm of the preconditioned matrix, and a lower bound on the distance of its field of values from the origin. We generalize the theory for the Helmholtz equation developed for the SORAS (Symmetrized Optimized Restricted Additive Schwarz) preconditioner, and we identify a list of assumptions and estimates that are sufficient to prove the two bounds needed for the convergence analysis for a general linear system. As an illustration of this technique, we prove estimates for the heterogenous reaction-convection-diffusion equation. An article on this topic is under preparation.

5.5. Diffusion MRI

J.-R. Li, K. V. Nguyen and T. N. Tran

Diffusion Magnetic Resonance Imaging (DMRI) is a promising tool to obtain useful information on microscopic structure and has been extensively applied to biological tissues.

We obtained the following results.

- The Bloch-Torrey partial differential equation can be used to describe the evolution of the transverse magnetization of the imaged sample under the influence of diffusion-encoding magnetic field gradients inside the MRI scanner. The integral of the magnetization inside a voxel gives the simulated diffusion MRI signal. This work proposes a finite element discretization on manifolds in order to efficiently simulate the diffusion MRI signal in domains that have a thin layer or a thin tube geometrical structure. The variable thickness of the three-dimensional domains is included in the weak formulation established on the manifolds. We conducted a numerical study of the proposed approach by simulating the diffusion MRI signals from the extracellular space (a thin layer medium) and from neurons (a thin tube medium), comparing the results with the reference signals obtained using a standard three-dimensional finite element discretization. We show good agreements between the simulated signals using our proposed method and the reference signals for a wide range of diffusion MRI parameters. The approximation becomes better as the diffusion time increases. The method helps to significantly reduce the required simulation time, computational memory, and difficulties associated with mesh generation, thus opening the possibilities to simulating complicated structures at low cost for a better understanding of diffusion MRI in the brain [12].
- The nerve cells of the Aplysia are much larger than mammalian neurons. Using the Aplysia ganglia to study the relationship between the cellular structure and the diffusion MRI signal can potentially shed light on this relationship for more complex organisms. We measured the dMRI signal of chemically-fixed abdominal ganglia of the Aplysia at several diffusion times. At the diffusion times measured and observed at low b-values, the dMRI signal is mono-exponential and can be accurately represented by the parameter ADC (Apparent Diffusion Coefficient). We performed numerical simulations of water diffusion for the large cell neurons in the abdominal ganglia after creating geometrical configurations by segmenting high resolution T2-weighted (T2w) images to obtain the cell outline and then incorporating a manually generated nucleus. The results of the numerical simulations validate the claim that water diffusion in the large cell neurons is in the short diffusion time regime at our experimental diffusion times. Then, using the analytical short time approximation (STA) formula for the ADC, we showed that in order to explain the experimentally observed behavior, it is necessary to consider the nucleus and the cytoplasm as two separate diffusion compartments. By using a two compartment STA model, we were able to illustrate the effect of the highly irregular shape of the cell nucleus on the ADC [13].
- The complex transverse water proton magnetization subject to diffusion-encoding magnetic field

gradient pulses in a heterogeneous medium can be modeled by the multiple compartment Bloch-Torrey partial differential equation. Under the assumption of negligible water exchange between compartments, the time-dependent apparent diffusion coefficient can be directly computed from the solution of a diffusion equation subject to a time-dependent Neumann boundary condition. This work describes a publicly available MATLAB toolbox called SpinDoctor that can be used 1) to solve the Bloch-Torrey partial differential equation in order to simulate the diffusion magnetic resonance imaging signal; 2) to solve a diffusion partial differential equation to obtain directly the apparent diffusion coefficient; 3) to compare the simulated apparent diffusion coefficient with a short-time approximation formula. The partial differential equations are solved by $P1$ finite elements combined with built-in MATLAB routines for solving ordinary differential equations. The finite element mesh generation is performed using an external package called Tetgen. SpinDoctor provides built-in options of including 1) spherical cells with a nucleus; 2) cylindrical cells with a myelin layer; 3) an extra-cellular space enclosed either a) in a box or b) in a tight wrapping around the cells; 4) deformation of canonical cells by bending and twisting; 5) permeable membranes; Built-in diffusion-encoding pulse sequences include the Pulsed Gradient Spin Echo and the Oscillating Gradient Spin Echo. We describe in detail how to use the SpinDoctor toolbox. We validate SpinDoctor simulations using reference signals computed by the Matrix Formalism method. We compare the accuracy and computational time of SpinDoctor simulations with Monte-Carlo simulations and show significant speed-up of SpinDoctor over Monte-Carlo simulations in complex geometries. We also illustrate several extensions of SpinDoctor functionalities, including the incorporation of $T2$ relaxation, the simulation of non-standard diffusion-encoding sequences, as well as the use of externally generated geometrical meshes [10].

- The numerical simulation of the diffusion MRI signal arising from complex tissue micro-structures is helpful for understanding and interpreting imaging data as well as for designing and optimizing MRI sequences. The discretization of the Bloch-Torrey equation by finite elements is a more recently developed approach for this purpose, in contrast to random walk simulations, which has a longer history. While finite element discretization is more difficult to implement than random walk simulations, the approach benefits from a long history of theoretical and numerical developments by the mathematical and engineering communities. In particular, software packages for the automated solutions of partial differential equations using finite element discretization, such as FEniCS, are undergoing active support and development. However, because diffusion MRI simulation is a relatively new application area, there is still a gap between the simulation needs of the MRI community and the available tools provided by finite element software packages. In this paper, we address two potential difficulties in using FEniCS for diffusion MRI simulation. First, we simplified software installation by the use of FEniCS containers that are completely portable across multiple platforms. Second, we provide a portable simulation framework based on Python and whose code is open source. This simulation framework can be seamlessly integrated with cloud computing resources such as Google Colaboratory notebooks working on a web browser or with Google Cloud Platform with MPI parallelization. We show examples illustrating the accuracy, the computational times, and parallel computing capabilities. The framework contributes to reproducible science and open-source software in computational diffusion MRI with the hope that it will help to speed up method developments and stimulate research collaborations [11].
- We performed simulations for a collaborative project with Demian Wassermann of the Parietal team on distinguishing between spindle and pyramidal neurons with Multi-shell Diffusion MRI [34].
- We continued in the simulation and modeling of heart diffusion MRI with the post-doc project of Imen Mekkaoui, funded by Inria-EPFL lab. The project is co-supervised with Jan Hesthaven, Chair of Computational Mathematics and Simulation Science (MCSS), EPFL. An article on this topic is under preparation.

5.6. Uncertainty Quantification methods

5.6.1. Acceleration of Domain Decomposition Methods for Stochastic Elliptic Equations

João F. Reis, Olivier P. Le Maître, Pietro M. Congedo, Paul Mycek

We propose a Monte Carlo based method to compute statistics from a solution of a stochastic elliptic equation. Solutions are computed through an iterative solver. We present a parallel construction of a robust stochastic preconditioner to accelerate the iterative scheme. This preconditioner is built before the sampling, at an offline stage, based on a decomposition of the geometric domain. Once constructed, a realisation of the preconditioner is generated for each sample and applied to an iterative method to solve the corresponding deterministic linear system. This approach is not restricted to a single iterative method and can be adapted to different iterative techniques. We demonstrate the efficiency of this approach with extensive numerical results, divided into two examples. The first example is a one-dimensional equation. The reduced dimension of the first example allows the construction of global operators and consequently, an extensive analysis of the convergence and stability properties of the proposed approach. The second example is an analogous two-dimensional version. We demonstrate the performance of the proposed preconditioner by comparison with other deterministic preconditioners based on the median of the coefficient fields. An article on this topic is under preparation.

5.6.2. Clustering based design of experiments for Systems of Gaussian processes

F. Sanson, O.P. Le Maitre, P.M. Congedo

Multi-physics problems in engineering can be often modeled using a System of Solvers (SoS), which is simply a set of solvers coupled together. SoS could be computationally expensive, for example in parametric studies, uncertainty quantification or sensitivity analysis, so typically requiring the construction of a global surrogate model of the SoS to perform such costly analysis. One recurrent strategy in literature consists of building a system of surrogate models where each solver is approximated with a local surrogate model. This approach can be efficient if good training sets for each surrogate can be generated, in particular on the intermediate variables (which are the outputs of an upstream solver and the inputs of a downstream one) that are a priori unknown. In this work, we propose a novel strategy to construct efficient training sets of the intermediate variables, using clustering-based techniques formulated for a systems of Gaussian processes (SoGP). In this way, improved coverage of the intermediate spaces is attained compared to randomly generated training sets. The performances of this approach are assessed on several test-cases showing that the clustering training strategy is systematically more efficient than randomly sampled training points [19].

5.6.3. Extension of AK-MCS for the efficient computation of very small failure probabilities

N. Razaaly, P.M. Congedo

We consider the problem of estimating a probability of failure p_f, defined as the volume of the excursion set of a complex (*e.g.* output of an expensive-to-run finite element model) scalar performance function J below a given threshold, under a probability measure that can be recast as a multivariate standard Gaussian law using an isoprobabilistic transformation. We propose a method able to deal with cases characterized by multiple failure regions, possibly very small failure probability p_f (say $\sim 10^{-6} - 10^{-9}$), and when the number of evaluations of J is limited. The present work is an extension of the popular Kriging-based active learning algorithm known as AK-MCS, permitting to deal with very low failure probabilities. The key idea merely consists in replacing the Monte-Carlo sampling, used in the original formulation to propose candidates and evaluate the failure probability, by a centered isotropic Gaussian sampling in the standard space, which standard deviation is iteratively tuned. This *extreme* AK-MCS (eAK-MCS) inherits its former multi-point enrichment algorithm allowing to add several points at each iteration step, and provide an estimated failure probability based on the Gaussian nature of the Kriging surrogate. Both the efficiency and the accuracy of the proposed method are showcased through its application to two to eight dimensional analytic examples, characterized by very low failure probabilities. Numerical experiments conducted with *unfavorable* initial *Design of Experiment* suggests the ability of the proposed method to detect failure domains [30].

5.6.4. An Efficient Kriging-Based Extreme Quantile Estimation suitable for expensive performance function

N. Razaaly, P.M. Congedo

We propose here a method for fast estimation of the quantiles associated with very small levels of probability, where the scalar performance function J is complex (e.g. output of an expensive-to-run finite element model), under a probability measure that can be recast as a multivariate standard Gaussian law using an isoprobabilistic transformation. A surrogate-based approach (Gaussian Processes) combined with adaptive experimental designs allows to iteratively increase the accuracy of the surrogate while keeping the overall number of J evaluations low. Direct use of Monte-Carlo simulation even on the surrogate model being too expensive, the key idea consists in using an Importance Sampling method based on an isotropic centered Gaussian with large Standard deviation permitting a cheap estimation of the quantiles of the surrogate. Similar to the strategy presented by Schobi and Sudret (2016), the surrogate is adaptively refined using a parallel infill refinement of an algorithm suitable for very small failure probability. We finally elaborate a multi-quantile selection approach allowing to exploit high-performance computing architectures further. We illustrate the performances of the proposed method on several two and six-dimensional cases. Accurate results are obtained with less than 100 evaluations of J. An article on this topic is under preparation.

5.7. Shape optimization under uncertainties

5.7.1. Non-Parametric Measure Approximations for Constrained Multi-Objective Optimisation under Uncertainty

M. Rivier, P.M. Congedo

In this paper, we propose non-parametric estimations of robustness and reliability measures to solve constrained multi-objective optimisation under uncertainty. These approximations with tunable fidelity permit to capture the Pareto front in a parsimonious way, and can be exploited within an adaptive refinement strategy. First, we build a non-Gaussian surrogate model of the objectives and constraints, allowing for more representativeness and detecting potential correlations. Additionally, we illustrate an efficient approach for obtaining joint representations of these robustness and reliability measures, which discriminates more sharply the Pareto-optimal designs from the others. Secondly, we propose an adaptive refinement strategy, using these tunable fidelity approximations to drive the computational effort towards the computation of the optimal area. To this extent, an adapted Pareto dominance rule and Pareto optimal probability computation are formulated. We assess the performance of the proposed strategy on several analytical test-cases against classical approaches in terms of the average distance to the Pareto front. Finally, we illustrate the performances of the method on the case of shape optimisation under uncertainty of an Organic Rankine Cycle turbine [26].

5.7.2. Optimization under Uncertainty of Large Dimensional Problems usingQuantile Bayesian Regression

C. Sabater, O. Le Maitre, P.M. Congedo, S. Goertz

When dealing with robust optimization problems, surrogate models are traditionally constructed to efficiently obtain the statistics of the random variable. However, when a large number of uncertainties are present, the required number of training samples to construct an accurate surrogate generally increases exponentially. The use of surrogates also requires the parametrization of the uncertainties. We present a novel approach for robust design insensitive to the number of uncertainties and that is able to deal with non-parametric uncertainties by leveraging a Bayesian formulation of quantile regression. The method does not require the use of any surrogate in the stochastic space. It is able to globally predict at every design point any given quantile of the random variable. In addition, it provides an estimation of the error in this prediction due to the limited sampling by making use of the posterior distribution of the model parameters.The framework includes an active infill that efficiently balances exploration with exploitation and accelerates the optimization process by increasing the accuracy of the statistic in the regions of interest. We validate the method in test functions and observe good convergence properties towards the determination of the location of the global optima. The framework is applied towards the aerodynamic robust design of an airfoil with a shock control bump under 382 geometrical and operational uncertainties. The framework is able to efficiently find the optimum configuration in complex, large-scale problems. An article on this topic is under preparation.

5.8. Application of Uncertainty Quantification studies to fluid-dynamics problems

5.8.1. Multi-fidelity surrogate-based optimization of transonic and supersonic axial turbines profiles

N. Razaaly, G. Persico, P.M. Congedo

This study presents a multifidelity surrogate-based approach for the optimization of the LS89 high pressure axial turbine vane to significantly reduce the computational cost associated to high fidelity CFD simulations while exploiting models of lower fidelity. A cokriging method is used to simultaneously take into account quantities of interest (QoI) coming from models of different fidelities providing a global surrogate model. A classic bayesian global optimization method permits to iteratively propose desing of interest. It relies on the maximization of the so-called Expected Improvement criterion. A geometrical parametrization technique based on B-splines is considered to describe the profile geometry. The mass-flow rate and the outlet angle are constrained. The optimization study reveals significant reduction in computational cost w.r.t. classic optimization frameworks based on a single fidelity, such as, adjoint-based and gradient-free methods, while providing similar improvements in term of fitness functions [23].

DISCO Project-Team

5. New Results

5.1. Multiplicity-induced-dominancy

Participants: Islam Boussaada, Guilherme Mazanti, Hugues Mounier [L2S, CentraleSupélec], Silviu-Iulian Niculescu.

The effects of multiplicity of spectral values on the exponential stability of reduced-order retarded differential equation were emphasized in recent works. In [13] the general class of second-order retarded differential equations is studied. A parametric multiplicity-induced-dominancy (MID) property is characterized, allowing a delayed stabilizing design with reduced complexity. The proposed approach is merely a delayed-output-feedback where the candidates' delays and gains result from the manifold defining the maximal multiplicity of a real spectral value, then, the dominancy is shown using the argument principle.

The work [52] considers retarded differential equations of arbitrary order with a single delay. The existence of a real root with maximal multiplicity is characterized in terms of the equation parameters. This root is shown to be always strictly dominant, determining thus the asymptotic behavior of the system. The dominancy proof is based on improved a priori bounds on the imaginary part of roots on the complex right half-plane and a suitable factorization of the characteristic function, which is an alternative technique to the argument principle.

In [53] we extend the MID property to a given pair of complex conjugate roots for a generic second-order retarded differential equation. Necessary and sufficient conditions for the existence of such a pair are provided, and it is also shown that such a pair is always necessarily dominant. It appears also that when the frequency corresponding to this pair of roots tends to 0, then the pair of roots collapse into a real root of maximal multiplicity. The latter property is exploited in the dominancy proof together with a study of crossing imaginary roots.

In [41] a control-oriented model of torsional vibrations occurring in rotary drilling process is proposed. More precisely, a wave equations with weak damping term is considered. An appropriate stabilizing controller with a reduced number of parameters is proposed for damping such torsional vibrations. Such a controller allows to further explore the effect of multiple roots with maximal admissible multiplicity for linear neutral system with a single delay.

5.2. Pole placement techniques for time-delay systems

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S, CentraleSupélec], Fazia Bedouhene [University Mouloud Mammeri de Tizi Ouzou, Algeria].

The interest in investigating multiple roots does not rely on the multiplicity itself, but rather on its connection with the dominance of this root, and the corresponding applications in stability analysis and control design. The work [31] extends the analytical characterization of the spectral abscissa for retarded time-delay system with real spectral values which are not necessarily multiple. The effect of the coexistence of such non oscillatory modes on the asymptotic stability of the trivial solution is explored. In particular, the coexistence of an appropriate number of real spectral values makes them rightmost-roots of the corresponding quasipolynomial. Furthermore, if they are negative, this guarantees the asymptotic stability of the trivial solution. As an application of the proposed rightmost-characteristic root assignment, the problem of the vibration damping for a thin flexible beam is considered in [33]. The considered beam is equipped with two piezoelectric patches: one of them works as a sensor and the other as an actuator. Each one of them is bonded on one side of the beam and both are collocated. The model of this system is obtained numerically thanks to a finite element modeling, leading to a linear state-space model. The design of a controller based on proportional and delayed-proportional actions on the input and output signals is proposed, where the properties of the proposed output feedback controller in terms of vibration damping and of robustness is discussed.

5.3. PID tuning for controlling delayed dynamics

Participants: Jie Chen [City University of Hong Kong], Jianqi Chen [City University of Hong Kong], Andong Liu [City University of Hong Kong], Dan Ma [Northeastern University, China], Silviu Niculescu.

Nowadays, the PID controller is the most used in controlling industrial processes. In [21] such a controller is further explored in the control of delayed dynamics. An explicit lower bound on the delay margin of second-order unstable delay systems achievable by PID control is established, which provides a priori a guaranteed range of delay values over which a second-order delay plant can be stabilized by a PID, and more generally, a finite-dimensional LTI controller. This is done by deriving lower bounds on the delay margin achievable by PD controllers, whereas this margin constitutes a lower bound on that achievable by PID controllers. Analysis shows that in most cases our results can be significantly less conservative than the lower bounds obtained elsewhere using more sophisticated, general LTI controllers.

5.4. Frequency-sweeping techniques in delayed dynamics analysis

Participants: Arben Cela [ESIEE Paris], Xu-Guang Li [Northeastern University, China], Xu Li [Northeastern University, China], Jiang-Chian Li [Northeastern University, China], Zhi-Zhong Mao [Shenyang University], Silviu Niculescu, Lu Zhang [Shenyang University].

The stability of linear systems with multiple (incommensurate) delays is investigated in [20], by extending a recently proposed frequency-sweeping approach. First, we consider the case where only one delay parameter is free while the others are fixed. The complete stability w.r.t. the free delay parameter can be systematically investigated by proving an appropriate invariance property. Next, we propose an iterative frequency-sweeping approach to study the stability under any given multiple delays. Moreover, we may effectively analyze the asymptotic behavior of the critical imaginary roots (if any) w.r.t. each delay parameter, which provides a possibility for stabilizing the system through adjusting the delay parameters. The approach is simple (graphical test) and can be applied systematically to the stability analysis of linear systems including multiple delays. A deeper discussion on its implementation is also proposed. Finally, various numerical examples complete the presentation.

In most of the numerical examples of time-delay systems proposed in the literature, the number of unstable characteristic roots remains positive before and after a multiple critical imaginary root (CIR) appears (as the delay, seen as a parameter, increases). This fact may lead to some misunderstandings: (i) A multiple CIR may at most affect the instability degree; (ii) It cannot cause any stability reversals (stability transitions from instability to stability). As far as we know, whether the appearance of a multiple CIR can induce stability is still unclear (in fact, when a CIR generates a stability reversal has not been specifically investigated). In [19], we provide a finer analysis of stability reversals and some new insights into the classification: the link between the multiplicity of a CIR and the asymptotic behavior with the stabilizing effect. Based on these results, we present an example illustrating that a multiple CIR's asymptotic behavior is able to cause a stability reversal. To the best of the authors' knowledge, such an example is a novelty in the literature on time-delay systems.

The work [30] focuses on the stability property of a class of distributed delay systems with constant coefficients. More precisely, we will discuss deeper the stability analysis with respect to the delay parameter. Our approach will allow to give new insights in solving the so-called complete stability problem. There are three technical issues need to be studied: First, the detection of the critical zero roots; second, the analysis of the asymptotic behavior of such critical zero roots; third, the asymptotic behavior analysis of the critical imaginary roots with respect to the infinitely many critical delays. We extended our recently-established frequency-sweeping approach, with which these technical issues can be effectively solved. More precisely, the main contributions of this paper are as follows: (i) Proposing a method for the detection of the critical zero roots. (ii) Proposing an approach for the asymptotic behavior analysis of such critical zero roots. (iii) The invariance property for the critical imaginary roots can be proved. Based on these results, a procedure was proposed, with which the complete stability analysis of such systems was accomplished systematically. Moreover, the procedure represents a unified approach: Most of the steps required by the complete stability problem may be fulfilled through observing the frequency-sweeping curves. Finally, some examples illustrate the effectiveness and advantages of the approach.

5.5. Weierstrass approach to asymptotic behavior of retarded differential equations

Participants: Jie Chen [City University of Hong Kong], Liliana Felix [University of San Luis Potosi], Alejandro Martinez-Gonzalez, Cesar F. Mendez-Barrios [University of San Luis Potosi], Silviu Niculescu.

The work [22] focuses on the analysis of the behavior of characteristic roots of time-delay systems, when the delay is subject to small parameter variations. The analysis is performed by means of the Weierstrass polynomial. More specifically, such a polynomial is employed to study the stability behavior of the characteristic roots with respect to small variations on the delay parameter. Analytic and splitting properties of the Puiseux series expansions of critical roots are characterized by allowing a full description of the cases that can be encountered. Several numerical examples encountered in the control literature are considered to illustrate the effectiveness of the proposed approach.

5.6. Some remarks on the Walton and Marshall method for neutral delay systems

Participants: Catherine Bonnet, Islam Boussaada, Le Ha Vy Nguyen.

The Walton and Marshall method allows to determine stability windows of delay systems of the retarded and neutral type. We noticed that some delay systems of the neutral type do not behave as claimed in [59] and analyzed carefully the position of the poles of such systems in the right half-plane. We have considered delay systems with characteristic equation being a quasi-polynomial with one delay and polynomials of degree one. It is shown that for a subclass of systems which have a chain of poles clustering the imaginary axis by the left, the procedure of Walton and Marshall fails: we prove the existence, for an infinitesimally small delay, of a positive real pole at infinity. This real pole is then proved to be the unique pole of the system in the closed right half-plane for all values of the delay. Some numerical examples illustrate the results [39]. We are currenlty extending those results to the general case of polynomials of degree $n > 1$.

5.7. $L2$ and BIBO Stability of systems with variable delays

Participants: Catherine Bonnet, Jonathan R. Partington [Univ of Leeds,U.K.].

There has been a growing interest in systems with time-varying delays in recent years and to the best of our knowledge, no study has been made of the input–output stability of a standard feedback scheme involving a system with time-varying delays. We have considered two versions of input–output stability: so-called Hinfinity and BIBO-stability. Retarded and neutral type systems with pointwise or distributed delays are studied here. We perform a stability analysis and discuss feedback stabilization. The results we derive yield very explicit estimates for stability margins [40].

5.8. Stability Analysis of Linear Partial Differential Equations

Participants: Giorgio Valmorbida, Aditya Gahlawat [University of Illinois at Urbana-Champaign].

We proposed a method to perform stability analysis of one-dimensional Partial Integro-Differential Equations. The relevance of the proposed results lies on the fact that we cast the Lyapunov inequalities as a differential inequality in two dimensions. The proposed structure for the inequalities is motivated by the same structure as the one used in the study of backstepping feedback laws, a successful strategy applied for several one-dimensional PDE systems. The advantage of the proposed Lyapunov analysis can be studied in a simpler manner as well as the fact that the backstepping law can be approximated by simpler laws and the stability can still be studied trhough the solution to the set of proposed inequalities.

We rely on Lyapunov analysis to establish the exponential stability of the systems. Then we present a test for the verification of the underlying Lyapunov inequalities, which relies on the existence of solutions of a system of coupled differential equations.

We illustrate the application of this method in several examples of PDEs defined by polynomial data, we formulate a numerical methodology in the form of a convex optimization problem which can be solved algorithmically. We show the effectiveness of the proposed numerical methodology using examples of different types of PDEs.

We are currently studying the extensions of coupled PDE-ODE systems.

5.9. Stability analysis of Piece-Wise Affine Systems

Participants: Giorgio Valmorbida, Leonardo Broering Groff, Joao Manoel Gomes Da Silva Jr [Universidade Federal do Rio Grande do Sul].

Piece-wise affine systems appear when linear dynamics are defined in different partitions of the state space. This type of system naturally appears whenever actuators have different stages or saturate or whenever non-linear control laws are obtained as the solution to a parameterised optimization problem as, for instance for systems with feedback laws based on the so-called explicit Model Predictive Control. Even though the dynamics is simple to describe, the stability analysis, performance assessment and robustness analysis are difficult to perform since, due to the often used explicit representation, the Lyapunov stability and dissipation tests are often described in terms of a number of inequalities that increase exponentially on the number of sets in the partition. Moreover regional stability and uncertainties corresponding to modification on the partition are difficult to study in this scenario.

To overcome these difficulties we have proposed an implicit representation for this class of systems in terms of ramp functions. The main advantage of such a representation lies on the fact that the ramp function can be exactly characterized in terms of linear inequalities and a quadratic equation, namely a linear complementarity condition. Thanks to the characterization of the ramp function and the implicit description of the PWA system the verification of Lyapunov inequalities related to piecewise quadratic functions can be cast as a pair of linear matrix inequalities.

The obtained formulation opens several possibilities to study the class of piecewise affine systems and their robustness properties. Indeed the fact that some partitions are uncertain is more easily coped with the proposed approach as they are described as parametric uncertainties of the implicit representation. Also, systems of larger dimension can be studied.

The stability analysis of the particular subclass of systems given by asymmetric saturation can also be performed with discontinuous Lyapunov functions for discrete-time systems.

5.10. Set Invariance for Descriptor Systems

Participants: Giorgio Valmorbida, Ye Wang [Universidade Federal do Rio Grande do Sul], Sorin Olaru [L2S, CentraleSupélec], Vicenç Puig [Universitat Politècnica de Catalunya], Gabriela Cembrano [Universitat Politècnica de Catalunya].

Some descriptor systems, characterized by a difference-algebraic relation, appear in economic systems. For such a class of systems we study robust invariant set characterizations of discrete-time descriptor systems and propose an active mode detection mechanism. The considered class of descriptor systems assumes regularity, stability and is affected by unknown-but-bounded disturbances.

As a first theoretical result, we establish a general framework for robust invariant sets for discrete-time descriptor systems in both causal and non-causal cases. Particular transformations are subsequently proposed for handling causal and non-causal descriptor systems and will be used to characterize the effects of disturbances. Based on these set-theoretic notions and a designed input signal for active set separations, we propose an active mode detection mechanism by exploiting the strong invariance properties.

5.11. New advances on backstepping

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Laurent Burlion [Rutgers Univ.].

We worked on the problem of improving a major control design technique for nonlinear continuous-time systems called backstepping by using a fundamentally new approach which uses as key ingredient the introduction in the control of artificial delays or the use of dynamic extensions.

In the paper [24], we adopted a technique which is based on the introduction of pointwise delays (and not of distributed terms) to solve a challenging input-to-state stabilization problem for a chain of saturated integrators when the variables are not accurately measured. Let us observe that classical backstepping does not apply in the considered case.

In the paper [23], we constructed bounded globally asymptotically stabilizing output feedbacks for a family of nonlinear systems, using a dynamic extension and a converging-input-converging-state assumption. We provided sufficient conditions for this assumption to hold, in terms of Lyapunov functions. The novelty is that our construction provides formulas for the control bounds while allowing uncertainties that prevent the use of classical backstepping in cases where only part of the state variable is available. We illustrated our work with an engineering application: the single-link direct-drive manipulator.

5.12. Finite time observers

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Saeed Ahmed [University of Kaiserslautern, Germany], Thach Dinh [CNAM], Tarek Raissi [CNAM].

Finite time observers are remarkably efficient when the value of the state is needed in a short time. By contrast with them, the solutions asymptotic observers may take a long time to be close to the solutions of the studied systems and may exhibit large transient errors. Motivated by this general fact, we produced three works.

In the work [12], we proposed finite time observers for time-varying nonlinear systems with delays in the outputs. When disturbances are present, we provide approximate values for the solutions which are expressed as upper bounds on the approximation errors after a suitable finite time. We illustrated our work via systems arising in the study of vibrating membranes, where time-varying coefficients can be used to represent intermittent measurements.

In paper [36], we use finite time reduced order continuous-discrete observers to solve an output feedback stabilization problem for a broad class of nonlinear systems whose output contains uncertainty. Unlike earlier works, our feedback control is discontinuous, but it does not contain any distributed terms, which is an advantage because the implementation of these terms may cause instability. We illustrated our main result by applying it to design a dynamic output feedback to solve a tracking problem for nonholonomic systems in chained form.

The paper [35] is devoted to the construction of finite time observers for discrete-time systems. We developped a new technique, which uses past values of the output. We considered the case where the systems are affected by additive disturbances and disturbances in the output. Exact estimation or approximate estimation have been achieved, depending on the absence or the presence of unknown but bounded uncertainties, respectively.

5.13. Observers with discrete measurements

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Saeed Ahmed [University of Kaiserslautern, Germany].

We studied the important case where the measurements of a system are discrete because output of this type may preclude the use of observers designed under the assumption that the measurements are continuous.

In the paper [25], we have studied time-varying linear systems in the difficult case where the inputs and outputs have sampling and delays, and where the systems and outputs contain uncertainties. The observers we have proposed are of continuous-discrete type and have no distributed terms. We allowed the delays to be arbitrarily large and proved that the observer in combination with a linear control result in an input-to-state stability, under delays and sampling. We illustrated our work in two examples including a DC motor model.

In the work [38], we have revisited a well-known contribution of observer design for continuous-time systems with discrete measurements which relies on a dynamic extension. Using a stability analysis which relies on the recent technique called "trajectory based approach", we proved that, for systems with asynchronous sampling, the proposed dynamic observer is converging even when the size of some (sufficiently scarce) intervals between 2 measurements is larger than the upper bound ensuring convergence of the observer that is provided in the literature. A scarcety condition on these intervals is exhibited.

5.14. Observer for a rigid body

Participants: Frédéric Mazenc, Maruthi Akella [University of Texas, USA], Hongyang Duong [Harbin Institute of Technology], Qinglei Hu [Beihang University].

In the work [15], observers are proposed for models of rigid bodies in the case where only a part of the state variables can be measured. The design is based on the dual-quaternion description. To achieve tracking control objectives, the proposed observer are combined with an independently designed proportional-derivative-like feedback control law (using full-state feedback), and a special Lyapunov "strictification" process is employed to ensure a separation property between the observer and the controller. Almost global asymptotic stability of the closed-loop dynamics is guaranteed. We performed numerical simulations for a prototypical spacecraft pose tracking mission application to illustrate the effectiveness and robustness of the proposed method.

5.15. Systems with pointwise delays

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Robledo Gonzalo [Univ. de Chile, Chile], Silviu Niculescu.

Frequently, the presence of delays is an obstacle to the stability analysis or the control of systems. Two of our works originate in the will to overcome this obstacle, in two distinct contexts.

The contribution [26] is devoted to the study of a model of a chain of two bio-reactors called 'chemostats'. One contains two microbial species in competition for a single limiting nutrient and receives an external input of the less advantaged competitor, which is cultivated in the other one. Pointwise delays are present. Under a condition on their size, we obtained sufficient conditions ensuring coexistence of all the species in competition. To prove the result, we adopted a Lyapunov based technique.

The contribution of [37] is twofold. In a first part, we exhibited a fundamental feature of the systems with a pointwise periodic time-varying delay: we have shown by a counterexample that the asymptotic stability of such a system cannot be deduced from the average value of the delay (even when the delay is 'rapidly' varying). In a second part, motivated by this counterexample, we proposed a new representation of systems with time-varying delays, which is helpful to carry out stability analyses and to develop a new state feedback stabilization method.

5.16. Control of an aircraft

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Laurent Burlion [Rutgers Univ.].

The work [34] adapts some ideas we published in previous contributions to a control problem for a chain of saturating integrators for dynamics with outputs that occurs in the vision based landing of aircraft. The major obstacle that we overcome is due to the fact that only imprecise output measurements are available. The control laws we designed are bounded by an arbitrarily small constant. The closed-loop systems we obtained possess the robustness property called "local input-to-state stability".

5.17. Effect of environment on population dynamics

Participants: Islam Boussaada, Silviu Niculescu, Jun-Xiu Chen [Nothestern University], Sette Diop [L2S, CentraleSupélec], Xu-Guang Li [Nothestern University], Paul Raynaud de Fitte [LMRS, Université de Rouen Normandie], Safia Slimani [LMRS, Université de Rouen Normandie], Sami Tliba [L2S, CentraleSupélec].

Competition in population dynamics is often considered to be governed by predator-prey models. In particular, Lotka-Volterra models are intensively used in this context.

A modified version of a prey-predator system with Leslie-Gower and Holling type II functional responses incorporating a refuge for preys is studied in [27]. Such a refuge substantially complicates the dynamics of the system. We study the local and global dynamics and the existence of limit-cycles. We also investigate conditions for extinction or existence of a stationary distribution, in the case of a stochastic perturbation of the system.

Most of the reported Lotka-Volterra examples have at most one stability interval for the delay parameters. Furthermore, the existing methods fall short in treating more general case studies. Inspired by some recent results for analyzing the stability of time-delay systems, this paper focuses on a deeper characterization of the stability of Lotka-Volterra systems w.r.t. the delay parameters. In [58], we introduced the recently-proposed frequency-sweeping approach to study the complete stability problem for a broad class of linearized Lotka-Volterra systems. As a result, the whole stability delay-set is analytically determined. Moreover, as a significant byproduct of the proposed approach, some Lotka-Volterra examples are found to have multiple stability delay-intervals. In some situations, a longer maturation period of species is helpful for the stability of a population system.

In another context, the effect of environment on yeast population dynamics is studied in [28]. In presence of oxygen cells usually adopt efficient metabolism in order to maximize energy production yield in poor diet. If nutrient resource increases, a metabolic shift from efficient metabolism (respiration) to inefficient metabolism (fermentation) is reflecting a minimal cost principle of living systems to optimize fitness. This is known as the Crabtree/Warburg effect. A model that describes the population dynamics of cells and the input growth condition is established. Proof of principle has been constructed using a battery of growth experiments on Crabtree-positive yeasts–Saccharomyces under various conditions of glucose in aerobic and micro-aerobic conditions. General cell growth model estimating metabolic shift has been constructed based on an Auto-Regressive approach.

5.18. Distributed Algorithms for Microbiological systems

Participants: Lotfi Baour, Catherine Bonnet, Da-Jung Cho, Walid Djema [BIOCORE project team], Lucas Leclerc, Matthias Fuegger [MEXICO project team], Frédéric Mazenc, Tomas Nowak [LRI, Univ Paris-Sud], Cristina Stoica [CentraleSupélec].

This project led by M. Fuegger and T. Nowak considers microbiological distributed systems such as bacterial cultures. Our goal is to develop algorithms to be used in such low-powered biological computing systems. We have considered a distributed computation model where bacteria communicate via concentrations of small signaling molecules. Algorithms designed for such a model are of importance to provide services like clock synchronization. Basic ODE models for well-mixed solutions are readily available from systems biology. This year, we have paid attention to ODE and PDE models presented in [56], [55]. We have analyzed the influence of model parameters on the stability of the system. Moreover, looking at the involved basic biochemical reactions we have considered some changes in the modelling.

EX-SITU Project-Team

7. New Results

7.1. Fundamentals of Interaction

Participants: Michel Beaudouin-Lafon [correspondant], Wendy Mackay, Cédric Fleury, Theophanis Tsandilas, Benjamin Bressolette, Julien Gori, Han Han, Yiran Zhang, Miguel Renom, Philip Tchernavskij, Martin Tricaud.

In order to better understand fundamental aspects of interaction, ExSitu conducts in-depth observational studies and controlled experiments which contribute to theories and frameworks that unify our findings and help us generate new, advanced interaction techniques. Our theoretical work also leads us to deepen or re-analyze existing theories and methodologies in order to gain new insights.

At the methodological level and in collaboration with University of Zurich (Switzerland), we have developed *Touchstone2* [19] (Best Paper award), a direct-manipulation interface for generating and examining trade-offs in experiment designs (Fig. 2). Based on interviews with experienced researchers, we developed an interactive environment for manipulating experiment design parameters, revealing patterns in trial tables, and estimating and comparing statistical power. We also developed TSL, a declarative language that precisely represents experiment designs. In two studies, experienced HCI researchers successfully used *Touchstone2* to evaluate design trade-offs and calculate how many participants are required for particular effect sizes. *Touchstone2* is freely available at https://touchstone2.org and we encourage the community to use it to improve the accountability and reproducibility of research by sharing TSL descriptions of their experimental designs.

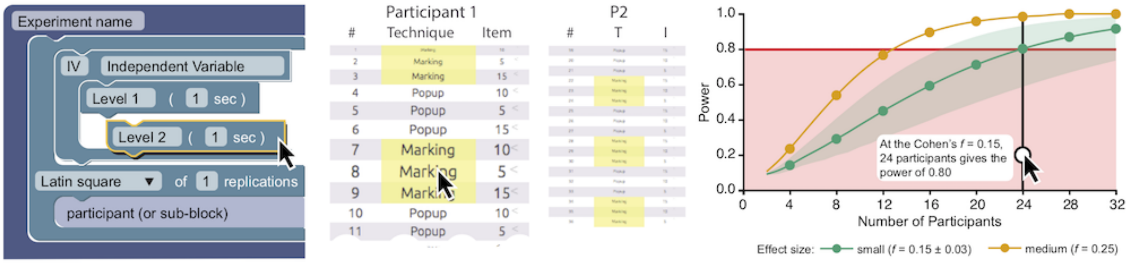

Figure 2. Touchstone2: visual language to specify an experimental design, trial table with fish-eye view, power plot.

The book “Sticky Creativity: Post-It Note Cognition, Interaction and Digitalization” [32], Academic Press, explores how the Post-It note has “become the most commonly used design material in creative design activities”, with research and use cases to illustrate its role creative activities. Wendy Mackay converted her one-day Master Class on participatory design methods into a book chapter, shifting the designer’s focus from static wireframes to prototyping how users will interact with a proposed new technology. The course takes the reader through a full interaction design cycle, with nine illustrated participatory design methods. It begins with a design brief: create an augmented sticky note inspired by observations of how people actually use paper sticky notes. Story-based interviews reveal both breakdowns and creative new uses of sticky notes. Brainstorming and video brainstorming, informed by the users’ stories, generate new ideas. Paper prototyping a design concept related to augmented sticky notes lets designers explore ideas for a future system to address an untapped need or desire. Shooting a video prototype, guided by titlecards and a storyboard, illustrates how future users will interact with the proposed system. Finally, a design walkthrough identifies key problems and suggests ideas for improvement.

At the theoretical level, we have continued our exploration of Information Theory as a design tool for HCI by analyzing past and current applications of Shannon's theory to HCI research to identify areas where information-theoretic concepts can be used to understand, design and optimize human-computer communication [30]. We have also continued our long-standing strand of work on pointing by evaluating several models for assessing pointing performance by participants with motor impairments [27]. Namely, we studied the strengths of weaknesses of various models, from traditional Fitts' Law to the WHo model, the EMG regression and the method of Positional Variance Profiles (PVPs), on datasets from abled participants vs. participants with dyspraxia.

In the context of the ERC ONE project on Unified Principles of Interaction, Philip Tchernavskij defended his Ph.D. thesis on malleable software [40]. The goal of malleable software is to make is as easy as possible for users themselves to change software, or to have it changed on their behalf in response to their developing needs. Current approaches do not address this issue adequately: software engineering promotes flexible code, but in practice this does not help end-users effect change in their software. Based on a study of a network of communities working with biodiversity data, we found that the mode of software production, i.e. the technologies and economic relations that produce software, is biased towards centralized, one-size-fits-all systems. Instead, we should seek to create infrastructures for plurality, i.e. tools that help multiple communities collaborate without forcing them to consolidate around identical interfaces or data representations. Malleable software seeks to maximize the kinds of modifications that can take place through regular interactions, e.g. direct manipulation of interface elements. By generalizing existing control structures for interaction under the concepts of co-occurrences and entanglements, we created an environment where interactions can be dynamically created and modified. The *Tangler* prototype illustrates the power of these concepts to create malleable software.

In collaboration with Aarhus University (Denmark), we created *Videostrates* [22] to explore the notion of an *interactive substrate* for video data. *Videostrates* is based on our joint previous work on *Webstrates* (https://webstrates.net) and supports both live and recorded video composition with a declarative HTML-based notation, combining both simple and sophisticated editing tools that can be used collaboratively. *Videostrates* is programmable and unleashes the power of the modern web platform for video manipulation. We demonstrated its potential through three use scenarios (Fig. 3): collaborative video editing with multiple tools and devices; orchestration of multiple live streams that are recorded and broadcast to a popular streaming platform; and programmatic creation of video using WebGL and shaders for blue screen effects. These scenarios demonstrate *Videostrates*' potential for novel collaborative video editors with fully programmable interfaces.

Figure 3. Videostrates examples: A) Two users collaboratively edit the same videostrate, one with a timeline-based editor and the other with a subtitle editor. The results appear in a live, interactive preview on a large screen. B) Videostrates aggregates, broadcasts and records multiple live streams, here from a statically mounted camera and a smartphone. C) A Videostrate-based computational notebook uses Codestrates to programmatically create a WebGL animation and synchronize its playback with recorded video composited with a green screen.

We conducted an in-depth observational study of landscape architecture students to reveal a new phenomenon in pen-and-touch surface interaction: *interstices* [24]. We observed that bimanual interactions with a pen and touch surface involved various sustained hand gestures, interleaved between their regular commands. Positioning of the non-preferred hand indicates anticipated actions, including: sustained hovering near the surface; pulled back but still floating above the surface; resting in their laps; and stabilizing the preferred hand while handwriting. These intersticial actions reveal anticipated actions and therefore should be taken into account in the design of novel interfaces.

We also started a study of blind or visually impaired people to better understand how they use graphical user interfaces [28]. The goal is to design multimodal interfaces for sighted users that do not rely on the visual channel as much as current GUIs.

In collaboration with the University of Paris Descartes and the ILDA Inria team, we investigated how to help users to query massive data series collections within interaction times. We demonstrated the importance of providing progressive whole-matching similarity search results on large time series collections (100 GB). Our experiments showed that there is a significant gap between the time the 1st Nearest Neighbor (1-NN) is found and the time when the search algorithm terminates [29]. In other words, users often wait without any improvement in their answers. We further showed that high-quality approximate answers are found very early, e.g., in less than one second, so they can support highly interactive visual analysis tasks. We discussed how to estimate probabilistic distance bounds, and how to help analysts evaluate the quality of their progressive results. The results of this collaboration have lead to Gogolou's Ph.D. thesis (ILDA Inria team) [38].

In the context of virtual reality, we explored how to integrate the real world surrounding users in the virtual environment. In many virtual reality systems, user physical workspace is superposed with a particular area of the virtual environment. This spatial consistency allows users to physically walk in the virtual environment and interact with virtual content through tangible objects. However, as soon as users perform virtual navigation to travel on a large scale (i.e. move their physical workspace in the virtual environment), they break this spatial consistency. We introduce two switch techniques to help users to recover the spatial consistency in some predefined virtual areas when using a teleportation technique for the virtual navigation [26]. We conducted a controlled experiment on a box-opening task in a CAVE-like system to evaluate the performance and usability of these switch techniques. The results highlight that helping the user to recover a spatially consistency ensures the accessibility of the entire virtual interaction space of the task. Consequently, the switch techniques decrease time and cognitive effort required to complete the task.

7.2. Human-Computer Partnerships

Participants: Wendy Mackay [correspondant], Baptiste Caramiaux, Téo Sanchez, Carla Griggio, Shu Yuan Hsueh, Wanyu Liu, Joanna Mcgrenere, Midas Nouwens.

ExSitu is interested in designing effective human-computer partnerships, in which expert users control their interaction with technology. Rather than treating the human users as the 'input' to a computer algorithm, we explore human-centered machine learning, where the goal is to use machine learning and other techniques to increase human capabilities. Much of human-computer interaction research focuses on measuring and improving productivity: our specific goal is to create what we call 'co-adaptive systems' that are discoverable, appropriable and expressive for the user.

In creative practices, human-centred machine learning facilitates the workflow for creatives to explore new ideas and possibilities. We compiled recent research and development advances in human-centred machine learning and artificial intelligence (AI), within the field of creative industries, in a white paper commissioned by the NEM (New European Media) initiative [35]. We explored the use of Deep Reinforcement Learning in the context of sound design with sound design experts [37]. We first conducted controlled studies where we compared manual exploration versus exploration by reinforcement. This helped us design a fully working system that we assessed in workshops with expert designers. We showed that an algorithmic sound explorer learning from human preferences enhances the creative process by allowing holistic and embodied exploration as opposed to analytic exploration afforded by standard interfaces.

We also explored how users create their own ecosystems of communication apps as a way to support rich, personalized forms of expression [12]. We wanted to gather data about how people customize apps to enable more personal forms of expression, and how such customizations shape their everyday communication. Given the increasing use of multiple apps with overlapping communication features, we were also interested in how customizing one app influences communication via other apps. We created a taxonomy of customization options based on interviews with 15 "extreme users" of communication apps. We found that participants tailored their apps to express their identities, organizational culture, and intimate bonds with others. They also experienced expression breakdowns: frustrations around barriers to transferring personal forms of expression across apps, which inspired inventive workarounds to maintain cross-app habits of expression, such as briefly switching apps to generate and export content for a particular conversation. We conclude with implications for personalized expression in ecosystems of communication apps.

We investigated the special communication practices between couples [20]. Research shows that sharing streams of contextual information, e.g. location and motion, helps couples coordinate and feel more connected. We studied how couples' communication changes when sharing multiple, persistent information streams. We designed *Lifelines*, a mobile-app technology probe that visualizes up to six streams on a shared timeline: closeness to home, battery level, steps, media playing, texts and calls. A month-long study with nine couples showed that partners interpreted information mostly from individual streams, but also combined them for more nuanced interpretations. Persistent streams allowed missing data to become meaningful and provided new ways of understanding each other. Unexpected patterns from any stream can trigger calls and texts, whereas seeing expected data can replace direct communication, which may improve or disrupt established communication practices.

Finally, we extended our earlier work on the *Expressive Keyboard* by adding animated emojis as a form of expressive output for messaging apps. An initial user study identified both the cumbersome nature of inserting emojis and the creative ways that users construct emoji sequences to convey rich, nuanced non-verbal expressions, including emphasis, change of expressions, and micro stories. We then developed *MojiBoard* [17], an emoji entry technique that lets users generate dynamic parametric emojis from a gesture keyboard. Here, the form of the user's gesture is transformed into an animation, allowing users to "draw" dynamic expressions through their own movements. *MojiBoard* lets users switch seamlessly between typing and parameterizing emojis. *MojiBoard* provides an example of how we can transform a user's gesture into an expressive output, which is reified into an emoji than can be interacted with again.

Wendy Mackay describes how the theoretical foundation of the CREATIV ERC Advance Grant, based on the principle of co-adaptation, influenced her research with musicians, choreographers, graphic designers and other creative professionals. The interview is published in the book "New Directions in Music and Human-Computer Interaction", Springer Nature, as a chapter entitled "HCI, Music and Art: An Interview with Wendy Mackay" [34]. Along the same lines, she contributed to a chapter "A Design Workbench for Interactive Music Systems" [33] that discusses possible links between the fields of computer music and human-computer interaction (HCI), particularly in the context of the MIDWAY project between Inria, France and McGill University, Canada. The goal of MIDWAY was to construct a "musical interaction design workbench" to facilitate the exploration and development of new interactive technologies for musical creation and performance by bringing together useful models, tools, and recent developments from computer music and HCI. These models and tools have helped expand the possibilities for enhancing musical expression, and provide HCI researchers with a better foundation for the design of tools for "extreme" users.

7.3. Creativity

Participants: Sarah Fdili Alaoui [correspondant], Carla Griggio, Shu Yuan Hsueh, Wendy Mackay, Baptiste Caramiaux, Joanna Mcgrenere, Midas Nouwens, Jean-Philippe Riviere, Nicolas Taffin, Philip Tchernavskij, Theophanis Tsandilas.

ExSitu is interested in understanding the work practices of creative professionals, particularly artists, designers, and scientists, who push the limits of interactive technology. We follow a multi-disciplinary participatory design approach, working with both expert and non-expert users in diverse creative contexts. We also create situations that cause users to reflect deeply on their activities in situ and collaborate to articulate new design problems.

We conducted an interview study of 23 contemporary music composers and choreographers where we focused on the role that physical artifacts play in shaping creative collaborations with performers [13]. We found that creators and performers form relationships where the creator acts as a author, a curator, a planner, or a researcher and the performer acts as an interpreter, a creator, an improvisor, or an informant. Furthermore, we found that creators sculpt, layer and remix artifacts, moving fluidly across these different forms of interaction throughout the creative process.

We studied Kinaesthetic creativity which refers to the body's ability to generate alternate futures [21]. We probe such creative process by studying how dancers interact with technology to generate ideas. We developed a series of parameterized interactive visuals and asked dance practitioners to use them in generating movement materials. From our study, we define a taxonomy that comprises different relationships and movement responses dancers form with the visuals. We describe resulting types of interaction patterns and demonstrate how dance creativity is driven by the ability to shift between these patterns.

We used technology probes to understand how dancers learned dance fragments from videos [15]. We introduced *MoveOn*, which lets dancers decompose video into short, repeatable clips to support their learning. This served as an effective analysis tool for identifying the changes in focus and understanding dancers decomposition and recomposition processes. Additionally we compared the teacher's and dancers' decomposition strategies, and how dancers learn on their own compared to teacher-created decompositions. We found that they all ungroup and regroup dance fragments, but with different foci of attention, which suggests that teacher-imposed decomposition is more effective for introductory dance students, whereas personal decomposition is more suitable for expert dancers.

We ran a workshop [25] at ACM *Creativity and Cognition* that explored how distributed forms of creativity arising in play can help guide and foster supportive research, game design, and technology. We brought together researchers, game designers, and others to examine theories of creativity and play, game design practices, and methods for studying creativity.

We developed a taxonomy [18] on technologies using Defamiliarization to to support Co-Creation in choreographic practices. Regarding intersection of choreographic practice and HCI, Sarah Fdili Alaoui [16] describe her research and creation journey of an interactive choreographic dance piece called SKIN. This generated a set of research questions that she addresses through experience explicitation interviews of both audience and creative team members on the lived experience of making and attending the performance and the emergent relationships between dance, media and interaction as well as the tensions and negotiations that emerged from integrating technology in art. She discusses her approach as anti-solutionist and argue for more openness in HCI to allow artists to contribute.

Finally, we assessed the inter-rater reliability of the Laban Movement Analysis system used in choreography and dance notation [11].

7.4. Collaboration

Participants: Cédric Fleury [correspondant], Michel Beaudouin-Lafon, Wendy Mackay, Carla Griggio, Yujiro Okuya, Arthur Fages.

ExSitu explores new ways of supporting collaborative interaction and remote communication. In particular, we studied co-located collaboration on large wall-sized display, video-conferencing systems for remote collaboration, and collaboration between professional designers and developers during the design of interactive systems.

Multi-touch wall-sized displays, as those of the Digiscope network (http://digiscope.fr/, afford collaborative exploration of large datasets and re-organization of digital content. In the context of industrial design, computer-aided design (CAD) is now an essential part of the design process allowing experts to evaluate and adjust product design using digital mock-ups. We investigated how a wall-sized display could be used

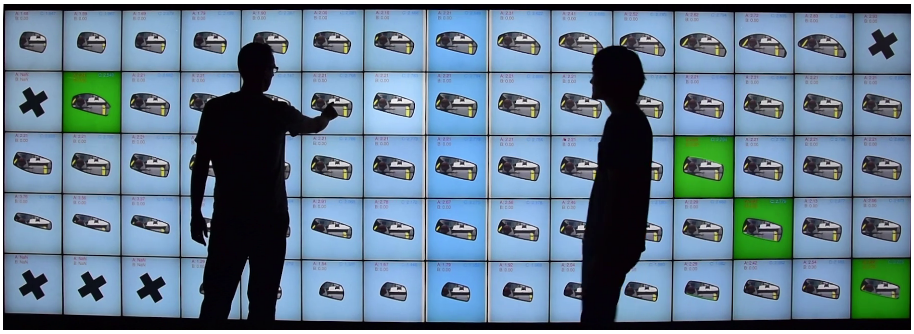

Figure 4. Collaborative exploration of multiple design alternatives of a car rear-view mirror on a wall-sized display.

to allow multidisciplinary collaborators (e.g. designers, engineers, ergonomists) to explore large number of design alternatives. In particular, we design a system which allows non-CAD expert to generate and distribute on a wall-sized display multiple various of a CAD model (Figure 4). We ran a usability study and a controlled experiment to assess the benefit of wall-sized displays in such context. Yujiro Okuya, under the supervision of Patrick Bourdot (LIMSI-CNRS) and Cédric Fleury, successfully defended his thesis *CAD Modification Techniques for Design Reviews on Heterogeneous Interactive Systems* [39] on this topic.

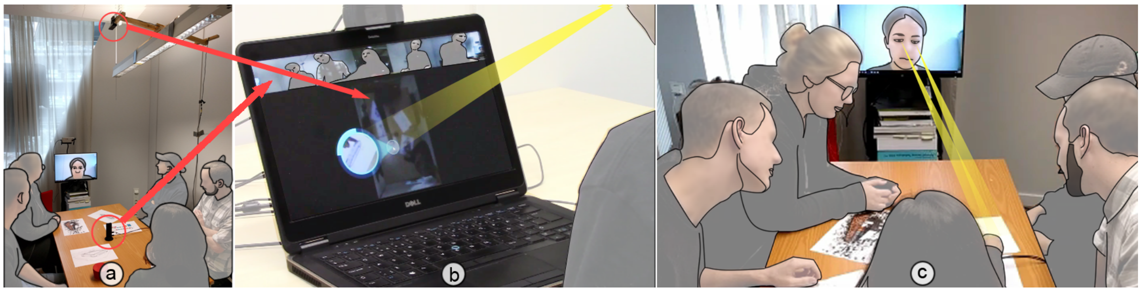

Figure 5. GazeLens system. (left) On the coworkers' side, a 360 camera on the table captures coworkers and a webcam mounted on the ceiling captures artifacts on the table. (middle) Video feeds from the two cameras are displayed on the screen of the remote satellite worker; a virtual lens strategically guides her/his attention towards a specific screen area according to the observed artifact. (right) The satellite's gaze, guided by the virtual lens, is aligned towards the observed artifact on the coworkers' space.

For remote collaboration using video, interpreting gaze direction is critical for communication between coworkers sitting around a table and a remote satellite colleague. However, 2D video distorts images and makes this interpretation inaccurate. We proposed GazeLens [23], a video conferencing system that improves coworkers' ability to interpret the satellite worker's gaze (Figure 5). A 360 camera captures the coworkers and a ceiling camera captures artifacts on the table. The system combines these two video feeds in an interface. Lens widgets strategically guide the satellite worker's attention toward specific areas of her/his screen allowing coworkers to clearly interpret her/his gaze direction. Controlled experiments showed that GazeLens increases coworkers' overall gaze interpretation accuracy in comparison to a conventional video conferencing system.

Finally, we also conducted an in-depth study of the collaboration patterns between designers and developers of interactive systems, and created a tool, *Enact*, to facilitate their work [14]. Professional designers and developers often struggle when transitioning between the design and implementation of an interactive system. We found that current practices induce unnecessary rework and cause discrepancies between design and implementation. We identified three recurring types of breakdowns: omitting critical details, ignoring edge cases, and disregarding technical limitations. We introduced four design principles to create tools that mitigate these problems: Provide multiple viewpoints, maintain a single source of truth, reveal the invisible and support design by enaction. We applied these principles to create *Enact*, a live environment for prototyping touch-based interactions (Fig. 6). We conducted two studies to assess *Enact* and compare it with current tools. Results suggest that *Enact* helps participants detect more edge cases, increases designers' participation and provides new opportunities for co-creation.

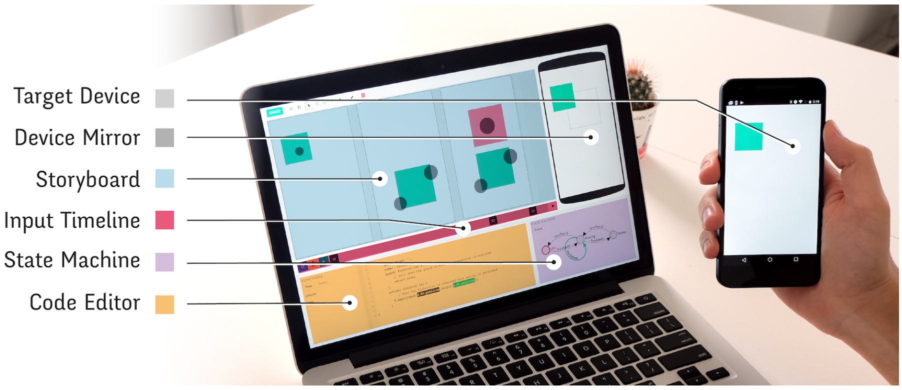

Figure 6. Enact uses a target mobile device and a desktop interface with five areas: a storyboard with consecutive screens, an event timeline with a handle for each screen, a state machine, a code editor and a device mirror.

GAMMA Project-Team

4. New Results

4.1. The meshing bible

Participants: Paul Louis George [correspondant], Frédéric Alauzet, Adrien Loseille, Loïc Maréchal.

Un projet important, initié en 2017, et toujours actif en 2020, consiste à écrire noir sur blanc un livre (en plusieurs volumes) et la motivation de ce travail est détaillée dans ce qui suit.

Pourquoi ce livre, pourquoi 2 volumes, pourquoi pas 3 volumes?

Notre dernier livre (généraliste) sur le maillage date de 2000 avec une mise à jour en 2008. Un collègue a commis un nouveau livre en 2015, très bien écrit mais assez classique dans son contenu, loin de préoccupations industrielles et (!) contenant quelques énormités (pas assez d'experience sur de vrais problèmes).

Ajoutons ma facilite (c'est P.L. G. qui parle) à écrire (bien ou mal, là n'est pas la question, il me suffit en effet de taper sur quelques touches d'un clavier), le désir de mon (premier) co-auteur de marquer le coup dans le domaine et la volonté (à leur corps defendant) des autres co-auteurs de participer à cette aventure. Le tout couplé avec les récents progrès dans le domaine (pensons aux éléments courbes et aux méthodes d'ordre élevé mais aussi à ce que peut être le HPC dans le domaine), tous les ingrédients sont là, on y va.

Le premier jet (un seul volume) se montre impossible à réaliser, il faudrait au minimum 800 pages, donc deux volumes a minima. Les deux volumes finis, ne reste il pas la place pour un troisième volume. Constatant avec effroi que nos étudiants (mais pas seulement) maitrisent bien force concepts mais sont incapables de voir, en pratique, comment les mettre en musique, le troisième volume est apparu comme une évidence (et on sera, au total, autour de 1000 pages).

A qui s'adresse ces volumes, bonne question. Ce n'est pas précisément de la littérature de gare mais nous nous sommes efforcé de prendre le malheureux lecteur par la main pour l'amener progressivement vers des concepts (très) avancés. Ainsi, le livre est très verbose et, en aucun cas, n'est un étalage savant de théorèmes et autres propositions, ce qui n'empêche pas de dire les choses. Par ailleurs, nous avons délibérément mis une part de subjectivité dans le propos pour suggérer (cela pouvant être contredit) que telle ou telle méthode n'avait pas notre faveur. A titre personnel, je pense que, bien que rares dans les livres, ces opinions ne peuvent qu'aider le lecteur a se former sa propre idée sur tel ou tel point.

Les livres sont publiés chez ISTE et écrits en français, eh oui, mais une traduction en anglais est avalable chez Wiley. La présence de la langue française dans la littérature scientifique me semble importante (et rejoint la politique de mon (notre) éditeur). Pour conclure, c'est plutôt satisfaisant de penser que ces livres (peut être destinés à faire référence sur le sujet) sont issus de l'Inria dans le neuf un.

4.2. Pixel-exact rendering for high-order meshes and solutions

Participants: Adrien Loseille [correspondant], Rémi Feuillet, Matthieu Maunoury.

Classic visualization software like ParaView [64], TecPlot [88], FieldView [60], Ensight [42], Medit [50], Vizir (OpenGL legacy based version) [67], Gmsh [57], ...historically rely on the display of linear triangles with linear solutions on it. More precisely, each element of the mesh is divided into a set of elementary triangles. At each vertex of the elementary triangle is attached a value and an associated color. The value and the color inside the triangle is then deduced by a linear interpolation inside the triangle. With the increase of high-order methods and high-order meshes, these softwares adapted their technology by using subdivision methods. If a mesh has high-order elements, these elements are subdivided into a set of linear triangles in order to approximate the shape of the high-order element [93]. Likewise, if a mesh has a high-order solution on it, each element is subdivided into smaller linear triangles in order to approximate the rendering of the high-order solution on it. The subdivision process can be really expensive if it is done in a naive way. For this reason, mesh adaptation procedures [80], [70], [71] are used to efficiently render high-order solutions and high-order elements using the standard linear rendering approaches. Even when optimized these approaches do have a huge RAM memory footprint as the subdivision is done on CPU in a preprocessing step. Also the adaptive subdivision process can be dependent on the palette (*i.e.* the range of values where the solution is studied) as the color only vary when the associated value is in this range. In this case, a change of palette inevitably imposes a new adaptation process. Finally, the use of a non conforming mesh adaptation can lead to a discontinuous rendering for a continuous solution.

Other approaches are specifically devoted to high-order solutions and are based on ray casting [75], [76], [78]. The idea is for a given pixel, to find exactly its color. To do so, for each pixel, rays are cast from the position of the screen in the physical space and their intersection with the scene determines the color for the pixel. If high-order features are taken into account, it determines the color exactly for this pixel. However, this method is based on two non-linear problems: the root-finding problem and the inversion of the geometrical mapping. These problems are really costly and do not compete with the interactivity of the standard linear rendering methods even when these are called with a subdivision process unless they are done conjointly on the GPU. However, synchronization between GPU and `OpenGL` buffer are non-trivial combination.

The proposed method intends to be a good compromise between both methods. It does guarantee pixel-exact rendering on linear elements without extra subdivision or ray casting and it keeps the interactivity of a classical method. Moreover, the subdivision of the curved entities is done on the fly on GPU which leaves the RAM memory footprint at the size of the loaded mesh.

4.3. High-order mesh generation

Participants: Frédéric Alauzet [correspondant], Adrien Loseille, Rémi Feuillet, Dave Marcum, Lucien Rochery.

For years, the resolution of numerical methods has consisted in solving Partial Derivative Equations by means of a piecewise linear representation of the physical phenomenon on linear meshes. This choice was merely driven by computational limitations. With the increase of the computational capabilities, it became possible to increase the polynomial order of the solution while keeping the mesh linear. This was motivated by the fact that even if the increase of the polynomial order requires more computational resources per iteration of the solver, it yields a faster convergence of the approximation error [0] [92] and it enables to keep track of unsteady features for a longer time and with a coarser mesh than with a linear approximation of the solution. However, in [46], [65], it was theoretically shown that for elliptic problems the optimal convergence rate for a high-order method was obtained with a curved boundary of the same order and in [44], evidence was given that without a high-order representation of the boundary the studied physical phenomenon was not exactly solved using a high-order method. In [95], it was even highlighted that, in some cases, the order of the mesh should be of a higher degree than the one of the solver. In other words, if the used mesh is not a high-order mesh, then the obtained high-order solution will never reliably represent the physical phenomenon.

Based on these issues, the development of high-order mesh generation procedures appears mandatory. To generate high-order meshes, several approaches exist. The first approach was tackled twenty years ago [47] for both surface and volume meshing. At this moment the idea was to use all the meshing tools to get a valid high-order mesh. The same problem was revisited a few years later in [86] for bio-medical applications. In these first approaches and in all the following, the underlying idea is to use a linear mesh and elevate it to the desired order. Some make use of a PDE or variational approach to do so [39], [79], [48], [73], [91], [94], [58], others are based on optimization and smoothing operations and start from a linear mesh with a constrained high-order curved boundary in order to generate a suitable high-order mesh [62], [51], [89]. Also, when dealing with Navier-Stokes equations, the question of generating curved boundary layer meshes (also called viscous meshes) appears. Most of the time, dedicated approaches are set-up to deal with this problem [74], [63]. In all these techniques, the key feature is to find the best deformation to be applied to the linear mesh and to optimize it. The prerequisite of these methods is that the initial boundary is curved and will be used as an input data. A natural question is consequently to study an optimal position of the high-order nodes on the curved boundary

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[0] The order of convergence is the degree of the polynomial approximation plus one.

starting from an initial linear or high-order boundary mesh. This can be done in a coupled way with the volume [81], [90] or in a preprocessing phase [82], [83]. In this process, the position of the nodes is set by projection onto the CAD geometry or by minimization of an error between the surface mesh and the CAD surface. Note that the vertices of the boundary mesh can move as well during the process. In the case of an initial linear boundary mesh with absence of a CAD geometry, some approaches based on normal reconstructions can be used to create a surrogate for the CAD model [93], [59]. Finally, a last question remains when dealing with such high-order meshes: Given a set of degrees of freedom, is the definition of these objects always valid ?. Until the work presented in [55], [61], [52], no real approach was proposed to deal in a robust way with the validity of high-order elements. The novelty of these approaches was to see the geometrical elements and their Jacobian as Bézier entities. Based on the properties of the Bézier representation, the validity of the element is concluded in a robust sense, while the other methods were only using a sampling of the Jacobian to conclude about its sign without any warranty on the whole validity of the elements.
In this context, several issues have been addressed : the analogy between high-order and Bézier elements, the development of high-order error estimates suitable for parametric high-order surface mesh generation andthe generalization of mesh optimization operators and their applications to curved mesh generation, moving-mesh methods, boundary layer mesh generation and mesh adaptation.

4.4. Unstructured anisotropic mesh adaptation for 3D RANS turbomachinery applications

Participants: Frédéric Alauzet, Loïc Frazza, Adrien Loseille [correspondant], Julien Vanharen.

The scope of this paper is to demonstrate the viability and efficiency of unstructured anisotropic mesh adaptation techniques to turbomachinery applications. The main difficulty in turbomachinery is the periodicity of the domain that must be taken into account inthe solution mesh-adaptive process. The periodicity is strongly enforced in the flow solver using ghost cells to minimize the impact on the source code. For the mesh adaptation, the local remeshing is done in two steps. First, the inner domain is remeshed with frozen periodic frontiers, and, second, the periodic surfaces are remeshed after moving geometrice ntities from one side of the domain to the other. One of the main goal of this work is to demonstrate how mesh adaptation, thanks to its automation, is able to generate meshes that are extremely difficult to envision and almost impossible to generate manually. This study only considers feature-based error estimate based on the standard multi-scale Lpinterpolation error estimate. We presents all the specific modifications that have been introduced in the adaptive process to deal with periodic simulations used for turbomachinery applications. The periodic mesh adaptation strategy is then tested and validated on the LS89 high pressure axial turbine vane and the NASA Rotor 37 test cases.

4.5. Hybrid mesh adaptation for CFD simulations

Participants: Frédéric Alauzet [correspondant], Lucille Tenkès, Julien Vanharen.

The aim of mesh adaptation is to generate the optimal mesh to perform a specific numerical simulation. It is nowadays a mature tool which is mathematically well-posed and fully automatic regarding tetrahedral meshes. Yet, there is still a strong demand for structured meshes, as many numerical schemes have proven to be more accurate on quadrilateral meshes than on triangular meshes, and as many favor structured elements in the boundary layer instead of tetrahedra to simulate viscous turbulent flows. Since no method can automatically provide pure hexahedral adapted meshes respecting alignment constraints, one solution is to use hybrid meshes, *i.e.* meshes containing both structured and unstructured elements. Accordingly, the following work focuses on hybrid metric-based mesh adaptation and CFD simulation on such meshes. Regarding hybrid mesh generation, the method relies on a preliminary mesh obtained through so-called metric-aligned and metric-orthogonal approaches. These approaches utilize the directional information held by a prescribed metric-field to generate right angled elements, that can be combined into structured elements to form a hybrid mesh. The result highly depends on the quality of the metric field. Thus, emphasis is put on the size gradation control performed beforehand. This process is re-designed to favor metric-orthogonal meshes. To validate the method, some CFD simulations are performed. The modifications brought to the existing Finite Volume solver to enable such computations has been developed.

4.6. Anisotropic mesh adaptation for fluid-structure interactions

Participants: Frédéric Alauzet, Adrien Loseille, Julien Vanharen [correspondant].

A new strategy for mesh adaptation dealing with Fluid-Structure Interaction (FSI) problems is presented using a partitioned approach. The Euler equations are solved by an edge-based Finite Volume solver whereas the linear elasticity equations are solved by the Finite Element Method using the Lagrange P^1 elements. The coupling between both codes is realized by imposing boundary conditions. Small displacements of the structure are assumed and so the mesh is not deformed. The computation of a well-documented FSI test case is finally carried out to perform validation of this new strategy.

GRACE Project-Team

6. New Results

6.1. Error Locating pairs

Participants: Alain Couvreur, Isabella Panaccione.

Algebraic codes such as Reed–Solomon codes and algebraic geometry codes benefit from efficient decoding algorithms permitting to correct errors up to half the minimum distance and sometimes beyond. In 1992, Pellikaan proved that many **unique** decoding could be unified using an object called *Error correcting pair*. In short, given an error correcting code $\mathcal{C}$, an error correcting pair for $\mathcal{C}$ is a pair of codes $(\mathcal{A}, \mathcal{B})$ whose component wise product $\mathcal{A} * \mathcal{B}$ is contained in the dual code $\mathcal{C}^{\perp}$ and such that $\mathcal{A}, \mathcal{B}$ satisfy some constraints of dimension and minimum distance.

On the other hand, in the late 90's, after the breakthrough of Sudan and Guruswami Sudan the question of list decoding permitting to decode beyond half the minimum distance. In a recently submitted article, A. Couvreur and I. Panaccione [15] proposed a unified point of view for probabilistic decoding algorithms decoding beyond half the minimum distance. Similarly to Pellikaan's result, this framework applies to any code benefiting from an *error locating pair* which is a relaxed version of error correcting pairs.

6.2. Factoring oracles

Participants: François Morain, Benjamin Smith, Guénaël Renault.

Integer factoring is an old topic, and the situation is as follows: in the classical world, we think integer factoring is hard and the algorithms we have are quite powerful though of subexponential complexity and factoring numbers with several hundred bits; whereas in the quantum world, it is assumed to be easy (i.e., there exists a quantum polynomial time algorithm) but never experienced and the record is something like a few bits. F. Morain, helped by B. Smith and G. Renault studied the theoretical problem of factoring integers given access to classical oracles, like the Euler totient function. They were able to give some interesting classes of numbers that could tackled, The manuscript [18] is currently being refereed.

ILDA Project-Team

7. New Results

7.1. Digital Ink and Data Manipulation

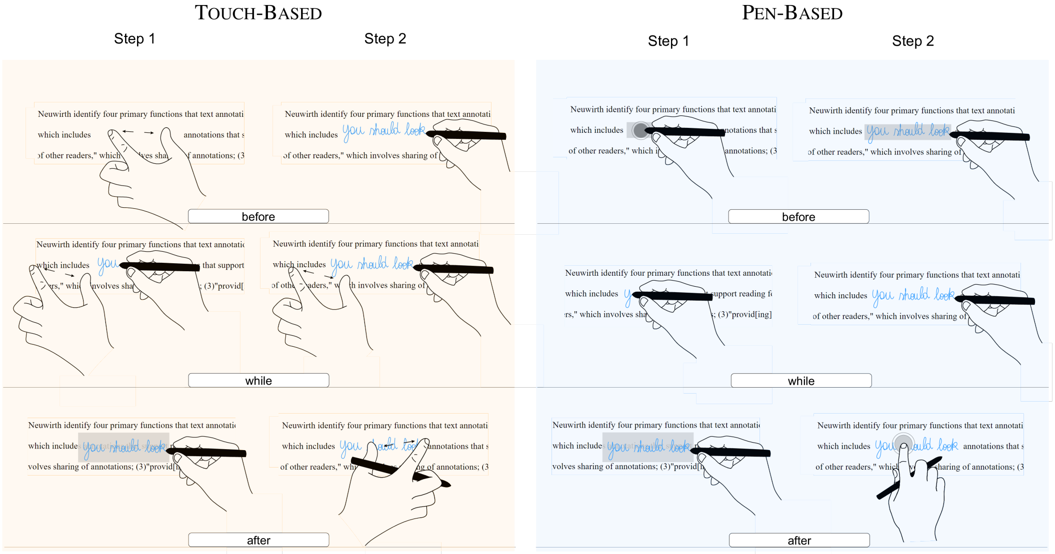


Figure 3. In the SpaceInk design space, both touch-based and pen-based techniques let users specify the strategy for creating white space at different moments: either before, while, or after annotating. With touch-based techniques, users are free to both gesture and write with a single hand (as illustrated in the after condition) or with two hands (as illustrated in the before condition).

We investigated how pen and touch could be best combined to facilitate the digital annotation of documents. When editing or reviewing a document, people directly overlay ink marks on content. For instance, they underline words, or circle elements in a figure. These overlay marks often accompany in-context annotations in the form of handwritten footnotes and marginalia. People tend to put annotations close to the content that elicited them, but have to compose with the often-limited whitespace. Based on these observations, we explored a design space – which we call SpaceInk (UIST 2019 [9]) – of pen+touch techniques that make room for in-context annotations by dynamically reflowing documents. We identified representative techniques in this design space, spanning both new ones and existing ones, as illustrated in Figure 3 . We evaluated them in a user study. The results of this study then informed the design of a prototype system which lets users concentrate on capturing fleeting thoughts, streamlining the overall annotation process by enabling the fluid inverleaving of space-making gestures with freeform ink.

Together with colleagues from the EPIC team at Microsoft Research (see Section 9.3.2.1), we also investigated the potential of digital inking for exploring heterogeneous datasets and trying to make sense of them. During sensemaking, people annotate insights: underlining sentences in a document or circling regions on a map. They jot down their hypotheses: drawing correlation lines on scatterplots or creating personal legends to track patterns. Based on these observations, we designed ActiveInk (CHI 2019 [22]), a system enabling people to seamlessly transition between exploring data and externalizing their thoughts using pen and touch as input

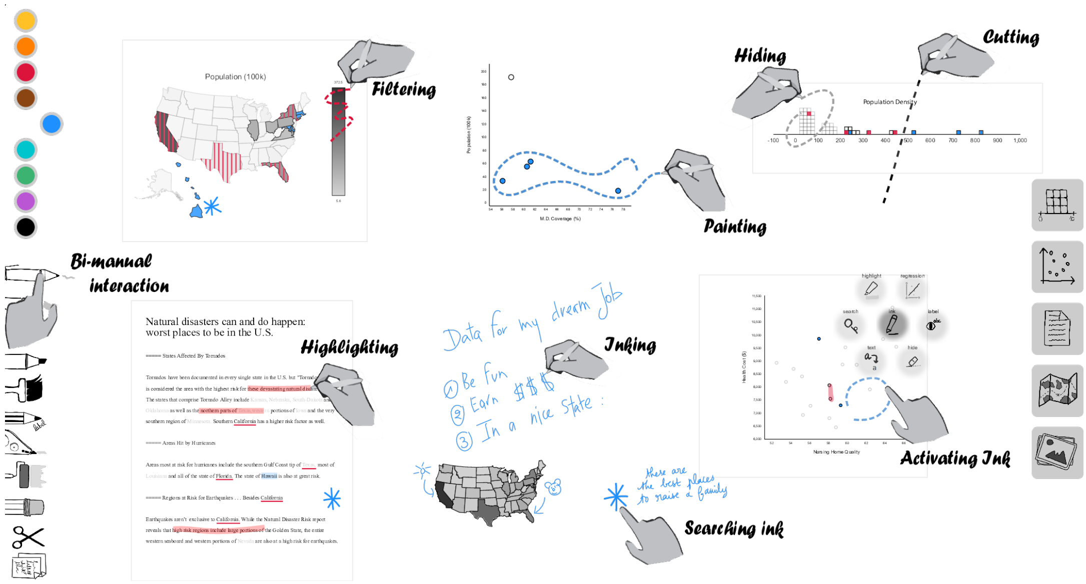


Figure 4. ActiveInk, a collaboration with Microsoft Research, affords smooth transition between using a digital pen for high-precision selections of heterogeneous data coming from multiple sources, and for externalizing thinking via notes and annotations. Ink strokes are leveraged to perform operations on underlying data.

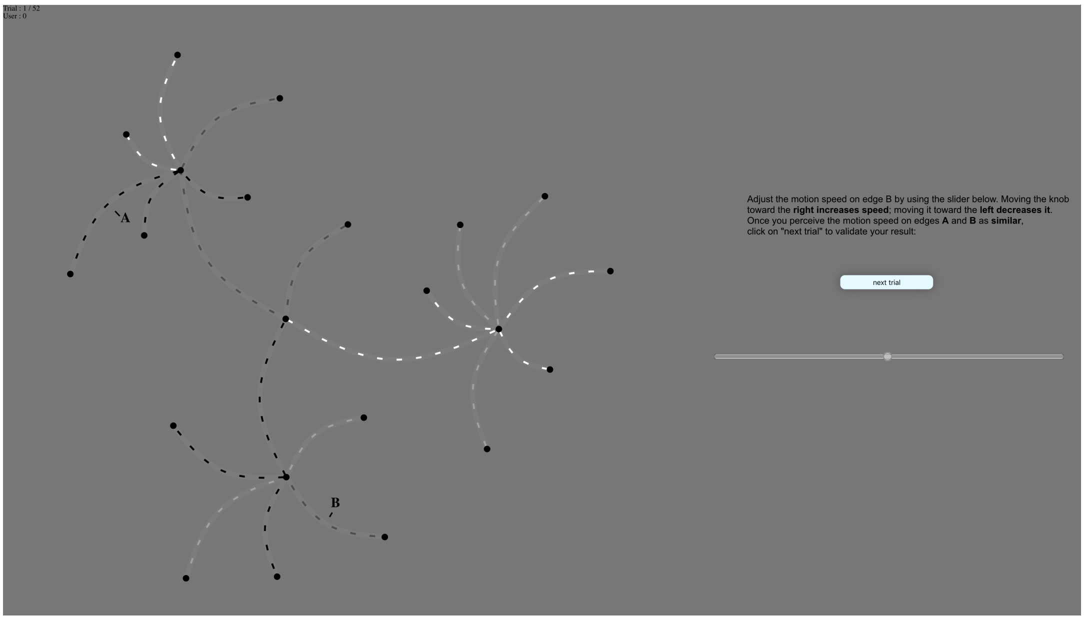
channels. ActiveInk, illustrated in Figure 4 , enables the natural use of pen for active reading behaviors, while supporting analytic actions by activating any of these ink strokes. Through a qualitative study with eight participants, we observed active reading behaviors during data exploration and design principles to support sensemaking.

7.2. Novel Forms of Input in Immersive Environments

ILDA researchers have started to investigate input techniques for the specific context of immersive environments, based on, e.g., virtual or augmented reality. These hardware devices enable displaying large amounts of data in space to better support data analysis, and there is a growing group of research focusing on Immersive Analytics in the HCI community. The question of input for data manipulation in these environments is crucial, but challenging because users must be able to activate various commands or adjust various values while remaining free to move. In this context, using the whole body as an input device offers several advantages: 1) the body provides physical support as an interactive surface, which improves accuracy and makes it less tiring to interact; 2) using the body does not impair mobility and avoids handling devices; 3) proprioception makes it possible to interact eyes-free, including when choosing values in a range; 4) by leveraging spatial memory, the body helps memorizing commands, thus interacting in expert mode (i.e., perform quick actions without visual feedback). ILDA team members participated to a position paper on this topic, which analyzes various ways of interacting with the body, discussing their pros and cons as well as associated challenges for immersive analytics [23].

7.3. Multivariate Network Visualization

Edges in networks often represent transfer relationships between vertices. When visualizing such networks as node-link diagrams, animated particles flowing along the links can effectively convey this notion of transfer. Variables that govern the motion of particles, their speed in particular, may be used to visually represent



Adjust the motion speed on edge B by using the slider below. Moving the knob toward the **right increases speed**; moving it toward the **left decreases it**. Once you perceive the motion speed on edges **A** and **B** as **similar**, click on "next trial" to validate your result:

Figure 5. Experimental task used in the study about the influence of color and size of moving particles on their perceived speed in node-link diagrams. Participants had to adjust the speed of particles on a specific edge so that it would match that of particles on another edge, using a slider.

edge data attributes. Few guidelines exist to inform the design of these particle-based network visualizations, however. Following up on our initial investigation of motion as an encoding channel for edge attributes in multivariate network visualization [75], we investigated the influence of color and size of moving particles on their perceived speed in node-link diagrams (INTERACT 2019 [20]). Empirical studies so far had only looked at the different motion variables in isolation, independently from other visual variables controlling the appearance of particles, such as their color or size. We ran a study of the influence of several visual variables on users' perception of the speed of particles. Part of the experimental setup is illustrated in Figure 5 . Our results show that particles' luminance, chromaticity and width do not interfere with their perceived speed. But variations in their length make it more difficult for users to compare the relative speed of particles across edges.

Figure 6. Graphies running on a tablet with support for pen+touch. Graphies is developed entirely using Web technologies.

Beyond questions of perception of information in multivariate network visualizations, we also investigated the problem of creating environments for the design of multivariate network visualizations, with a focus on expressive design. Expressive design environments enable visualization designers not only to specify chart types and visual mappings, but also to customize individual graphical marks, as they would in a vector graphics drawing tool. Prior work had mainly investigated how to support the expressive design of a wide range of charts generated from tabular data: bar charts, scatterplots, maps, *etc*. But multivariate network data structures raise specific challenges and opportunities in terms of visual design and interactive authoring. Together with company TKM (see Section 8.1), we developed an expressive design environment for node-link diagrams generated from multivariate networks called Graphies (TVCG 2019, [15]), illustrated in Figure 6 . We followed a user-centered design approach, involving expert analysts from TKM, and validated the approach through a study in which participants successfully reproduced several expressive designs, and created their own designs as well.

7.4. Visualization in Specific Application Areas

Finally, we worked in collaboration with other researchers on projects aimed at investigating how visualization can support experts in different application areas.

In the area of geovisualization, we performed a comparison of visualization techniques to help analysts identify correlation between variables over space and time (TVCG/InfoVis 2019, [6]). Observing the relationship between two or more variables over space and time is essential in many application domains. For instance, looking, for different countries, at the evolution of both the life expectancy at birth and the fertility rate will give an overview of their demographics. The choice of visual representation for such multivariate data is key to enabling analysts to extract patterns and trends. We conducted a study comparing three techniques that are representative of different strategies to visualize geo-temporal multivariate data. Participants performed a series of tasks that required them to identify if two variables were correlated over time and if there was a pattern in their evolution. Our results showed that a visualization's effectiveness depends strongly on the task to be carried out. Based on this study's findings, we derived a set of design guidelines about geo-temporal visualization techniques for communicating correlation.

Together with researchers from INRA, we performed an exploratory study about the visual exploration of model simulations for a range of experts (CHI 2019, [16]). Experts in different domains rely increasingly on simulation models of complex processes to reach insights, make decisions, and plan future projects. These models are often used to study possible trade-offs, as experts try to optimize multiple conflicting objectives in a single investigation. Understanding all the model intricacies, however, is challenging for a single domain expert. This project introduced a simple approach to support multiple experts when exploring complex model results, working concurrently on a shared visualization surface. The results of an observational study focusing on the link between expertise and insight generation during the analysis process, revealed the different exploration strategies and multi-storyline approaches that domain experts adopt during trade-off analysis. This eventually led to recommendations for collaborative model exploration systems.

We collaborated with researchers in databases from Université Paris Descartes on progressive similarity search on time-series data (BigVis 2019 workshop, [24]). Time-series data are increasing at a dramatic rate, yet their analysis remains highly relevant in a wide range of human activities. Due to their volume, existing systems dealing with time-series data cannot guarantee interactive response times, even for fundamental tasks such as similarity search. This paper presented our vision to develop analytic approaches that support exploration and decision making by providing progressive results, before the final and exact ones have been computed. Findings from our experiment indicated that there is a gap between the time the most similar answer is found and the time when the search algorithm terminates, resulting in inflated waiting times without any improvement. These findings led to preliminary ideas about computing probabilistic estimates of the final results that could help users decide when to stop the search process.

In the field of Education, we contributed to EduClust, an online visualization application for teaching clustering algorithms (EuroGraphics 2019, [18]). EduClust combines visualizations, interactions, and animations to facilitate the understanding and teaching of clustering steps, parameters, and procedures. Traditional classroom settings aim for cognitive processes like remembering and understanding. We designed EduClust for expanded educational objectives like applying and evaluating. The application can be used by both educators to prepare teaching material and examples, and by students to explore clustering differences and discover algorithmic subtleties.

LIFEWARE Project-Team

7. New Results

7.1. CRN design by program compilation

Participants: Elisabeth Degrand, François Fages, Mathieu Hemery, Wei-Chih Huang [NTU Taiwan], Sylvain Soliman.

One goal of synthetic biology is to implement useful functions with biochemical reactions, either by reprogramming living cells or programming artificial vesicles. In this perspective, we consider Chemical Reaction Networks (CRN) as a programming language, and investigate the CRN program synthesis problem. Recent work has shown that CRN interpreted by differential equations are Turing-complete and can be seen as analog computers where the molecular concentrations play the role of information carriers. Any real function that is computable by a Turing machine in arbitrary precision can thus be computed by a CRN over a finite set of molecular species. The proof of this result gives a numerical method to generate a finite CRN for implementing a real function presented as the solution of a Polynomial Initial Values Problem (PIVP).

The compilation of high-level imperative programming languages in CRN requires however an efficient implementation of program control flows using threshold functions. The biochemical threshold function is also a crucial component in the biosensor circuits to be deployed in living cells or synthetic vesicles for disease diagnosis. In [5], based on the zero-order ultrasensitivity, we propose an economic biochemical implementation of threshold functions with reconfigurable threshold values. We show that the so-constructed threshold function module well approximates the unit step function and allows robust composition with other function modules for complex computation tasks. This is now implemented in BIOCHAM-4 for the compilation of sequentiality and conditionals in CRNs.

7.2. CRN design by artificial evolution

Participants: Elisabeth Degrand, François Fages, Mathieu Hemery, Sylvain Soliman.

In [4], [12], we study an alternative method based on artificial evolution to build a CRN that approximates a real function given on finite sets of input values. We present a nested search algorithm that evolves the structure of the CRN and optimizes the kinetic parameters at each generation. We evaluate this algorithm on the Heaviside and Cosine functions both as functions of time and functions of input molecular species. We then compare the CRN obtained by artificial evolution both to the CRN generated by the numerical method from a PIVP definition of the function, and to the natural CRN found in the BioModels repository for switches and oscillators.

On a Heaviside function of time, the results obtained by artificial evolution lead to a remarkably simple CRN of 3 molecular species and 5 reactions with double catalysts which provide a very stiff transition although using mass action law kinetics. This solution is more economical than the CRN generated by the PIVP method for sigmoid functions. On a Heaviside function of input, the CRN found by evolution are slightly more complicated than the bistable switch found in cell cycle CRN for instance, but much less complex than the MAPK signaling network that plays a similar role.

On the cosine function of time, the best CRN found by evolution contains an annihilation reaction similar to the CRN generated by the numerical method for positive and negative variables, but one less reaction thanks to an intriguing non symmetric use of the two variables which preserves the limit cycle. Interestingly, the evolved and the PIVP generated structures could be compared to prokaryote and eukaryote models of the circadian clock found in BioModels.

On the cosine function of input, a CRN surprisingly emerges with the structure of the CRN for cosine function of time, using the same trick as for PIVP compilation to stop time at the desired input value.

In [2], we use a genetic algorithm to evolve biochemical networks displaying a direct logarithmic response. Numerous biological systems are known to harbour a form of logarithmic behaviour, from Weber's law to bacterial chemotaxis. Working on a logarithmic scale allows the organism to respond appropriately to large variations in a given input at a modest cost in terms of metabolism. Interestingly, a quasi-perfect log-response implemented by the same simple core network evolves in a convergent way across our different replications. The best network is able to fit a logarithm over 4 order of magnitude with an accuracy of the order of 1%. At the heart of this network, we show that a logarithmic approximation may be implemented with one single non-linear interaction, that can be interpreted either as a phosphorylation or as a ligand induced multimerization and provide an analytical explanation of the effect. Biological log-response might thus be easier to implement than usually assumed.

7.3. CRN learning from data time series

Participants: François Fages, Jeremy Grignard, Julien Martinelli, Sylvain Soliman.

With the automation of biological experiments and the increase of quality of single cell data that can now be obtained by phosphoproteomic and time lapse videomicroscopy, automating the building of mechanistic models from these data time series becomes conceivable and a necessity for many new applications. While learning numerical parameters to fit a given model structure to observed data is now a quite well understood subject, learning the structure of the model is a more challenging problem that previous attempts failed to solve without relying quite heavily on prior knowledge about that structure. In [8], [7], we consider mechanistic models based on chemical reaction networks (CRN) with their continuous dynamics based on ordinary differential equations, and finite time series about the time evolution of concentration of molecular species for a given time horizon and a finite set of perturbed initial conditions. We present a greedy heuristics unsupervised statistical learning algorithm to infer reactions with a time complexity for inferring one reaction in $O(t.n^2)$where n is the number of species and t the number of observed transitions in the traces. We evaluate this algorithm both on simulated data from hidden CRNs, and on real videomicroscopy single cell data about the circadian clock and cell cycle progression of NIH3T3 embryonic fibroblasts. In all cases, our algorithm is able to infer meaningful reactions, though generally not a complete set for instance in presence of multiple time scales or highly variable traces.

7.4. CRN reductions

Participants: Orianne Bargain, Eléonore Bellot, François Fages, Eva Philippe, Sylvain Soliman.

We have shown in the past that model reduction relationships between CRNs can be detected on a large scale by the graph matching notion of subgraph epimorphism [0], furthermore quite efficiently using constraint programming or SAT solving techniques. Nevertheless, establishing whether two models are linked through a SEPI is an NP-complete problem which can be computationally expensive in some practical cases. Furthermore, the number of SEPIs can be huge, and some of them may not have a biological interpretation. In [11], we have improved the SEPI framework in this respect in three ways: by introducing optimization criteria to restrict the set of solutions, by restricting merge operations to some notion of neighborhood, and by preprocessing the CRN graphs in normal form in order to eliminate some common model reduction patterns.

Furthermore, in the framework of the ANR-DFG SYMBIONT project we investigate mathematical justification of SEPI reductions based on Tikhonov's theorem and their computation using tropical algebra methods and constraint programming techniques [0].

7.5. CRN modeling of biological systems

Participants: Auriane Cozic, Elisabeth Degrand, François Fages, Eléa Greugny, Jeremy Grignard, Constance Le Gac, Léna Le Quellec, Paul Remondeau, Sylvain Soliman.

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[0] Steven Gay, François Fages, Thierry Martinez, Sylvain Soliman, Christine Solnon. On the subgraph Epimorphism Problem. Discrete Applied Mathematics, 162:214–228, 2014.

[0] Sylvain Soliman, François Fages, Ovidiu Radulescu. A constraint solving approach to model reduction by tropical equilibration. Algorithms for Molecular Biology, 9(24), 2014.

This year, beyond implementation work on hybrid simulations in BIOCHAM and on antithetic feedback control in CRNs, we have started the computational modelling of three biological systems with important potential applications in biomedicine.

The first is about erythrocytes (i.e. red blood cells). Their most obvious function concerns the respiratory system since erythrocytes allow gas exchanges at the level of the organism by transporting dioxygen and carbon dioxide between the lungs and the tissues. However, red blood cells also have an important buffer function in the blood, which is necessary to keep blood pH in the physiological range. Modelling the red blood cells with CRNs using BIOCHAM gives us insight as to which biological objects are necessary to allow the cell to process its functions correctly. At the level of Systems Biology, it also allows us to understand the links between the different biological functions of erythrocytes.

The second concerns microtubules and their post-translational modifications involved in major cellular processes such as: mitosis, cardiomyocyte contraction, and neuronal differentiation. More precisely, in neurons, the post-translational modifications of detyrosination and tyrosination are crucial for neuronal plasticity, axon regeneration, recruitment and transports of proteins and correct neuronal wiring. We hypothesize that the decrease of density and length of microtubules and the loss of neuronal structures such as synapses, dendritic spine and growth cone which are correlated with the progressive cognitive decline [9,10] may be the consequence of the dysregulation of the cycle detyrosination/tyrosination in neurodegenerative disorder. This hypothesis is investigated in collaboration with Servier by combining experimental approaches with mathematical modelling.

The third concerns inflammation processes in skin. Skin protects the body against external agents, for instance pathogens, irritants, or UV radiation, that can trigger inflammation. Inflammation is a complex phenomenon that is classified in two main types, acute and chronic. They are distinguished by different parameters such as the duration, the underlying mechanisms, the components involved like the type of immune cells, and the nature and intensity of the associated clinical signs. The computational models developed in collaboration with Johnson&Johnson France, combine mathematical and multi-agent modelling using BIOCHAM and EPISIM modelling tools.

7.6. Automated Inference of Boolean models from molecular interaction maps

Participant: Sylvain Soliman.

Molecular interaction maps have emerged as a meaningful way of representing biological mechanisms in a comprehensive and systematic manner. However, their static nature provides limited insights to the emerging behavior of the described biological system under different conditions. Computational modeling provides the means to study dynamic properties through *in silico* simulations and perturbations.

In collaboration with Anna Niarakis (Université d'Évry, GenHotel) we have started developing the CaSQ Python package, by defining simplification rules and logical formulas for the inferred Boolean models according to the topology and the annotations of the starting molecular interaction maps. We used CaSQ to produce executable files of existing molecular maps notably a big map of the Rheumatoid Arthritis that is at the core of Évry team's work.

A publication on the inference process has already been submitted to Bioinformatics but work continues on the applications side to fine-tune the automatically generated model and analyze its dynamical properties.

7.7. Optimal control of an artificial microbial differentiation system for protein bioproduction

Participants: Élise Weill Duflos, Virgile Andréani, Chetan Aditya, Pierre Martinon [EPI Commands], Jakob Ruess, Grégory Batt, J. Frédéric Bonnans [EPI Commands].

The growth of microorganisms is controlled by strategies for the dynamical allocation of available resources over different cellular functions. Synthetic biology approaches are considered nowadays to artificially modify these strategies and turn microbial populations into biotechnological factories for the production of metabolites of interest. In our recent work, we have studied dynamics of microbial resource allocation and growth in terms of coarse-grained self-replicator models described by ordinary differential equations, and proposed artificial control strategies for the optimization of metabolite production based on the reengineering of resource allocation. In this contribution, we elaborated on our earlier results and further investigate synthetic resource allocation control strategies [9]. Using numerical simulation, we studied the effect on growth and bioproduction of the (biological or technological) costs associated with discontinuous control strategies, and of the time allotted to optimal substrate utilization. Results provided novel insight into the most favorable synthetic control strategies.

7.8. Can optimal experimental design serve as a tool to characterize highly non-linear synthetic circuits?

Participants: Maxim Kryukov [Pasteur Institute], Arthur Carcano, Grégory Batt, Jakob Ruess.

One of the most crippling problems in quantitative and synthetic biology is that models aiming to describe the real mechanisms of biochemical processes inside cells typically contain too many unknown parameters to be reliably inferable from available experimental data. Recent years, however, have seen immense progress in the development of experimental platforms that allow not only to measure biological systems more precisely but also to administer external control inputs to the cells. Optimal experimental design has been identified as a tool that can be used to decide how to best choose these control inputs so as to excite the systems in ways that are particularly useful for learning the biochemical rate constants from the corresponding data. Unfortunately, the experiment that is best to learn the parameters of a system depends on the precise values of these parameters, which are naturally unknown at the time at which experiments need to be designed. Here, we used a recently constructed genetic toggle switch as a case study to investigate how close to the best possible experiment we can hope to get with the most widely used optimal design approaches in the field. We found that, for strongly nonlinear systems such as the toggle switch, reliably predicting the information that can be gained from a priori fixed experiments can be difficult if the system parameters are not known very precisely [6]. This suggests that a better strategy to guarantee informative experiments might be to use feedback control and to adjust the experimental plan in real time.

7.9. Molecular noise of innate immunity shapes bacteria-phage ecologies

Participant: Jakob Ruess.

Mathematical models have been used successfully at diverse scales of biological organization, ranging from ecology and population dynamics to stochastic reaction events occurring between individual molecules in single cells. Generally, many biological processes unfold across multiple scales, with mutations being the best studied example of how stochasticity at the molecular scale can influence outcomes at the population scale. In many other contexts, however, an analogous link between micro-and macro-scale remains elusive, primarily due to the challenges involved in setting up and analyzing multi-scale models. In [3], we employed such a model to investigate how stochasticity propagates from individual biochemical reaction events in the bacterial innate immune system to the ecology of bacteria and bacterial viruses. We showed analytically how the dynamics of bacterial populations are shaped by the activities of immunity-conferring enzymes in single cells and how the ecological consequences imply optimal bacterial defense strategies against viruses. Our results suggest that bacterial populations in the presence of viruses can either optimize their initial growth rate or their population size, with the first strategy favoring simple immunity featuring a single restriction modification system and the second strategy favoring complex bacterial innate immunity featuring several simultaneously active restriction modification systems.

7.10. Estimating information in time-varying signals

Participant: Jakob Ruess.

Across diverse biological systems - ranging from neural networks to intracellular signaling and genetic regulatory networks - the information about changes in the environment is frequently encoded in the full temporal dynamics of the network nodes. A pressing data-analysis challenge has thus been to efficiently estimate the amount of information that these dynamics convey from experimental data. In [1], we developed and evaluated decoding-based estimation methods to lower bound the mutual information about a finite set of inputs, encoded in single-cell high-dimensional time series data. For biological reaction networks governed by the chemical Master equation, we derived model-based information approximations and analytical upper bounds, against which we benchmarked our proposed model-free decoding estimators. In contrast to the frequently-used k-nearest-neighbor estimator, decoding-based estimators robustly extract a large fraction of the available information from high-dimensional trajectories with a realistic number of data samples. We applied these estimators to previously published data on Erk and Ca^{2+} signaling in mammalian cells and to yeast stress-response, and found that substantial amount of information about environmental state can be encoded by non-trivial response statistics even in stationary signals. We argued that these single-cell, decoding-based information estimates, rather than the commonly-used tests for significant differences between selected population response statistics, provide a proper and unbiased measure for the performance of biological signaling networks.

M3DISIM Project-Team

6. New Results

6.1. Mathematical and Mechanical Modeling

6.1.1. Stochastic modeling of chemical-mechanical coupling in striated muscles

Participants: Matthieu Caruel, Philippe Moireau, Dominique Chapelle [correspondant].

In [18] we propose a chemical–mechanical model of myosin heads in sarcomeres, within the classical description of rigid sliding filaments. In our case, myosin heads have two mechanical degrees-of-freedom (dofs)—one of which associated with the so-called power stroke—and two possible chemical states, i.e., bound to an actin site or not. Our major motivations are twofold: (1) to derive a multiscale coupled chemical–mechanical model and (2) to thus account—at the macroscopic scale—for mechanical phenomena that are out of reach for classical muscle models. This model is first written in the form of Langevin stochastic equations, and we are then able to obtain the corresponding Fokker–Planck partial differential equations governing the probability density functions associated with the mechanical dofs and chemical states. This second form is important, as it allows to monitor muscle energetics and also to compare our model with classical ones, such as the Huxley'57 model to which our equations are shown to reduce under two different types of simplifying assumptions. This provides insight and gives a Langevin form for Huxley'57. We then show how we can calibrate our model based on experimental data—taken here for skeletal muscles—and numerical simulations demonstrate the adequacy of the model to represent complex physiological phenomena, in particular the fast isometric transients in which the power stroke is known to have a crucial role, thus circumventing a limitation of many classical models.

6.1.2. Upscaling of elastic network models

Participant: Patrick Le Tallec.

This work is done in collaboration with Julie Diani from École Polytechnique. The purpose of the approach is to develop general upscaling strategy for deriving macroscopic constitutive laws for rubberlike materials from the knowledge of the network distribution and a mechanical description of the individual chains and of their free energy. It is based on a variational approach in which the microscopic configuration is described by the position of the crosslinks and is obtained not by an affine assumption but by minimizing the corresponding free energy on stochastic large Representative Volume Elements with adequate boundary conditions. This general framework is then approximated by using a microsphere (directional) description of the network and by performing a local minimisation of the network free energy on this simplified configuration space under a maximal advance path kinematic constraint. This approximation framework takes into account anisotropic damage and is extended to handle situations with tube like constraints and stress induced cristallisation. For more detail see [23].

6.1.3. Stochastic construction of surrogate multiphase materials

Participant: Patrick Le Tallec.

Random microstructures of heterogeneous materials play a crucial role in the material macroscopic behavior and in predictions of its effective properties. A common approach to modeling random multiphase materials is to develop so-called surrogate models approximating statistical features of the material. However, the surrogate models used in fatigue analysis usually employ simple microstructure, consisting of ideal geometries such as ellipsoidal inclusions, which generally does not capture complex geometries. In our work , we introduce a simple but flexible surrogate microstructure model for two-phase materials through a level-cut of a Gaussian random field with covariance of Matern class. In addition to the traditional morphology descriptors such as porosity, size and aspect ratio of inclusions, our approach provides control of the regularity of the inclusions interface and sphericity. These parameters are estimated from a small number of real material images using

Bayesian inversion. An efficient process of evaluating the samples, based on the Fast Fourier Transform, makes possible the use of Monte-Carlo methods to estimate statistical properties for the quantities of interest in a given material class. This work in progress is done in collaboration with Andrei Constantinescu (École Polytechnique), Ustim Khristenko and Barbara Wohlmuth (Technical University Munich) and Tinsley Oden (University of Texas at Austin). This work has been submitted for publication in an international journal.

6.1.4. Apprehending the effects of mechanical deformations in cardiac electrophysiology – A homogenization approach

Participants: Annabelle Collin [MONC], Sébastien Imperiale, Philippe Moireau, Jean-Frédéric Gerbeau [Inria Siège], Dominique Chapelle [correspondant].

In this work [22], we follow a formal homogenization approach to investigate the effects of mechanical deformations in electrophysiology models relying on a bidomain description of ionic motion at the microscopic level. To that purpose, we extend these microscopic equations to take into account the mechanical deformations, and proceed by recasting the problem in the frame- work of classical two-scale homogenization in periodic media, and identifying the equations satisfied by the first coefficients in the formal expansions. The homogenized equations reveal some interesting effects related to the microstructure – and associated with a specific cell problem to be solved to obtain the macroscopic conductivity tensors – in which mechanical deformations play a non-trivial role, i.e. do not simply lead to a standard bidomain problem posed in the deformed configuration. We then present detailed numerical illustrations of the homogenized model with coupled cardiac electrical-mechanical simulations – all the way to ECG simulations – albeit without taking into account the abundantly-investigated effect of mechanical deformations in ionic models, in order to focus here on other effects. And in fact our numerical results indicate that these other effects are numerically of a comparable order, and therefore cannot be disregarded.

6.1.5. Patient-specific pulmonary mechanics - Modelling and estimation. Application to pulmonary fibrosis.

Participants: Cecile Patte [correspondant], Martin Genet, Dominique Chapelle.

Interstitial pulmonary diseases, like Idiopathic Pulmonary Fibrosis (IPF), affect the alveolar structure of lung tissue, which impacts lung mechanical properties and pulmonary functions. In this work [43], we aim to better understand the pulmonary mechanics in order to improve IPF diagnosis. We developped a poromechanical model for the lung at the organ scale and at the breathing scale. This model is then used to estimate regional mechanical parameters based on clinical data. In the future, this process can be used as an augmented diagnosis tool for clinicians. This work has been presented at the CSMA conference.

6.1.6. Energy preserving cardiac circulation models: formulation, reduction, coupling, inversion, and discretization

Participants: Jessica Manganotti, Philippe Moireau, Sébastien Imperiale [correspondant], Miguel Fernandez [Inria Paris, COMMEDIA].

The modeling of the heart cannot be satisfying if not coupled to the body circulation, and at least to the arterial circulation, which is its direct output “boundary condition”. But more importantly in the clinical context, it is still difficult – ant very invasive – to access the ventricular pressure, which is absolutely necessary for specifying the heart activity. By comparison, more and more devices allow to register non-invasively a distal pressure, for instance at the wrist or the finger, which could be used to estimate the ventricular pressure by inversion of a well adapted arterial circulation model. Such relation is of major interest for clinicians, for example anesthetists, since it could allow real-time monitoring and prediction of the effects of injected drugs during a clinical intervention. Models of the arterial circulation is a well-known subject where dimension reduction has been widely studied for more than half a century. However, the question remains of formulating energy-consistent formulations that can be consistently maintained during the reduction, when coupled to a heart model, and also when discretized. Yet the question is crucial for a better understanding of the physical phenomena of blood flow ejection from the heart as well as the propagation in the arterial network. Moreover, as these models are non-linear, energy-preserving approaches are one of the few tools at our disposal to mathematically justify modeling, discretization or inversion approaches. Finally, inverting this unsteady model for estimation purposes of medical data also benefits from energy-preserving formulation as the inverse approach should also satisfy some stability properties. The subject here is twofold and part of the thesis of J. Manganotti. First we plan to develop accurate models, coupling strategies and robust numerical methods of the arterial network propagation coupled to the heart. Second, we want to develop observer-based strategies that will allow to easily feed these models with measurements in order to perform state estimation of hidden variables or identify key biophysical parameters.

6.1.7. Hierarchical modeling of force generation in cardiac muscle

Participants: Matthieu Caruel, François Kimmig [correspondant].

Performing physiologically relevant simulations of the beating heart in clinical context requires to develop detailed models of the microscale force generation process. These models however may be difficult to implement in practice due to their high computational costs and complex calibration. We propose a hierarchy of three interconnected cardiac muscle contraction models – from the more refined to the more simplified – that are rigorously and systematically related with each other, offering a way to select, for a specific application, the model that yields the best trade-off between physiological fidelity, computational cost and calibration complexity. Our starting model takes into account the stochastic dynamics of the molecular motors force producing conformational changes– and in particular the power stroke – and captures all the timescales of appearing in classical experimental isotonic responses of a heart papillary muscle submitted to rapid load changes. Adiabatic elimination of fast relaxing variables of the stochastic model yields a formulation based on partial differential equations (PDEs) that falls into the family of the Huxley'57 model, while embedding some properties of the process occurring at the fastest timescales. The third family of models is deduced from the PDE model by making minimal assumptions on the parameters, which leads to a computationally light formulation based on ordinary differential equations only. The three models families are compared to the same set of experimental data to systematically assess what physiological indicators can be reproduced or not and how these indicators constrain the model parameters. Finally, we discuss the applicability of these models for heart simulation. This work has been submitted for publication in an international journal.

6.1.8. A relaxed growth modeling framework for controlling growth-induced residual stresses

Participant: Martin Genet.

Background Constitutive models of the mechanical response of soft tissues have been established and are widely accepted, but models of soft tissues remodeling are more controversial. Specifically for growth, one important question arises pertaining to residual stresses: existing growth models inevitably introduce residual stresses, but it is not entirely clear if this is physiological or merely an artifact of the modeling framework. As a consequence, in simulating growth, some authors have chosen to keep growth-induced residual stresses, and others have chosen to remove them. **Methods** In this work, we introduce a novel "relaxed growth" framework allowing for a fine control of the amount of residual stresses generated during tissue growth. It is a direct extension of the classical framework of the multiplicative decomposition of the transformation gradient, to which an additional sub-transformation is introduced in order to let the original unloaded configuration evolve, hence relieving some residual stresses. We provide multiple illustrations of the framework mechanical response, on time-driven constrained growth as well as the strain-driven growth problem of the artery under internal pressure, including the opening angle experiment. **Findings** The novel relaxed growth modeling framework introduced in this paper allows for a better control of growth-induced residual stresses compared to standard growth models based on the multiplicative decomposition of the transformation gradient. **Interpretation** Growth-induced residual stresses should be better handled in soft tissues biomechanical models, especially in patient-specific models of diseased organs that are aimed at augmented diagnosis and treatment optimization. See [27] for more detail.

6.1.9. Multiscale population dynamics in reproductive biology: singular perturbation reduction in deterministic and stochastic models

Participants: Frédérique Clément [correspondant], Romain Yvinec.

During the supervision of a CEMRACS2018 project performed by Céline Bonnet (CMAP) and Keltoum Chahour (LERMA and JLAD), we have described (with Marie Postel, Sorbonne Université and Romain Yvinec, INRA) different modeling approaches for ovarian follicle population dynamics, based on either ordinary (ODE), partial (PDE) or stochastic (SDE) differential equations, and accounting for interactions between follicles [50]. We have put a special focus on representing the population-level feedback exerted by growing ovarian follicles onto the activation of quiescent follicles. We have taken advantage of the timescale difference existing between the growth and activation processes to apply model reduction techniques in the framework of singular perturbations. We have first studied the linear versions of the models to derive theoretical results on the convergence to the limit models. In the nonlinear cases, we have provided detailed numerical evidence of convergence to the limit behavior. We have reproduced the main semi-quantitative features characterizing the ovarian follicle pool, namely a bimodal distribution of the whole population, and a slope break in the decay of the quiescent pool with aging.

6.1.10. Stochastic nonlinear model for somatic cell population dynamics during ovarian follicle activation

Participants: Frédérique Clément [correspondant], Frédérique Robin, Romain Yvinec.

In mammals, female germ cells are sheltered within somatic structures called ovarian follicles, which remain in a quiescent state until they get activated, all along reproductive life. We have investigated the sequence of somatic cell events occurring just after follicle activation [54]. We have introduced a nonlinear stochastic model accounting for the joint dynamics of two cell types, either precursor or proliferative cells. The initial precursor cell population transitions progressively to a proliferative cell population, by both spontaneous and self-amplified processes. In the meantime, the proliferative cell population may start either a linear or exponential growing phase. A key issue is to determine whether cell proliferation is concomitant or posterior to cell transition, and to assess both the time needed for all precursor cells to complete transition and the corresponding increase in the cell number with respect to the initial cell number. Using the probabilistic theory of first passage times, we have designed a numerical scheme based on a rigorous Finite State Projection and coupling techniques to assess the mean extinction time and the cell number at extinction time. We have also obtained analytical formulas for an approximating branching process. We have calibrated the model parameters using an exact likelihood approach using both experimental and in-silico datasets. We have carried out a comprehensive comparison between the initial model and a series of submodels, which help to select the critical cell events taking place during activation. We have finally interpreted these results from a biological viewpoint.

6.1.11. A multiscale mathematical model of cell dynamics during neurogenesis in the mouse cerebral cortex

Participant: Frédérique Clément.

This work is a collaboration with Marie Postel and Sylvie Schneider-Maunoury (Sorbonne Université), Alice Karam (Sorbonne Universités), Guillaume Pézeron (MNHN).

Neurogenesis in the murine cerebral cortex involves the coordinated divisions of two main types of progenitor cells, whose numbers, division modes and cell cycle durations set up the final neuronal output. In this work [33] we aim at understanding the respective roles of these factors in the neurogenesis process, we have combined experimental in vivo studies with mathematical modeling and numerical simulations of the dynamics of neural progenitor cells. A special focus is put on the population of intermediate progenitors (IPs), a transit amplifying progenitor type critically involved in the size of the final neuron pool. A multiscale formalism describing IP dynamics allows one to track the progression of cells along the subsequent phases of the cell cycle, as well as the temporal evolution of the different cell numbers. Our model takes into account the dividing apical progenitors (AP) engaged into neurogenesis, both neurogenic and proliferative IPs, and the newborn neurons. The transfer rates from one population to another are subject to the mode of division (symmetric, asymmetric, neurogenic) and may be time-varying. The model outputs have been successfully fitted to experimental cell numbers from mouse embryos at different stages of cortical development, taking into account IPs and neurons, in order to adjust the numerical parameters. Applying the model to a mouse mutant for Ftm/Rpgrip1l, a gene involved in human ciliopathies with severe brain abnormalities, reveals a shortening of the neurogenic period associated with an increased influx of newborn IPs from apical progenitors at mid-neurogenesis. Additional information is provided on cell kinetics, such as the mitotic and S phase indexes, and neurogenic fraction. Our model can be used to study other mouse mutants with cortical neurogenesis defects and can be adapted to study the importance of progenitor dynamics in cortical evolution and human diseases.

6.2. Numerical Methods

6.2.1. Numerical analysis for an energy-stable total discretization of a poromechanics model with inf-sup stability

Participants: Dominique Chapelle [correspondant], Philippe Moireau.

In this joint work with Bruno Burtschell [16], we consider a previously proposed general nonlinear poromechanical formulation, and we derive a linearized version of this model. For this linearized model, we obtain an existence result and we propose a complete discretization strategy–in time and space–with a special concern for issues associated with incompressible or nearly-incompressible behavior. We provide a detailed mathematical analysis of this strategy, the main result being an error estimate uniform with respect to the compressibility parameter. We then illustrate our approach with detailed simulation results and we numerically investigate the importance of the assumptions made in the analysis, including the fulfillment of specific inf-sup conditions.

6.2.2. Conservative and entropy controlled remap for multi-material ALE simulations

Participant: Patrick Le Tallec.

For many multi-material problems such as fluid-structure interaction, impact or implosion problems, materials are in very large strains due to their nature or to the applied forces. In our situations of interest, we also have a strong coupling between energy and momentum conservation laws, due to intense transfers between internal and kinetic energies and to strong advection effects. Such situations are classically governed by the Euler's equations, written in Lagrangian form, and using a multi-material, single velocity framework, but their numerical solution demands a strict control of energy conservation and entropy production, which is hard to achieve in situations where dynamic remeshing is mandatory. In this framework, our approach deals with the analysis of the impact of a second-order staggered remap using an intersection-based approach on conservation properties and on the entropy control. We show that an accurate remap with exact mesh intersections and exact integrations affects both the momentum and the kinetic energy because of node mass re-localizations and node velocity remap. We propose therefore a staggered remapping strategy in order to take into account these discrepancies at a low computational cost. While preserving the strict conservation of total energy, our strategy allows to recover a proper entropy control at the expense of strict momentum conservation and monotonicity losses. This work [32] is done in collaboration with Alexandra Claisse (CEA DAM) and Alexis Marboeuf (École Polytechnique and CEA DAM).

6.2.3. Multipatch isogeometric analysis for complex structures

Participant: Patrick Le Tallec.

This work – done in collaboration with Nicolas Adam (École Polytechnique and PSA) and Malek Zarroug (PSA) – introduces, analyzes and validates isogeometric mortar methods for the solution of thick shells problems which are set on a multipatch geometry. It concerns industrial parts of complex geometries for which the effects of transverse shear cannot be neglected. For this purpose, Reissner-Mindlin model was retained and rotational degrees of freedom (DOF) of the normal are taken into account. A particular attention is devoted to the introduction of a proper formulation of the coupling conditions at patches interfaces, with a particular interest on augmented lagrangian formulations, to the choice and validation of mortar spaces, and to the derivation of adequate integration rules. The relevance of the proposed approach is assessed numerically on various significative examples of industrial relevance. This work has been submitted for publication in an international journal.

6.2.4. *Mathematical and numerical study of transient wave scattering by obstacles with the Arlequin Method*

Participant: Sébastien Imperiale.

In this work [14] we extend the Arlequin method to overlapping domain decomposition technique for transient wave equation scattering by obstacles. The main contribution of this work is to construct and analyze from the continuous level up to the fully discrete level some variants of the Arlequin method. The constructed discretizations allow to solve wave propagation problems while using non-conforming and overlapping meshes for the background propagating medium and the surrounding of the obstacle respectively. Hence we obtain a flexible and stable method in terms of the space discretization – an inf-sup condition is proven – while the stability of the time discretization is ensured by energy identities.

6.2.5. *Construction and analysis of fourth-order, energy consistent, family of explicit time discretizations for dissipative linear wave equations*

Participants: Juliette Chabassier [MAGIQUE-3D], Julien Diaz [MAGIQUE-3D], Sébastien Imperiale [correspondant].

This work and the corresponding article [19], deal with the construction of a family of fourth order, energy consistent, explicit time discretizations for dissipative linear wave equations. The schemes are obtained by replacing the inversion of a matrix, that comes naturally after using the technique of the Modified Equation on the second order Leap Frog scheme applied to dissipative linear wave equations, by explicit approximations of its inverse. The stability of the schemes are studied using an energy analysis and a convergence analysis is carried out. Numerical results in 1D illustrate the space/time convergence properties of the schemes and their efficiency is compared to more classical time discretizations.

6.2.6. *Energy decay and stability of a perfectly matched layer For the wave equation*

Participants: Sébastien Imperiale [correspondant], Maryna Kachanovska [POEMS].

We follow a previous work where PML formulations was proposed for the wave equation in its standard second-order form. In the present work [15], energy decay and L^2 stability bounds in two and three space dimensions are rigorously proved both for continuous and discrete formulations with constant damping coefficients. Numerical results validate the theory.

6.2.7. *A high-order spectral element fast Fourier transform for the poisson equation*

Participants: Federica Caforio, Sébastien Imperiale [correspondant].

The aim of this work [17] is to propose a novel, fast solver for the Poisson problem discretised with High-Order Spectral Element Methods (HO-SEM) in canonical geometries (rectangle in 2D, rectangular parallelepiped in 3D). This method is based on the use of the Discrete Fourier Transform to reduce the problem to the inversion of the symbol of the operator in the frequency space. The proposed solver is endowed with several properties. First, it preserves the efficiency of the standard FFT algorithm; then, the matrix storage is drastically reduced (in particular, it is independent of the space dimension); a pseudo-explicit Singular Value Decomposition (SVD) is used for the inversion of the symbols; finally, it can be extended to non-periodic boundary conditions. Furthermore, due to the underlying HO-SEM discretisation, the multi-dimensional symbol of the operator can be efficiently computed from the one-dimensional symbol by tensorisation.

6.2.8. *Thermodynamic properties of muscle contraction models and associated discrete-time principles*

Participants: François Kimmig, Dominique Chapelle [correspondant], Philippe Moireau.

Considering a large class of muscle contraction models accounting for actin-myosin interaction, we present a mathematical setting in which solution properties can be established, including fundamental thermodynamic balances. Moreover, we propose a complete discretization strategy for which we are also able to obtain discrete versions of the thermodynamic balances and other properties. Our major objective is to show how the thermodynamics of such models can be tracked after discretization, including when they are coupled to a macroscopic muscle formulation in the realm of continuum mechanics. Our approach allows to carefully identify the sources of energy and entropy in the system, and to follow them up to the numerical applications. See [30] for more detail.

6.2.9. Mechanical and imaging models-based image registration

Participants: Radomir Chabiniok, Martin Genet [correspondant].

Image registration plays an increasingly important role in many fields such as biomedical or mechanical engineering. Generally speaking, it consists in deforming a (moving) source image to match a (fixed) template image. Many approaches have been proposed over the years; if new model-free machine learning-based approaches are now beginning to provide robust and accurate results, extracting motion from images is still most commonly based on combining some statistical analysis of the images intensity and some model of the underlying deformation as initial guess or regularizer. These approaches may be efficient even for complex type of motion; however, any artifact in the source image (e.g., partial voluming, local decrease of signal-to-noise ratio or even local signal void), drastically deteriorates the registration. This work introduces a novel approach of extracting motion from biomedical image series, based on a model of the imaging modality. It is, to a large extent, independent of the type of model and image data – the pre-requisite is to incorporate biomechanical constraints into the motion of the object (organ) of interest and being able to generate data corresponding to the real image, i.e., having an imaging model at hand. We will illustrate the method with examples of synthetically generated 2D tagged magnetic resonance images. This work was presented at the VipIMAGE 2019 conference. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD. See [44] for more detail. This work was done in collaboration with Katerina Skardova (Czech Technical University in Prague) and Matthias Rambausek (École Polytechnique).

6.2.10. Validation of finite element image registration-based cardiac strain estimation from magnetic resonance images

Participants: Martin Genet [correspondant], Philippe Moireau.

Accurate assessment of regional and global function of the heart is an important readout for the diagnosis and routine evaluation of cardiac patients. Indeed, recent clinical and experimental studies suggest that compared to global metrics, regional measures of function could allow for more accurate diagnosis and early intervention for many cardiac diseases. Although global strain measures derived from tagged magnetic resonance (MR) imaging have been shown to be reproducible for the majority of image registration techniques, the measurement of regional heterogeneity of strain is less robust. Moreover, radial strain is underestimated with the current techniques even globally. Finite element (FE)-based techniques offer a mechanistic approach for the regularization of the ill-posed registration problem. This work presents the validation of a recently proposed FE-based image registration method with mechanical regularization named equilibrated warping. For this purpose, synthetic 3D-tagged MR images are generated from a reference biomechanical model of the left ventricle (LV). The performance of the registration algorithm is consequently tested on the images with different signal-to-noise ratios (SNRs), revealing the robustness of the method. See [35] for more detail.

6.3. Inverse Problems

6.3.1. Analysis of an observer strategy for initial state reconstruction of wave-like systems in unbounded domains

Participants: Sébastien Imperiale, Philippe Moireau [correspondant].

In [29] we are interested in reconstructing the initial condition of a wave equation in an unbounded domain configuration from measurements available in time on a subdomain. To solve this problem, we adopt an iterative strategy of reconstruction based on observers and time reversal adjoint formulations. We prove the convergence of our reconstruction algorithm with perfect measurements and its robustness to noise. Moreover, we develop a complete strategy to practically solve this problem on a bounded domain using artificial transparent boundary conditions to account for the exterior domain. Our work then demonstrates that the consistency error introduced by the use of approximate transparent boundary conditions is compensated by the stabilisation properties obtained from the use of the available measurements, hence allowing to still be able to reconstruct the unknown initial condition.

6.3.2. Analysis and numerical simulation of an inverse problem for a structured cell population dynamics model

Participants: Frédérique Clément, Frédérique Robin [correspondant].

We have studied (with Béatrice Laroche, INRA) a multiscale inverse problem associated with a multi-type model for age structured cell populations [20] (see also [21] for another application). In the single type case, the model is a McKendrick-VonFoerster like equation with a mitosis-dependent death rate and potential migration at birth. In the multi-type case, the migration term results in a unidirectional motion from one type to the next, so that the boundary condition at age 0 contains an additional extrinsic contribution from the previous type. We consider the inverse problem of retrieving microscopic information (the division rates and migration proportions) from the knowledge of macroscopic information (total number of cells per layer), given the initial condition. We have first shown the well-posedness of the inverse problem in the single type case using a Fredholm integral equation derived from the characteristic curves, and we have used a constructive approach to obtain the lattice division rate, considering either a synchronized or non-synchronized initial condition. We have taken advantage of the unidirectional motion to decompose the whole model into nested submodels corresponding to self-renewal equations with an additional extrinsic contribution. We have again derived a Fredholm integral equation for each submodel and deduced the well-posedness of the multi-type inverse problem. In each situation, we illustrate numerically our theoretical results.

6.3.3. Inverse problem based on data assimilation approaches for protein aggregation

Participants: Philippe Moireau [correspondant], Cécile Della Valle [MAMBA], Marie Doumic [MAMBA].

Estimating reaction rates and size distributions of protein polymers is an important step for understanding the mechanisms of protein misfolding and aggregation. In a depolarization configuration, we here extend some previous results obtained during the PhD Thesis of A. Armiento. Now, the depolarization rate is time-dependent or in the presence of an additional vanishing viscosity term. We continue to develop our framework mixing inverse problems methodologies and optimal control approaches typically encountered in data assimilation, allowing to justify mathematically the methods but also to adopt efficient numerical strategies. Publications of this work will be soon submitted.

6.3.4. Front shape similarity measure for data-driven simulations of wildland fire spread based on state estimation: Application to the RxCADRE field-scale experiment

Participants: Annabelle Collin [MONC], Philippe Moireau [correspondant].

Data-driven wildfire spread modeling is emerging as a cornerstone for forecasting real-time fire behavior using thermal-infrared imaging data. One key challenge in data assimilation lies in the design of an adequate measure to represent the discrepancies between observed and simulated firelines (or “fronts”). A first approach consists in adopting a Lagrangian description of the flame front and in computing a Euclidean distance between simulated and observed fronts by pairing each observed marker with its closest neighbor along the simulated front. However, this front marker registration approach is difficult to generalize to complex front topology that can occur when fire propagation conditions are highly heterogeneous due to topography, biomass fuel and micrometeorology. To overcome this issue, we investigate in this paper an object-oriented approach derived from the Chan–Vese contour fitting functional used in image processing. The burning area is treated as a moving object that can undergo shape deformations and topological changes. We combine this non-Euclidean measure with a state estimation approach (a Luenberger observer) to perform simulations of the time-evolving fire front location driven by discrete observations of the fireline. We apply this object-oriented data assimilation method to the three-hectare RxCADRE S5 field-scale experiment. This collaboration with CERFACS (M. Rochoux) and University of Maryland (C. Zhang and A. Trouvé) led to a publication [34] in the Proceedings of the Combustion Institute.

6.3.5. Model assessment through data assimilation of realistic data in cardiac electrophysiology

Participants: Antoine Gerard [CARMEN], Annabelle Collin [MONC], Gautier Bureau, Philippe Moireau [correspondant], Yves Coudière [CARMEN].

We consider a model-based estimation procedure – namely a data assimilation algorithm – of the atrial depolarization state of a sub- ject using data corresponding to electro-anatomical maps. Our objective is to evaluate the sensitivity of such a model-based reconstruction with respect to model choices. The followed data assimilation approach is capable of using electrical activation times to adapt a monodomain model simulation, thanks to an ingenious model-data fitting term inspired from image processing. The resulting simulation smoothes and completes the activation maps when they are spatially incomplete. Moreover, conductivity parameters can also be inferred. The model sensitivity assessment is performed based on synthetic data generated with a validated realistic atria model and then inverted using simpler modeling ingredients. In particular, the impact of the muscle fibers definition and corresponding anisotropic conductivity parameters is studied. Finally, an application of the method to real data is presented, showing promising results. This collaborative work has been published, see [37].

6.4. Experimental Assessments

6.4.1. Combination of traction assays and multiphoton imaging to quantify skin biomechanics

Participant: Jean-Marc Allain.

An important issue in tissue biomechanics is to decipher the relationship between the mechanical behavior at macroscopic scale and the organization of the collagen fiber network at microscopic scale. We have formalized a definitive protocol [46] to combine traction assays with multiphoton microscopy in ex vivo murine skin. This multiscale approach provides simultaneously the stress/stretch response of a skin biopsy and the collagen reorganization in the dermis by use of second harmonic generation (SHG) signals and appropriate image processing.

6.4.2. Monitoring dynamic collagen reorganization during skin stretching with fast polarization-resolved second harmonic generation imaging

Participant: Jean-Marc Allain.

The mechanical properties of biological tissues are strongly correlated to the specific distribution of their collagen fibers. Monitoring the dynamic reorganization of the collagen network during mechanical stretching is however a technical challenge, because it requires mapping orientation of collagen fibers in a thick and deforming sample. In this work [24], a fast polarization-resolved second harmonic generation microscope is implemented to map collagen orientation during mechanical assays. This system is based on line-to-line switching of polarization using an electro-optical modulator and works in epi-detection geometry. After proper calibration, it successfully highlights the collagen dynamic alignment along the traction direction in ex vivo murine skin dermis. This microstructure reorganization is quantified by the entropy of the collagen orientation distribution as a function of the stretch ratio. It exhibits a linear behavior, whose slope is measured with a good accuracy. This approach can be generalized to probe a variety of dynamic processes in thick tissues.

6.4.3. Multiscale characterisation of skin mechanics through in-situ imaging

Participant: Jean-Marc Allain.

The complex mechanical properties of skin have been studied intensively over the past decades. They are intrinsically linked to the structure of the skin at several length scales, from the macroscopic layers (epidermis, dermis and hypodermis) down to the microstructural organization at the molecular level. Understanding the link between this microscopic organization and the mechanical properties is of significant interest in the cosmetic and medical fields. Nevertheless, it only recently became possible to directly visualize the skin's microstructure during mechanical assays, carried out on the whole tissue or on isolated layers. These recent observations have provided novel information on the role of structural components of the skin in its mechanical properties, mainly the collagen fibers in the dermis, while the contribution of others, such as elastin fibers, remains elusive. We performed in [45] a systematic review of the current methods used to observe skin's microstructure during a mechanical assay, along with their strengths and limitations, as well as a review of the unique information they provide on the link between structure and function of the skin.

6.4.4. Root Hair Sizer: an algorithm for high throughput recovery of different root hair and root developmental parameters

Participant: Jean-Marc Allain.

The root is an important organ for water and nutrient uptake, and soil anchorage. It is equipped with root hairs (RHs) which are elongated structures increasing the exchange surface with the soil. RHs are also studied as a model for plant cellular development, as they represent a single cell with specific and highly regulated polarized elongation. For these reasons, it is useful to be able to accurately quantify RH length employing standardized procedures. Methods commonly employed rely on manual steps and are therefore time consuming and prone to errors, restricting analysis to a short segment of the root tip. Few partially automated methods have been reported to increase measurement efficiency. However, none of the reported methods allow an accurate and standardized definition of the position along the root for RH length measurement, making data comparison difficult. In this work [28] we are developing an image analysis algorithm that semi-automatically detects RHs and measures their length along the whole differentiation zone of roots. This method, implemented as a simple automated script in ImageJ/Fiji software that we termed Root Hair Sizer, slides a rectangular window along a binarized and straightened image of root tips to estimate the maximal RH length in a given measuring interval. This measure is not affected by heavily bent RHs and any bald spots. RH length data along the root are then modelled with a sigmoidal curve, generating several biologically significant parameters such as RH length, positioning of the root differentiation zone and, under certain conditions, RH growth rate. Image analysis with Root Hair Sizer and subsequent sigmoidal modelling of RH length data provide a simple and efficient way to characterize RH growth in different conditions, equally suitable to small and large scale phenotyping experiments.

6.4.5. Calcium and plasma membrane force-gated ion channels behind development

Participant: Jean-Marc Allain.

During development, tissues are submitted to high variation of compression and tension forces. The roles of the cell wall, the cytoskeleton, the turgor pressure and the cell geometry during this process have received due attention. In contrast, apart from its role in the establishment of turgor pressure, the involvement of the plasma membrane as a transducer of mechanical forces during development has been under studied. Force-gated (FG) or Mechanosensitive (MS) ion channels embedded in the bilayer represent 'per se' archetypal mechanosensor able to directly and instantaneously transduce membrane forces into electrical and calcium signals. We reviewed in [26] how their fine-tuning, combined with their ability to detect micro-curvature and local membrane tension, allows FG channels to transduce mechanical cues into developmental signals.

6.5. Clinical Applications

6.5.1. Cardiac displacement tracking with data assimilation combining a biomechanical model and an automatic contour detection

Participants: Radomir Chabiniok, Gautier Bureau, Dominique Chapelle, Philippe Moireau [correspondant].

Data assimilation in computational models represents an essential step in building patient-specific simulations. This work aims at circumventing one major bottleneck in the practical use of data assimilation strategies in cardiac applications, namely, the difficulty of formulating and effectively computing adequate data-fitting term for cardiac imaging such as cine MRI. We here provide a proof-of-concept study of data assimilation based on automatic contour detection. The tissue motion simulated by the data assimilation framework is then assessed with displacements extracted from tagged MRI in six subjects, and the results illustrate the performance of the proposed method, including for circumferential displacements, which are not well extracted from cine MRI alone. This work was presented at the Functional Imaging and Modeling of Heart Conference (FIMH2019, Bordeaux, France) and published in [36].

6.5.2. Minimally-invasive estimation of patient-specific end-systolic elastance using a biomechanical heart model

Participants: Arthur Le Gall, Fabrice Vallée, Dominique Chapelle, Radomir Chabiniok [correspondant].

The end-systolic elastance (E_{es}) – the slope of the end-systolic pressure-volume relationship (ESPVR) at the end of ejection phase – has become a reliable indicator of myocardial functional state. The estimation of E_{es} by the original multiple-beat method is invasive, which limits its routine usage. By contrast, non-invasive single-beat estimation methods, based on the assumption of the linearity of ESPVR and the uniqueness of the normalised time-varying elastance curve $E^N(t)$ across subjects and physiology states, have been applied in a number of clinical studies. It is however known that these two assumptions have a limited validity, as ESPVR can be approximated by a linear function only locally, and $E^N(t)$ obtained from a multi-subject experiment includes a confidence interval around the mean function. Using datasets of 3 patients undergoing general anaesthesia (each containing aortic flow and pressure measurements at baseline and after introducing a vasopressor noradrenaline), we first study the sensitivity of two single-beat methods — by Sensaki et al. and by Chen et al. — to the uncertainty of $E^N(t)$. Then, we propose a minimally-invasive method based on a patient-specific biophysical modelling to estimate the whole time-varying elastance curve $E^{model}(t)$. We compare E_{es}^{model} with the two single-beat estimation methods, and the normalised varying elastance curve $E^{N,model}(t)$ with $E^N(t)$ from published physiological experiments. This work was presented at the Functional Imaging and Modeling of Heart conference (FIMH2019, Bordeaux, France) and published in [38].

6.5.3. Model-based indices of early-stage cardiovascular failure and its therapeutic management in Fontan patients

Participant: Radomir Chabiniok.

Investigating the causes of failure of Fontan circulation in individual patients remains challenging despite detailed combined invasive cardiac catheterisation and magnetic resonance (XMR) exams at rest and during stress. In this work, we use a biomechanical model of the heart and Fontan circulation with the components of systemic and pulmonary beds to augment the diagnostic assessment of the patients undergoing the XMR stress exam. We apply our model in 3 Fontan patients and one biventricular “control" case. In all subjects, we obtained important biophysical factors of cardiovascular physiology – contractility, contractile reserve and changes in systemic and pulmonary vascular resistance – which contribute to explaining the mechanism of failure in individual patients. Finally, we used the patient-specific model of one Fontan patient to investigate the impact of changes in pulmonary vascular resistance, aiming at in silico testing of pulmonary vasodilation treatments. This work (in collaboration with Bram Ruijsink and Kuberan Pushparajah from St Thomas Hospital, King’s College London) was presented at the Functional Imaging and Modeling of Heart conference (FIMH2019, Bordeaux, France) and published in [40]. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.4. Dobutamine stress testing in patients with Fontan circulation augmented by biomechanical modeling

Participants: Philippe Moireau, Dominique Chapelle, Radomir Chabiniok [correspondant].

Understanding (patho)physiological phenomena and mechanisms of failure in patients with Fontan circulation — a surgically established circulation for patients born with a functionally single ventricle — remains challenging due to the complex hemodynamics and high inter-patient variations in anatomy and function. In this work, we present a biomechanical model of the heart and circulation to augment the diagnostic evaluation of Fontan patients with early-stage heart failure. The proposed framework employs a reduced-order model of heart coupled with a simplified circulation including venous return, creating a closed-loop system. We deploy this framework to augment the information from data obtained during combined cardiac catheterization and magnetic resonance exams (XMR), performed at rest and during dobutamine stress in 9 children with Fontan circulation and 2 biventricular controls. We demonstrate that our modeling framework enables patient-specific investigation of myocardial stiffness, contractility at rest, contractile reserve during stress and changes in vascular resistance. Hereby, the model allows to identify key factors underlying the pathophysiological response to stress in these patients. In addition, the rapid personalization of the model to patient data and fast simulation of cardiac cycles makes our framework directly applicable in a clinical workflow. We conclude that the proposed modeling framework is a valuable addition to the current clinical diagnostic XMR exam that helps to explain patient-specific stress hemodynamics and can identify potential mechanisms of failure in patients with Fontan circulation. This work has been submitted for publication in an international journal. This work (in collaboration with Bram Ruijsink and Kuberan Pushparajah from St Thomas Hospital, King's College London and Tarique Hussain, UT Southwestern Medical Center Dallas) also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.5. Signed-distance function based non-rigid registration of image sequences with varying image intensity

Participant: Radomir Chabiniok.

In this work we deal with non-rigid registration of the image series acquired by the Modified Look-Locker Inversion Recovery (MOLLI) magnetic resonance imaging sequence, which is used for a pixel-wise estimation of T_1 relaxation time. The spatial registration of the images within the series is necessary to compensate the patient's imperfect breath-holding. The evolution of intensities and a large variation of the image contrast within the MOLLI image series, together with the myocardium of left ventricle (the object of interest) typically not being the most distinct object in the scene, makes the registration challenging. We propose a method for locally adjusted optical flow-based registration of multimodal images, which uses the segmentation of the object of interest and its representation by the signed-distance function. We describe all the components of the proposed OF^{dist} method and their implementation. The OF^{dist} method is then compared to the performance of a standard mutual information maximization-based registration method, applied either to the original image (MIM) or to the signed-distance function (MIM^{dist}). Several experiments with synthetic and real MOLLI images are carried out. On synthetic image with a single object, MIM performed the best, while OF^{dist} and MIM^{dist} provided better results on synthetic images with more than one object and on real images. When applied to signed-distance function of two objects of interest, MIM^{dist} provided a larger registration error (but more homogeneously distributed) compared to OF^{dist}. For the real MOLLI image sequence with left ventricle pre-segmented using level-set method, the proposed OF^{dist} registration performed the best, as is demonstrated visually and by measuring the increase of mutual information in the object of interest and its neighborhood. This collaborative work (Katerina Skardova, Czech Technical University, Institute of Clinical and Experimental Medicine in Prague) has been submitted for publication in an international journal. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.6. Estimation of left ventricular pressure-volume loop using hemodynamic monitoring augmented by a patient-specific biomechanical model. An observational study

Participants: Arthur Le Gall, Fabrice Vallée, Dominique Chapelle, Radomir Chabiniok [correspondant].

Background During general anaesthesia, direct analysis of the arterial pressure or aortic flow waveforms may be confusing in complex haemodynamic situations. Patient-specific biomechanical modelling allows to simulate Pressure-Volume (PV) loops and obtain functional indicators of the cardiovascular (CV) system, such as ventricular-arterial coupling (Vva), cardiac efficiency (CE) or myocardial contractility. It therefore augments the information obtained by monitoring and could help in medical decision-making. **Methods** Patients undergoing GA for neuroradiological procedure were included in this prospective observational study. A biomechanical model of heart and vasculature specific to each patient was built using transthoracic echocardiography and aortic pressure and flow signals. If intraoperative hypotension (IOH) appeared, diluted noradrenaline (NOR) was administered and the model readjusted. **Results** The model was calibrated for 29 (64%) normotensive and for 16 (36%) hypotensive patients before and after NOR administration. The simulated mean aortic pressure (MAP) and stroke volume (SV) were equivalent to the measurements (Percentage Error: 6% for MAP and 18% for SV) in all 45 datasets at baseline. After NOR administration, the percentage of concordance with 10% exclusion zone between measurement and simulation was > 95% for both MAP and SV. The modelling results showed a decreased Vva (0.64±0.37 vs 0.88±0.43; p=0.039), and an increased CE (0.8±0.1 vs 0.73±0.11; p=0.042) in hypotensive as compared with normotensive patients. After NOR administration, Vva increased by 92±101%, CE decreased by 13±11% (p<0.001 for both) and contractility increased by 14±11% (p=0.002). **Conclusions** The numerical models built for individual patients were applied to estimate patients' PV loops and functional indicators of CV system during haemodynamic alterations and during restoration by NOR. This study demonstrates the feasibility of patient-specific cardiovascular modelling using clinical data readily available during GA and paves the way for model-augmented haemodynamic monitoring at operating theatres and intensive care units. This work is about to be submitted for publication in an international journal. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.7. Investigation of phase contrast magnetic resonance imaging underestimation of turbulent flow through the aortic valve phantom: Experimental and computational study by using lattice Boltzmann method

Participant: Radomir Chabiniok.

Work in collaboration with Radek Fucik, Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague.

Objective The accuracy of phase-contrast magnetic resonance imaging (PC-MRI) measurement is investigated using a computational fluid dynamics (CFD) model with the objective to determine the magnitude of the flow underestimation due to turbulence behind a narrowed valve in a phantom experiment. **Materials and Methods** An acrylic stationary flow phantom is used with three insertable plates mimicking aortic valvular stenoses of varying degrees. Positive and negative horizontal fluxes are measured at equidistant slices using standard PC-MRI sequences by 1.5T and 3T systems. The CFD model is based on the 3D lattice Boltzmann method (LBM). The experimental and simulated data are compared using the Bland-Altman-derived limits of agreement. Based on the LBM results, the turbulence is quantified and confronted with the level of flow underestimation. **Results** Matching results of PC-MRI flow were obtained for valves up to moderate stenosis on both field strengths. The flow magnitude through a severely stenotic valve was underestimated due to signal void in the regions of turbulent flow behind the valve, consistently with the level of quantified turbulence intensity. **Discussion** Flow measured by PC-MRI is affected by noise and turbulence. LBM can simulate turbulent flow efficiently and accurately, it has therefore the potential to improve clinical interpretation of PC-MRI. This collaborative work (Czech Technical University, Institute of Clinical and Experimental Medicine in Prague and Inria) has been submitted for publication in an international journal. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.8. Left ventricular torsion obtained using equilibrated warping in patients with repaired Tetralogy of Fallot

Participants: Martin Genet, Radomir Chabiniok [correspondant].

Work in collaboration with Katerina Skardova, Department of Mathematics, Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague and Tarique Hussain UT Southwestern Medical Center Dallas.

Background Patients after surgical repair of Tetralogy of Fallot (rTOF) have right ventricular (RV) dysfunction and may subsequently suffer a decrease in left ventricular (LV) function. Previous studies evaluating the assessment of LV torsion have shown poor reproducibility using cardiovascular magnetic resonance imaging (CMR). The aim of our study is to evaluate a novel finite element method of image registration to assess LV torsion in patients with rTOF and explore the relationship between LV torsion and cardiac parameters routinely obtained with CMR. **Methods** The assessment of torsion is based on the finite element method for image registration, and the equilibrium gap principle for problem regularization, known as equilibrated warping developed by M. Genet (Inria Saclay). It has been shown to be able to predict global torsion in regular cine images as well in 3D tagged images, despite low contrast. Seventy-six cases of rTOF and ten controls were included. The group of control patients were assessed for reproducibility using equilibrated warping and standard tissue tracking software (cvi42, version 5.10.1, Calgary, Canada). RV end-systolic volume (RVESV), RV end-diastolic volume (RVEDV), RV ejection fraction (RVEF), LVESV, LVEDV, LVEF, LV peak systolic torsion and peak systolic torsion gradient (normalized by mesh length) were obtained for each patient with rTOF. Patients were dichotomized into two groups: those with normal torsion (systolic basal clockwise rotation and apical counterclockwise rotation, representative example is shown in Image 1) and those with loss of torsion, defined as a reversal of normal systolic basal clockwise rotation (representative example is shown in Image 2). **Results** Torsion by equilibrated warping was successfully obtained in 68 of 76 (89%) patients with rTOF and 9 of 10 (90%) normal controls. For equilibrated warping, the intra- and inter-observer coefficients of variation were 0.095 and 0.117, respectively; compared to 0.668 and 0.418 for tissue tracking by standard clinical software. The intra- and inter-observer intraclass correlation coefficients for equilibrated warping were 0.862 and 0.831, respectively; compared to 0.250 and 0.621 for tissue tracking. Loss of torsion was noted in 32 of the 68 (47%) patients with rTOF and there was a significant difference in peak systolic torsion gradient between patients with normal torsion and loss of torsion. There was no difference in LV or RV volumes or function between these groups. **Conclusion** The equilibrated warping method of image registration to assess LV torsion is feasible in patients with rTOF and shows good reliability. Loss of torsion is common in patients with rTOF. In our study, there was no significant association between loss of torsion and other ventricular parameters indicative of a worsening cardiac condition. Future studies committed to the long- term follow-up of this population are needed to assess the role of torsion in predicting ventricular dysfunction and death. This work was accepted for presentation at SCMR conference 2020 (Society for Cardiovascular Magnetic Resonance). It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.9. Volume administration protocol to assess ventricular mechanics during interventional cardiac magnetic resonance procedures

Participant: Radomir Chabiniok.

Work in collaboration with Joshua Greer and Tarique Hussain UT Southwestern Medical Center Dallas.

Background Failure in Fontan circulation occurs with supposed normal ventricular systolic and diastolic function, including normal ventricular end-diastolic pressures and ventricular ejection fraction. This highlights the difficulty in assessing systolic and diastolic ventricular function in patients with single ventricle physiology. Interventional cardiac magnetic resonance (CMR) provides an opportunity for simultaneous acquisition of pressure and volume measurements that may lend itself well to analysis of ventricular mechanics in this population. We aim to develop a protocol of volume administration to assess ventricular pressure and volume during the cardiac cycle to construct pressure-volume loops under different loading conditions and perform their biomechanical interpretation. **Methods** This is a single center prospective study conducted on single ventricle patients with Glenn or Fontan circulation referred for interventional CMR procedures. With a catheter advanced into the ventricle, a pressure tracing and a cine sequence accelerated by kt-BLAST is obtained. Two 2.5 mL/kg fluid boluses are then rapidly administered into the catheter sheath with repeated acquisition of the pressure tracing and cine imaging immediately following each. Cine images are post-processed after the procedure to obtain ventricular volumes. The data are combined to construct pressure-volume loops and plot the end-diastolic pressure-volume relationship (EDPVR). **Results** The protocol has been performed in six patients. Ventricular end-diastolic pressure readings increased by a median of 2.5 mmHg (range of 1-3 mmHg) after the first volume administration and a median of 1.5 mmHg (range of 1-8 mmHg) after the second volume administration. Ventricular end-diastolic volumes increased by a median of 4.1 mL (range of 1.7-19.3 mL) after the first volume administration and a median of 1.5 mL (range of 0.4-24.2 mL) after the second volume administration. The data obtained during simultaneous volume and pressure measurements allowed for the construction of ventricular pressure-volume loops. Ventricular stroke work increased by a median of 0.0825 Joules (range of 0.010-0.167 Joules) after the first volume administration then decreased by a median of -0.062 Joules (range of -0.083 to 0.005 Joules) after the second volume administration. EDPVR curves were derived from the pressure-volume loops and differentiated patients with similar starting end-diastolic pressures. **Conclusions** We present a novel method for the acquisition of data to construct pressure-volume loops. Our protocol focuses on rapid volume administration and fast data acquisition with the goal of increasing preload but recording data prior to compensatory changes in afterload. In each patient, administration of 2.5 mL/kg fluid boluses achieved measurable increases in ventricular end-diastolic pressure and ventricular end-diastolic volume. The construction of pressure-volume loops with varying loading may facilitate in-depth assessment of ventricular mechanics in patients with single ventricle heart disease. The variation of preload may allow for the assessment of EDPVR, therefore ventricular stiffness, and to some extent also the contractile response in such a physiology-modifying situation. This work was submitted to the CHOP 2020 conference. It also represents a part of the objectives supported by the Inria-UTSW Associated Team TOFMOD.

6.5.10. Computational quantification of patient specific changes in ventricular dynamics associated with pulmonary hypertension

Participant: Martin Genet.

Pulmonary arterial hypertension (PAH) causes an increase in the mechanical loading imposed on the right ventricle (RV) that results in progressive changes to its mechanics and function. Here, we quantify the mechanical changes associated with PAH by assimilating clinical data consisting of reconstructed three-dimensional geometry, pressure, and volume waveforms, as well as regional strains measured in patients with PAH ($n = 12$) and controls ($n = 6$) within a computational modeling framework of the ventricles. Modeling parameters reflecting regional passive stiffness and load-independent contractility as indexed by the tissue active tension were optimized so that simulation results matched the measurements. The optimized parameters were compared with clinical metrics to find usable indicators associated with the underlying mechanical changes. Peak contractility of the RV free wall (RVFW) $\gamma_{RVFW,max}$ was found to be strongly correlated and had an inverse relationship with the RV and left ventricle (LV) end-diastolic volume ratio (i.e., RVEDV/LVEDV) (RVEDV/LVEDV)+0.44, $R^2 = 0.77$). Correlation with RV ejection fraction ($R^2 = 0.50$) and end-diastolic volume index ($R^2 = 0.40$) were comparatively weaker. Patients with $RVEDV/LVEDV > 1.5$ had 25% lower $\gamma_{RVFW,max}$ ($P < 0.05$) than that of the control. On average, RVFW passive stiffness progressively increased with the degree of remodeling as indexed by RVEDV/LVEDV. These results suggest a mechanical basis of using RVEDV/LVEDV as a clinical index for delineating disease severity and estimating RVFW contractility in patients with PAH. See [25] for more detail.

6.5.11. Validation of equilibrated warping-image registration with mechanical regularization-on 3D ultrasound images

Participant: Martin Genet.

Image registration plays a very important role in quantifying cardiac motion from medical images, which has significant implications in the diagnosis of cardiac diseases and the development of personalized cardiac computational models. Many approaches have been proposed to solve the image registration problem; however, due to the intrinsic ill-posedness of the image registration problem, all these registration techniques, regardless of their variabilities, require some sort of regularization. An efficient regularization approach was recently proposed based on the equilibrium gap principle, named equilibrated warping. Compared to previous work, it has been formulated at the continuous level within the finite strain hyperelasticity framework and solved using the finite element method. Regularizing the image registration problem using this principle is advantageous as it produces a realistic solution that is close to that of an hyperelastic body in equilibrium with arbitrary boundary tractions, but no body load.The equilibrated warping method has already been extensively validated on both tagged and untagged magnetic resonance images. In this paper, we provide full validation of the method on 3D ultrasound images, based on the 2011 MICCAI Motion Tracking Challenge data. See [39] for more detail.

MEXICO Project-Team

7. New Results

7.1. Generalized Alignment-Based Trace Clustering of Process Behavior

Process mining techniques use event logs containing real process executions in order to mine, align and extend process models. The partition of an event log into trace variants facilitates the understanding and analysis of traces, so it is a common pre-processing in process mining environments. Trace clustering automates this partition; traditionally it has been applied without taking into consideration the availability of a process model. In this paper we extend our previous work on process model based trace clustering, by allowing cluster centroids to have a complex structure, that can range from a partial order, down to a subnet of the initial process model. This way, the new clustering framework presented in [28] is able to cluster together traces that are distant only due to concurrency or loop constructs in process models. We show the complexity analysis of the different instantiations of the trace clustering framework, and have implemented it in a prototype tool that has been tested on different datasets.

7.2. The involution tool for accurate digital timing and power analysis

In [23] we introduce the prototype of a digital timing simulation and power analysis tool for integrated circuit (Involution Tool) which employs the involution delay model introduced by Fuegger et al. at DATE'15. Unlike the pure and inertial delay models typically used in digital timing analysis tools, the involution model faithfully captures pulse propagation. The presented tool is able to quantify for the first time the accuracy of the latter by facilitating comparisons of its timing and power predictions with both SPICE-generated results and results achieved by standard timing analysis tools. It is easily customizable, both w.r.t. different instances of the involution model and different circuits, and supports automatic test case generation, including parameter sweeping. We demonstrate its capabilities by providing timing and power analysis results for three circuits in varying technologies: an inverter tree, the clock tree of an open-source processor, and a combinational circuit that involves multi-input NAND gates. It turns out that the timing and power predictions of two natural types of involution models are significantly better than the predictions obtained by standard digital simulations for the inverter tree and the clock tree. For the NAND circuit, the performance is comparable but not significantly better. Our simulations thus confirm the benefits of the involution model, but also demonstrate shortcomings for multi-input gates.

7.3. Transistor-level analysis of dynamic delay models

Delay estimation is a crucial task in digital circuit design as it provides the possibility to assure the desired func-tionality, but also prevents undesired behavior very early. For this purpose elaborate delay models like the Degradation Delay Model (DDM) and the Involution Delay Model (IDM) have been proposed in the past, which facilitate accurate dynamic timing analysis: Both use delay functions that determine the delay of the current input transition based on the time difference T to the previous output one. Currently, however, extensive analog simulations are necessary to determine the (parameters of the) delay function, which is a very time-consuming and cumbersome task and thus limits the applicability of these models. In [21], we therefore thoroughly investigate the characterization procedures of a CMOS inverter on the transistor level in order to derive analytical expressions for the delay functions. Based on reasonably simple transistor models we identify three operation regions, each described by a different estimation function. Using simulations with two independent technologies, we show that our predictions are not only accurate but also reasonably robust w.r.t. variations. Our results furthermore indicate that the exponential fitting proposed for DDM is actually only partially valid, while our analytic approach can be applied on the whole range. Even the more complex IDM is predicted reasonably accurate.

7.4. A faithful binary circuit model

[Fuegger et al., IEEE TC 2016] proved that no existing digital circuit model, including those based on pure and inertial delay channels, faithfully captures glitch propagation: For the Short-Pulse Filtration (SPF) problem similar to that of building a one-shot inertial delay, they showed that every member of the broad class of bounded single-history channels either contradicts the unsolvability of SPF in bounded time or the solvability of SPF in unbounded time in physical circuits. In [12], we propose binary circuit models based on novel involution channels that do not suffer from this deficiency. Namely, in sharp contrast to bounded single-history channels, SPF cannot be solved in bounded time with involution channels, whereas it is easy to provide an unbounded SPF implementation. Hence, binary-valued circuit models based on involution channels allow to solve SPF precisely when this is possible in physical circuits. Additionally, using both Spice simulations and physical measurements of an inverter chain instrumented by high-speed analog amplifiers, we demonstrate that our model provides good modeling accuracy with respect to real circuits as well. Consequently , our involution channel model is not only a promising basis for sound formal verification, but also allows to seamlessly improve existing dynamic timing analysis.

7.5. Concurrency in Boolean networks

Boolean networks (BNs) are widely used to model the qualitative dynamics of biological systems. Besides the logical rules determining the evolution of each component with respect to the state of its regulators, the scheduling of component updates can have a dramatic impact on the predicted behaviours. In [10], we explore the use of Read (contextual) Petri Nets (RPNs) to study dynamics of BNs from a concurrency theory perspective. After showing bi-directional translations between RPNs and BNs and analogies between results on synchronism sensitivity, we illustrate that usual updating modes for BNs can miss plausible behaviours, i.e., incorrectly conclude on the absence/impossibility of reaching specific configurations. We propose an encoding of BNs capitalizing on the RPN semantics enabling more behaviour than the generalized asynchronous updating mode. The proposed encoding ensures a correct abstraction of any multivalued refinement, as one may expect to achieve when modelling biological systems with no assumption on its time features.

7.6. Sequential Reprogramming of Boolean Networks Made Practical

We address the sequential reprogramming of gene regulatory networks modelled as Boolean networks.

- Cellular reprogramming, a technique that opens huge opportunities in modern and regenerative medicine, heavily relies on identifying key genes to perturb. Most of the existing computational methods for controlling which attractor (steady state) the cell will reach focus on finding mutations to apply to the initial state. However, it has been shown, and is proved in our article [14], that waiting between perturbations so that the update dynamics of the system prepares the ground, allows for new reprogramming strategies. To identify such sequential perturbations, we consider a qualitative model of regulatory networks, and rely on Binary Decision Diagrams to model their dynamics and the putative perturbations. Our method establishes a set identification of sequential perturbations, whether permanent (mutations) or only temporary, to achieve the existential or inevitable reachability of an arbitrary state of the system. We apply an implementation for temporary perturbations on models from the literature, illustrating that we are able to derive sequential perturbations to achieve trans-differentiation.
- In [22], we develop an attractor-based sequential reprogramming method to compute all sequential reprogramming paths from a source attractor to a target attractor, where only attractors of the network are used as intermediates. Our method is more practical than existing reprogramming methods as it incorporates several practical constraints: (1) only biologically observable states, viz. attractors, can act as intermediates; (2) certain attractors, such as apoptosis, can be avoided as intermediates; (3) certain nodes can be avoided to perturb as they may be essential for cell survival or difficult to perturb with biomolecular techniques; and (4) given a threshold k, all sequential reprogramming paths with no more than k perturbations are computed. We compare our method with the minimal one-step

reprogramming and the minimal sequential reprogramming on a variety of biological networks. The results show that our method can greatly reduce the number of perturbations compared to the one-step reprogramming, while having comparable results with the minimal sequential reprogramming. Moreover, our implementation is scalable for networks of more than 60 nodes.

7.7. Parameter Space Abstraction and Unfolding Semantics of Discrete Regulatory Networks.

The modelling of discrete regulatory networks combines a graph specifying the pairwise influences between the variables of the system, and a parametrisation from which can be derived a discrete transition system. Given the influence graph only, the exploration of admissible parametrisations and the behaviours they enable is computationally demanding due to the combinatorial explosions of both parametrisation and reachable state space. In [13], we introduce an abstraction of the parametrisation space and its refinement to account for the existence of given transitions, and for constraints on the sign and observability of influences. The abstraction uses a convex sub-lattice containing the concrete parametrisation space specified by its infimum and supremum parametrisations. It is shown that the computed abstractions are optimal, i.e., no smaller convex sublattice exists. Although the abstraction may introduce over-approximation, it has been proven to be conservative with respect to reachability of states. Then, an unfolding semantics for Parametric Regulatory Networks is defined, taking advantage of concurrency between transitions to provide a compact representation of reachable transitions. A prototype implementation is provided: it has been applied to several examples of Boolean and multi-valued networks, showing its tractability for networks with numerous components.

7.8. Combining Refinement of Parametric Models with Goal-Oriented Reduction of Dynamics

Parametric models abstract part of the specification of dynamical models by integral parameters. They are for example used in computational systems biology, notably with parametric regulatory networks, which specify the global architecture (interactions) of the networks, while parameterising the precise rules for drawing the possible temporal evolutions of the states of the components. A key challenge is then to identify the discrete parameters corresponding to concrete models with desired dynamical properties. Our work [20] addresses the restriction of the abstract execution of parametric regulatory (discrete) networks by the means of static analysis of reachability properties (goal states). Initially defined at the level of concrete parameterised models, the goal-oriented reduction of dynamics is lifted to parametric networks, and is proven to preserve all the minimal traces to the specified goal states. It results that one can jointly perform the refinement of parametric networks (restriction of domain of parameters) while reducing the necessary transitions to explore and preserving reachability properties of interest.

7.9. Autonomous Transitions Enhance CSLTA Expressiveness and Conciseness

CSLTA is a stochastic temporal logic for continuous-time Markov chains (CTMC) where formulas similarly to those of CTL* are inductively defined by nesting of timed path formulas and state formulas. In particular a timed path formula of CSLTA is specified by a single-clock Deterministic Timed Automaton (DTA). Such a DTA features two kinds of transitions: synchronizing transitions triggered by CTMC transitions and autonomous transitions triggered by time elapsing that change the location of the DTA when the clock reaches a given threshold. It has already been shown that CSLTA strictly includes stochastic logics like CSL and asCSL. An interesting variant of CSLTA consists in equipping transitions rather than locations by boolean formulas. In [27], we answer the following question: do autonomous transitions and/or boolean guards on transitions enhance expressiveness and/or conciseness of DTAs? We show that this is indeed the case. In establishing our main results we also identify an accurate syntactical characterization of DTAs for which the autonomous transitions do not add expressive power but lead to exponentially more concise DTAs.

7.10. Coverability and Termination in Recursive Petri Nets

In the early two-thousands, Recursive Petri nets have been introduced in order to model distributed planning of multi-agent systems for which counters and recursivity were necessary. Although Recursive Petri nets strictly extend Petri nets and stack automata, most of the usual property problems are solvable but using non primitive recursive algorithms, even for coverability and termination. For almost all other extended Petri nets models containing a stack the complexity of coverability and termination are unknown or strictly larger than EXPSPACE. In contrast, we establish in [18] that for Recursive Petri nets, the coverability and termination problems are EXPSPACE-complete as for Petri nets. From an expressiveness point of view, we show that coverability languages of Recursive Petri nets strictly include the union of coverability languages of Petri nets and context-free languages. Thus we get for free a more powerful model than Petri net.

OPIS Project-Team

7. New Results

7.1. General risk measures for robust machine learning

Participants: Emilie Chouzenoux, Jean-Christophe Pesquet (Collaboration: Henri Gérard, ENPC, Paris)
A wide array of machine learning problems are formulated as the minimization of the expectation of a convex loss function on some parameter space. Since the probability distribution of the data of interest is usually unknown, it is is often estimated from training sets, which may lead to poor out-of-sample performance. In the work [11], we bring new insights in this problem by using the framework which has been developed in quantitative finance for risk measures. We show that the original min-max problem can be recast as a convex minimization problem under suitable assumptions. We discuss several important examples of robust formulations, in particular by defining ambiguity sets based on φ-divergences and the Wasserstein metric. We also propose an efficient algorithm for solving the corresponding convex optimization problems involving complex convex constraints. Through simulation examples, we demonstrate that this algorithm scales well on real data sets.

7.2. Deep Latent Factor Model for Collaborative Filtering

Participants: Emilie Chouzenoux (Collaboration: Aanchal Mongia, Neha Jhamb, Angshul Majumdar, IIIT Delhi, India)
Latent factor models have been used widely in collaborative filtering based recommender systems. In recent years, deep learning has been successful in solving a wide variety of machine learning problems. Motivated by the success of deep learning, we propose in [44], [23] a deeper version of latent factor model. Experiments on benchmark datasets shows that our proposed technique significantly outperforms all stateof-the-art collaborative filtering techniques.

7.3. A Proximal Interior Point Algorithm with Applications to Image Processing

Participants: Emilie Chouzenoux, Marie-Caroline Corbineau, Jean-Christophe Pesquet
In the work [10], we introduce a new proximal interior point algorithm (PIPA). This algorithm is able to handle convex optimization problems involving various constraints where the objective function is the sum of a Lipschitz differentiable term and a possibly nonsmooth one. Each iteration of PIPA involves the minimization of a merit function evaluated for decaying values of a logarithmic barrier parameter. This inner minimization is performed thanks to a finite number of subiterations of a variable metric forward-backward method employing a line search strategy. The convergence of this latter step as well as the convergence the global method itself are analyzed. The numerical efficiency of the proposed approach is demonstrated in two image processing applications.

7.4. Deep Unfolding of a Proximal Interior Point Method for Image Restoration

Participants: Emilie Chouzenoux, Marie-Caroline Corbineau, Jean-Christophe Pesquet (Collaboration: Carla Bertocchi, Marco Prato, Universita di Modena, Italy)

Variational methods are widely applied to ill-posed inverse problems for they have the ability to embed prior knowledge about the solution. However, the level of performance of these methods significantly depends on a set of parameters, which can be estimated through computationally expensive and time consuming methods. In contrast, deep learning offers very generic and efficient architectures, at the expense of explainability, since it is often used as a black-box, without any fine control over its output. Deep unfolding provides a convenient approach to combine variational-based and deep learning approaches. Starting from a variational formulation for image restoration, we developped in [36], [5], iRestNet, a neural network architecture obtained by unfolding a proximal interior point algorithm. Hard constraints, encoding desirable properties for the restored image, are incorporated into the network thanks to a logarithmic barrier, while the barrier parameter, the stepsize, and the penalization weight are learned by the network. We derive explicit expressions for the gradient of the proximity operator for various choices of constraints, which allows training iRestNet with gradient descent and backpropagation. In addition, we provide theoretical results regarding the stability of the network for a common inverse problem example. Numerical experiments on image deblurring problems show that the proposed approach compares favorably with both state-of-the-art variational and machine learning methods in terms of image quality.

7.5. Preconditioned P-ULA for Joint Deconvolution-Segmentation of Ultrasound Images

Participants: Emilie Chouzenoux, Marie-Caroline Corbineau, Jean-Christophe Pesquet (Collaboration: Denis Kouamé, Jean-Yves Tourneret, IRIT, Toulouse)
Joint deconvolution and segmentation of ultrasound images is a challenging problem in medical imaging. By adopting a hierarchical Bayesian model, we propose in [15] an accelerated Markov chain Monte Carlo scheme where the tissue reflectivity function is sampled thanks to a recently introduced proximal unadjusted Langevin algorithm. This new approach is combined with a forward-backward step and a preconditioning strategy to accelerate the convergence, and with a method based on the majorization-minimization principle to solve the inner nonconvex minimization problems. As demonstrated in numerical experiments conducted on both simulated and in vivo ultrasound images, the proposed method provides high-quality restoration and segmentation results and is up to six times faster than an existing Hamiltonian Monte Carlo method.

7.6. A Random Block-Coordinate Douglas-Rachford Splitting Method with Low Computational Complexity for Binary Logistic Regression

Participants: Emilie Chouzenoux, Jean-Christophe Pesquet (Collaboration: Giovanni Chierchia, ESIEE Paris, Luis Bricenos Arias, Universidad Técnica Federico Santa Maria, Valparaiso, Chile)
In the paper [6], we proposed a new optimization algorithm for sparse logistic regression based on a stochastic version of the Douglas-Rachford splitting method. Our algorithm sweeps the training set by randomly selecting a mini-batch of data at each iteration, and it allows us to update the variables in a block coordinate manner. Our approach leverages the proximity operator of the logistic loss, which is expressed with the generalized Lambert W function. Experiments carried out on standard datasets demonstrate the efficiency of our approach w.r.t. stochastic gradient-like methods.

7.7. A probabilistic incremental proximal gradient method

Participant: Emilie Chouzenoux (Collaboration: Omer Deniz Akyildiz, Alan Turing Institute, London, UK, Victor Elvira, University of Edinburgh, Joaquin Miguez, Universidad Carlos III de Madrid, Spain)
In the paper [3], we proposed a probabilistic optimization method, named probabilistic incremental proximal gradient (PIPG) method, by developing a probabilistic interpretation of the incremental proximal gradient algorithm. We explicitly model the update rules of the incremental proximal gradient method and develop a systematic approach to propagate the uncertainty of the solution estimate over iterations. The PIPG algorithm takes the form of Bayesian filtering updates for a state-space model constructed by using the cost function. Our framework makes it possible to utilize well-known exact or approximate Bayesian filters, such as Kalman or extended Kalman filters, to solve large scale regularized optimization problems.

7.8. Optimal Multivariate Gaussian Fitting with Applications to PSF Modeling in Two-Photon Microscopy Imaging

Participants: Emilie Chouzenoux, Jean-Christophe Pesquet (Collaboration: Claire Lefort, XLIM, Limoges, Tim Tsz-Kit Lau, Northwestern University, USA)

Fitting Gaussian functions to empirical data is a crucial task in a variety of scientific applications, especially in image processing. However, most of the existing approaches for performing such fitting are restricted to two dimensions and they cannot be easily extended to higher dimensions. Moreover, they are usually based on alternating minimization schemes which benefit from few theoretical guarantees in the underlying nonconvex setting. In the paper [12], we provided a novel variational formulation of the multivariate Gaussian fitting problem, which is applicable to any dimension and accounts for possible non-zero background and noise in the input data. The block multiconvexity of our objective function leads us to propose a proximal alternating method to minimize it in order to estimate the Gaussian shape parameters. The resulting FIGARO algorithm is shown to converge to a critical point under mild assumptions. The algorithm shows a good robustness when tested on synthetic datasets. To demonstrate the versatility of FIGARO, we also illustrate its excellent performance in the fitting of the Point Spread Functions of experimental raw data from a two-photon fluorescence microscope.

7.9. Calibration-less parallel imaging compressed sensing reconstruction based on OSCAR regularization

Participants: Emilie Chouzenoux, Loubna El Gueddari (Collaboration: Philippe Ciuciu, Alexandre Vignaut, Inria Saclay, Parietal)

Over the last decade, the combination of parallel imaging (PI) and compressed sensing (CS) in magnetic resonance imaging (MRI) has allowed to speed up acquisition while maintaining a good signal-to-noise ratio (SNR) for millimetric resolution. Self-calibrating techniques such as L1-ESPiRIT have emerged as a standard approach to estimate the coil sensitivity maps that are required at the reconstruction stage. Although straightforward in Cartesian acquisitions, these approaches become more computationally demanding in non-Cartesian scenarios especially for high resolution imaging (e.g. 500 μm in plane). Instead, calibration-less techniques no longer require this prior knowledge to perform multi-channel image reconstruction from undersampled k-space data. In this work, we introduce a new calibration-less PI-CS reconstruction method that is particularly suited to non-Cartesian data. It leverages structure sparsity of the multi-channel images in a wavelet transform domain while adapting to SNR inhomogeneities across receivers thanks to the OSCAR-norm regularization. Comparison and validation on 8 to 20-fold prospectively accelerated high-resolution ex-vivo human brain MRI data collected at 7 Tesla shows that the subbandwise OSCAR-norm regularization achieves the best trade-off between image quality and computational cost at the reconstructions stage compared to other tested versions (global, scalewise and pixelwise). This approach provides slight to moderate improvement over its state-of-the-art competitors (self-calibrating ‘1-ESPIRiT method and calibration-less AC-LORAKS and CaLM methods) in terms of closeness to the Cartesian reference magnitude image. Importantly, it also preserves much better phase information compared to other approaches [37], [57], [62].

7.10. Proximal approaches for matrix optimization problems: Application to robust precision matrix estimation

Participants: Emilie Chouzenoux, Jean-Christophe Pesquet (Collaboration: Alessandro Benfenati, Universita di Milano)

In recent years, there has been a growing interest in mathematical models leading to the minimization, in a symmetric matrix space, of a Bregman divergence coupled with a regularization term. We address problems of this type within a general framework where the regularization term is split into two parts, one being a spectral function while the other is arbitrary. A Douglas–Rachford approach is proposed to address such problems, and a list of proximity operators is provided allowing us to consider various choices for the fit–to–data functional and for the regularization term. Based on our theoretical results, two novel approaches are proposed for the noisy graphical lasso problem, where a covariance or precision matrix has to be statistically estimated in presence of noise. The Douglas–Rachford approach directly applies to the estimation of the covariance matrix. When the precision matrix is sought, we solve a nonconvex optimization problem. More precisely, we propose a majorization–minimization approach building a sequence of convex surrogates and solving the inner optimization subproblems via the aforementioned Douglas–Rachford procedure. We establish conditions for the convergence of this iterative scheme. We illustrate the good numerical performance of the proposed approaches with respect to state–of–the–art approaches on synthetic and real-world datasets [4].

7.11. Representation Learning on Real-World Graphs

Participants: Fragkiskos Malliaros, Abdulkadir Çelikkanat
Network representation learning (NRL) methods aim to map each vertex into a low dimensional space by preserving both local and global structure of a given network. In recent years, various approaches based on random walks have been proposed to learn node embeddings – thanks to their success in several challenging problems. In this work, we have introduced two methodologies to compute latent representations of nodes based on random walks.

In particular, we have proposed *Kernel Node Embeddings* (KernelNE) [53], a model that aims to bring together two popular approaches for NRL, namely matrix factorization and random walk-based models. KernelNE is a weighted matrix factorization model which encodes random walk-based information about the nodes of the graph. The main benefit of this formulation is that it allows to utilize kernel functions on the computation of the embeddings.

Our second approach is motivated by the fact that the popular Skip-Gram algorithm models the conditional distribution of nodes within a random walk based on the softmax function, which might prohibit to capture richer types of interaction patterns among nodes that co-occur within a random walk. Here we argue that considering more expressive conditional probability models to relate nodes within a random walk sequence, might lead to more informative representations. That way, we have introduced the *Exponential Family Graph Embedding* (EFGE) model [54], that capitalizes on exponential family distribution models to capture interactions between nodes.

We have evaluated our methods on two downstream tasks: node classification and link prediction in social, information and biological networks. The experimental results demonstrate that random walk-based models accompanied with kernels as well as exponential family distributions outperform widely-known baseline NRL methods.

7.12. Semi-supervised Learning for Misinformation Detection

Participants: Fragkiskos Malliaros (Collaboration: Adrien Benamira, Benjamin Devillers, Etienne Lesot, Ayush K. Ray, Manal Saadi, CentraleSupélec)
Social networks have become the main platforms for information dissemination. Nevertheless, due to the increasing number of users, social media platforms tend to be highly vulnerable to the propagation of disinformation – making the detection of fake news a challenging task. In our work, we have focused on content-based methods for detecting fake news – casting the problem to a binary text classification one (an article corresponds to either fake news or not). The main challenge here stems from the fact that the number of labeled data is limited; very few articles can be examined and annotated as fake. To this extend, we opted for semi-supervised learning approaches. In particular, we have proposed a graph-based semi-supervised fake news detection method, based on graph neural networks [34]. Our intuition is that, graphs are expressive

models that are able to capture contextual dependencies among articles, alleviating the label scarcity constraint. On a high level, our framework is composed of three components: i) embedding of articles in the Euclidean space; ii) construction of an article similarity graph; iii) inference of missing labels using graph learning techniques. The experimental results indicate that the proposed methodology achieves better performance compared to traditional classification techniques, especially when trained on limited number of labeled articles.

7.13. A Perturb and Combine Approach to Analyze Real-World Graphs

Participants: Fragkiskos Malliaros (Collaboration: Antoine J.-P. Tixier, Maria Evgenia G. Rossi, Jesse Read, Michalis Vazirgiannis, École Polytechnique)

Influential spreaders are nodes that can diffuse information to the largest part of the network in a minimum amount of time. Detecting influential spreaders is an important task with numerous real-world applications. Nevertheless, some of the most effective influential spreader detection algorithms (e.g., the k-core decomposition) are unstable to small perturbations of the network structure. Inspired by bagging in Machine Learning, we have proposed the first Perturb and Combine (P&C) procedure for networks [51]. It (1) creates many perturbed versions of a given graph, (2) applies a node scoring function separately to each graph, and (3) combines the results. Experiments conducted on real-world networks of various sizes with the k-core, generalized k-core, and PageRank algorithms reveal that P&C brings substantial improvements. Moreover, this performance boost can be obtained at almost no extra cost through parallelization. Finally, a bias-variance analysis suggests that P&C works mainly by reducing bias, and that therefore, it should be capable of improving the performance of all vertex scoring functions, including stable ones.

7.14. Stochastic quasi-Fejér block-coordinate fixed point iterations with random sweeping: Mean-square and linear convergence

Participant: Jean-Christophe Pesquet (Collaboration: Patrick Louis Combettes, North Carolina University, USA)

In our previous work, we investigated the almost sure weak convergence of block-coordinate fixed point algorithms and discussed their applications to nonlinear analysis and optimization. This algorithmic framework features random sweeping rules to select arbitrarily the blocks of variables that are activated over the course of the iterations and it allows for stochastic errors in the evaluation of the operators. The paper [14] establishes results on the mean-square and linear convergence of the iterates. Applications to monotone operator splitting and proximal optimization algorithms are presented.

7.15. Rational optimization for non- linear reconstruction with approximate ℓ_0 penalization

Participants: Marc Castella, Arthur Marmin, Jean-Christophe Pesquet

Recovering nonlinearly degraded signal in the presence of noise is a challenging problem. In this work, this problem is tackled by minimizing the sum of a non convex least-squares fit criterion and a penalty term. We assume that the nonlinearity of the model can be accounted for by a rational function. In addition, we suppose that the signal to be sought is sparse and a rational approximation of the ℓ_0 pseudo-norm thus constitutes a suitable penalization. The resulting composite cost function belongs to the broad class of semi-algebraic functions. To find a globally optimal solution to such an optimization problem, it can be transformed into a generalized moment problem, for which a hierarchy of semidefinite programming relaxations can be built. Global optimality comes at the expense of an increased dimension and, to overcome computational limitations concerning the number of involved variables, the structure of the problem has to be carefully addressed. A situation of practical interest is when the nonlinear model consists of a convolutive transform followed by a componentwise nonlinear rational saturation. We then propose to use a sparse relaxation able to deal with up to several hundreds of optimized variables. In contrast with the naive approach consisting of linearizing the model, our experiments show that the proposed approach offers good performance [7].

7.16. Deep neural network structures solving variational inequalities

Participant: Jean-Christophe Pesquet (Collaboration: Patrick Louis Combettes, North Carolina University, USA)
Motivated by structures that appear in deep neural networks, we investigate nonlinear composite models alternating proximity and affine operators defined on different spaces. We first show that a wide range of activation operators used in neural networks are actually proximity operators. We then establish conditions for the averagedness of the proposed composite constructs and investigate their asymptotic properties. It is shown that the limit of the resulting process solves a variational inequality which, in general, does not derive from a minimization problem [13].

7.17. Generation of patient-specific cardiac vascular networks: a hybrid image-based and synthetic geometric model

Participant: Hugues Talbot (Collaboration: Clara Jaquet, Laurent Najman, ESIEE Paris, Leo Grady, Michiel Schaap, Buzzy Spain, Hyun Kim, Charles Taylor, HeartFlow Inc, Irene Vignon-Clementel, Inria Paris)
In this work, we have proposed a blood-vessel generation procedure for extending known patient vasculature over and within the heart ventricle [19]. It is patient-specific, in the sense that it extend the known, segmented patient vasculature, and it is consistent with physics-based blood vessels characteristics (i.e. derived from CFD) and known vessel physiology. The generated vascular network bridges the gap between the vasculature that can be imaged and assessed via classical means (CT or MRI) and perfusion maps that can be imaged with specific modalities (radiotracer injected scintigraphy or PET). One objective of this work is to eventually propose a forward model for perfusion map generation, that can be used to solved the associated inverse problem of finding the cause of observed perfusion deficits associated with coronary diseases that cannot be imaged directly.

7.18. High throughput automated detection of axial malformations in Medaka fish embryo

Participant: Hugues Talbot (Collaboration: Diane Genest, Élodie Puybareau, Jean Cousty, ESIEE Paris, Marc Léonard, Noémie de Crozé, L'Oréal Recherche)
Fish embryos are used throughout the cosmetics industry to assess the toxicity of the components of their products, as well as more generally in waterways pollution measurements. Indeed pollution is often detectable in trace amounts when they hinder, stop or cause malformations during fish embryo development. In this work, we propose a high-throughput procedure for detecting most important malformations in fish embryo. For examples those affecting the tail or the eyes, based on image analysis and machine learning [16]. We have also proposed an atlas-based automated procedure for detecting swim bladder malformations, which are very difficult to assess manually [39].

These malformation are among the most difficult to assess but very common in various degrees of severity. Our procedure provide similar error rate as trained and careful humans operators, as assessed on thousands of images acquired in partneship with L'Oréal. We also show that our procedure is much faster and more consistent than human operators. It is now used in production by our partner.

7.19. Quantitative PET in the context of lymphoma

Participant: Hugues Talbot (Collaboration: Eloïse Grossiord, Laurent Najman, ESIEE Paris, Benoît Naegel, iCube, Strasbourg, Nicolas Passat, CRESTIC, Reims)
Lymphoma is type of cancer affecting the lymph system. Similar to blood disorders, these cancers can be difficult to cure because they affect a large portion of the body and metastasize easily. In contrast to leukemia, lymphoma also affects organs: the lymph nodes. Assessing the effectiveness of therapies implies to follow the impact of treatment on lymph nodes. This requires segmenting a large number of lesion, often several dozens. In [17], we have proposed an automated procedure based on hierarchical mathematical morphology, which has been extensively validated, and is now available as a plug-in for ImageJ/FIJI.

7.20. nD variational restoration of curvilinear structures with prior-based directional regularization

Participant: Hugues Talbot (Collaboration: Odyssée Merveille, Benoît Naegel, iCube, Strasbourg, Nicolas Passat, CRESTIC, Reims)

Curvilinear structure restoration in image processing procedures is a difficult task, which can be compounded when these structures are thin, i.e., when their smallest dimension is close to the resolution of the sensor. Many recent restoration methods involve considering a local gradient-based regularization term as prior, assuming gradient sparsity. An isotropic gradient operator is typically not suitable for thin curvilinear structures, since gradients are not sparse for these. In this paper [22], we propose a mixed gradient operator that combines a standard gradient in the isotropic image regions, and a directional gradient in the regions where specific orientations are likely. In particular, such information can be provided by curvilinear structure detectors (e.g., RORPO or Frangi filters). Our proposed mixed gradient operator, that can be viewed as a companion tool of such detectors, is proposed in a discrete framework and its formulation/computation holds in any dimension; in other words, it is valid in Z^n, $n \geq 1$. We show how this mixed gradient can be used to construct image priors that take edge orientation, as well as intensity, into account, and then involved in various image processing tasks while preserving curvilinear structures. The experiments carried out on 2D, 3D, real, and synthetic images illustrate the relevance of the proposed gradient, and its use in variational frameworks for both denoising and segmentation tasks.

7.21. Skin aging automated assessment

Participant: Hugues Talbot (Collaboration: Julie Robic, Alex Nkengne, Clarins laboratories, Benjamin Perret, Michel Couprie, ESIEE Paris)

With aging, human skin becomes drier, thinner and more irregular, but these characteristics are highly person-dependent, and can be brought about via exposure to heat, cold or Sun. It is important to the cosmetics industry to assess objectively the effect of their products on skin aging. With our partner Clarins laboratory, we have proposed a series of automated procedures based on graph-based image analysis. We have in particular proposed to detect the surface that correspond to the dermal-epidermal junction [25], and a series or procedures to link the appearance of this surfact to aging characteristics [48]. Both have been validated by dermatologists specialized in skin aging.

7.22. Particle tracking

Participant: Hugues Talbot (Collaboration: Alessandro Benfenati, Universita di Milano, Francesco Bonacci, Laboratoire Navier, Tarik Bourouina, ESIEE Paris)

Fluorescent bead tracking is important in biomedical application related to biomechanics, rheology and fluid dynamics. We have made several contributions for the detection and tracking of micrometer-scale fluorescent bead in 3D confocal microscopy [47], [61]. Many software packages exist for 2D tracking but almost none exist for 3D. It is a harder problem because in general beads are not fixed and move between plane acquisitions, due to the relatively slow scanning characteristics of confocal microscopy.

7.23. Artificial Intelligence Applications for Thoracic imaging

Participants: Guillaume Chassagnon, Maria Vakalopoulou (Collaboration: Marie-Pierre Revel and Nikos Paragios, AP-HP - Hopital Cochin Broca Hotel Dieu, Therapanacea)

Relevance and penetration of machine learning in clinical practice is a recent phenomenon with multiple applications being currently under development. Deep learning –and especially convolutional neural networks (CNNs)– is a subset of machine learning, which has recently entered the field of thoracic imaging. The structure of neural networks, organized in multiple layers, allows them to address complex tasks. For several clinical situations, CNNs have demonstrated superior performance as compared with classical machine learning algorithms and in some cases achieved comparable or better performance than clinical experts. Chest radiography, a high-volume procedure, is a natural application domain because of the large amount of stored images and reports facilitating the training of deep learning algorithms. Several algorithms for automated reporting have been developed. The training of deep learning algorithm CT images is more complex due to the dimension, variability, and complexity of the 3D signal. The role of these methods is likely to increase in clinical practice as a complement of the radiologist's expertise. The objective of these two reviews [9], [26] is to provide definitions for understanding the methods and their potential applications for thoracic imaging.

7.24. Use of Elastic Registration in Pulmonary MRI for the Assessment of Pulmonary Fibrosis in Patients with Systemic Sclerosis

Participants: Guillaume Chassagnon, Maria Vakalopoulou (Collaboration: Charlotte Martin, Rafael Marini Silva, Alexis Régent, Luc Mouthon, Nikos Paragios and Marie-Pierre Revel, AP-HP - Hopital Cochin Broca Hotel Dieu, Therapanacea)

Elastic registration of inspiratory and expiratory MRI revealed qualitative and quantitative differences in lung deformation in study participants with systemic sclerosis compared with healthy volunteers. Current imaging methods are not sensitive to changes in pulmonary function resulting from fibrosis. MRI with ultrashort echo time can be used to image the lung parenchyma and lung motion. To evaluate elastic registration of inspiratory to expiratory lung MRI for the assessment of pulmonary fibrosis in study participants with systemic sclerosis (SSc). This prospective study [8] was performed from September 2017 to March 2018 and recruited healthy volunteers and participants with SSc and high-resolution CT (within the previous 3 months) of the chest for lung MRI. Two breath-hold, coronal, three-dimensional, ultrashort–echo-time, gradient-echo sequences of the lungs were acquired after full inspiration and expiration with a 3.0-T unit. Images were registered from inspiration to expiration by using an elastic registration algorithm. Jacobian determinants were calculated from deformation fields and represented on color maps. Similarity between areas with marked shrinkage and logarithm of Jacobian determinants were compared between healthy volunteers and study participants with SSc. Receiver operating characteristic curve analysis was performed to determine the best Dice similarity coefficient threshold for diagnosis of fibrosis. Sixteen participants with SSc (seven with pulmonary fibrosis at high-resolution CT) and 11 healthy volunteers were evaluated. Areas of marked shrinkage during expiration with logarithm of Jacobian determinants less than -0.15 were found in the posterior lung bases of healthy volunteers and in participants with SSc without fibrosis, but not in participants with fibrosis. The sensitivity and specificity of MRI for presence of fibrosis at high-resolution CT were 86% and 75%, respectively (area under the curve, 0.81; $P = .04$) by using a threshold of 0.36 for Dice similarity coefficient. Elastic registration of inspiratory to expiratory MRI shows less lung base respiratory deformation in study participants with systemic sclerosis related pulmonary fibrosis compared with participants without fibrosis.

7.25. U-ReSNet: Ultimate Coupling of Registration and Segmentation with Deep Nets

Participants: Théo Estienne, Enzo Battistella, Marvin Lerousseau, Roger Sun, Maria Vakalopoulou (Collaboration: Stergios Christodoulidis, Alexandre Carre, Guillaume Klausner, Stavroula Mougiakakou, Charlotte Robert, Nikos Paragios and Eric Deutsch, Institute Gustave Roussy, University of Bern, Therapanacea)

We proposed in [58] a 3D deep neural network called U-ReSNet, a joint framework that can accurately register and segment medical volumes. The proposed network learns to automatically generate linear and elastic deformation models, trained by minimizing the mean square error and the local cross correlation similarity metrics. In parallel, a coupled architecture is integrated, seeking to provide segmentation maps for anatomies or tissue patterns using an additional decoder part trained with the dice coefficient metric. U-ReSNet is trained in an end to end fashion, while due to this joint optimization the generated network features are more informative leading to promising results compared to other deep learning-based methods existing in the literature. We evaluated the proposed architecture using the publicly available OASIS 3 dataset, measuring the dice coefficient metric for both registration and segmentation tasks. Our promising results indicate the potentials of our method which is composed from a convolutional architecture that is extremely simple and light in terms of parameters.

7.26. Gene Expression High-Dimensional Clustering Towards a Novel, Robust, Clinically Relevant and Highly Compact Cancer Signature

Participants: Enzo Battistella, Théo Estienne, Marvin Lerousseau, Roger Sun, Maria Vakalopoulou (Collaboration: Charlotte Robert, Nikos Paragios and Eric Deutsch, Institute Gustave Roussy, Therapanacea)

Precision medicine, a highly disruptive paradigm shift in healthcare targeting the personalizing treatment, heavily relies on genomic data. However, the complexity of the biological interactions, the important number of genes as well as the lack of substantial patient's clinical data consist a tremendous bottleneck on the clinical implementation of precision medicine. In this work [32], we introduce a generic, low dimensional gene signature that represents adequately the tumor type. Our gene signature is produced using LP-stability algorithm, a high dimensional center-based unsupervised clustering algorithm working in the dual domain, and is very versatile as it can consider any arbitrary distance metric between genes. The gene signature produced by LP-stability reports at least 10 times better statistical significance and 35% better biological significance than the ones produced by two referential unsupervised clustering methods. Moreover, our experiments demonstrate that our low dimensional biomarker (27 genes) surpass significantly existing state of the art methods both in terms of qualitative and quantitative assessment while providing better associations to tumor types than methods widely used in the literature that rely on several omics data.

7.27. A Novel Object-Based Deep Learning Framework for Semantic Segmentation of Very High-Resolution Remote Sensing Data: Comparison with Convolutional and Fully Convolutional Networks

Participants: Maria Papadomanolaki and Maria Vakalopoulou (Collaboration: Konstantinos Karantzalos, National Technical University of Athens)

Deep learning architectures have received much attention in recent years demonstrating state-of-the-art performance in several segmentation, classification and other computer vision tasks. Most of these deep networks are based on either convolutional or fully convolutional architectures. In this study [24], we propose a novel object-based deep-learning framework for semantic segmentation in very high-resolution satellite data. In particular, we exploit object-based priors integrated into a fully convolutional neural network by incorporating an anisotropic diffusion data preprocessing step and an additional loss term during the training process. Under this constrained framework, the goal is to enforce pixels that belong to the same object to be classified at the same semantic category. We compared thoroughly the novel object-based framework with the currently dominating convolutional and fully convolutional deep networks. In particular, numerous experiments were conducted on the publicly available ISPRS WGII/4 benchmark datasets, namely Vaihingen and Potsdam, for validation and inter-comparison based on a variety of metrics. Quantitatively, experimental results indicate that, overall, the proposed object-based framework slightly outperformed the current state-of-the-art fully convolutional networks by more than 1% in terms of overall accuracy, while intersection over union results are improved for all semantic categories. Qualitatively, man-made classes with more strict geometry such as buildings were the ones that benefit most from our method, especially along object boundaries, highlighting the great potential of the developed approach.

7.28. A multi-task deep learning framework coupling semantic segmentation and image reconstruction for very high resolution imagery

Participants: Maria Papadomanolaki and Maria Vakalopoulou (Collaboration: Konstantinos Karantzalos, National Technical University of Athens)

Semantic segmentation, especially for very high-resolution satellite data, is one of the pillar problems in the remote sensing community. Lately, deep learning techniques are the ones that set the state-of-the-art for a number of benchmark datasets, however, there are still a lot of challenges that need to be addressed, especially in the case of limited annotations. To this end, in this study [45], we propose a novel framework based on deep neural networks that is able to address concurrently semantic segmentation and image reconstruction in an end to end training. Under the proposed formulation, the image reconstruction acts as a regularization, constraining efficiently the solution in the entire image domain. This self-supervised component helps significantly the generalization of the network for the semantic segmentation, especially in cases of a low number of annotations. Experimental results and the performed quantitative evaluation on the publicly available ISPRS (WGIII/4) dataset indicate the great potential of the developed approach.

7.29. Detecting Urban Changes with Recurrent Neural Networks from Multitemporal Sentinel-2 Data

Participants: Maria Papadomanolaki, Sagar Verma and Maria Vakalopoulou (Collaboration: Siddharth Gupta and Konstantinos Karantzalos, Granular AI and National Technical University of Athens)

The advent of multitemporal high resolution data, like the Copernicus Sentinel-2, has enhanced significantly the potential of monitoring the earth's surface and environmental dynamics. In this study [45], we present a novel deep learning framework for urban change detection which combines state-of-the-art fully convolutional networks (similar to U-Net) for feature representation and powerful recurrent networks (such as LSTMs) for temporal modeling. We report our results on the recently publicly available bi-temporal Onera Satellite Change Detection (OSCD) Sentinel-2 dataset, enhancing the temporal information with additional images of the same region on different dates. Moreover, we evaluate the performance of the recurrent networks as well as the use of the additional dates on the unseen test-set using an ensemble cross-validation strategy. All the developed models during the validation phase have scored an overall accuracy of more than 95%, while the use of LSTMs and further temporal information, boost the F1 rate of the change class by an additional 1.5%.

7.30. Image Registration of Satellite Imagery with Deep Convolutional Neural Networks

Participants: Maria Vakalopoulou and Mihir Sahasrabudhe (Collaboration: Stergios Christodoulidis, Stavroula Mougiakakou and Nikos Paragios, University of Bern and Therapanacea)

Image registration in multimodal, multitemporal satellite imagery is one of the most important problems in remote sensing and essential for a number of other tasks such as change detection and image fusion. In this study [52], inspired by the recent success of deep learning approaches we propose a novel convolutional neural network architecture that couples linear and deformable approaches for accurate alignment of remote sensing imagery. The proposed method is completely unsupervised, ensures smooth displacement fields and provides real time registration on a pair of images. We evaluate the performance of our method using a challenging multitemporal dataset of very high resolution satellite images and compare its performance with a state of the art elastic registration method based on graphical models. Both quantitative and qualitative results prove the high potentials of our method.

7.31. Lifting AutoEncoders: Unsupervised Learning of a Fully-Disentangled 3D Morphable Model Using Deep Non-Rigid Structure From Motion

Participants: Mihir Sahasrabudhe (Collaboration: Eqward Bartrum, Riza Alp Guler, Dimitris Samaras and Iasonas Kokkinos, Stony Brook, UCL and Ariel AI)

We introduced, in [49], Lifting Autoencoders, a generative 3D surface-based model of object categories. We bring together ideas from non-rigid structure from motion, image formation, and morphable models to learn a controllable, geometric model of 3D categories in an entirely unsupervised manner from an unstructured set of images. We exploit the 3D geometric nature of our model and use normal information to disentangle appearance into illumination, shading, and albedo. We further use weak supervision to disentangle the non-rigid shape variability of human faces into identity and expression. We combine the 3D representation with a differentiable renderer to generate RGB images and append an adversarially trained refinement network to obtain sharp, photorealistic image reconstruction results. The learned generative model can be controlled in terms of interpretable geometry and appearance factors, allowing us to perform photorealistic image manipulation of identity, expression, 3D pose, and illumination properties.

PARIETAL Project-Team

7. New Results

7.1. The visual word form area (VWFA) is part of both language and attention circuitry

While predominant models of visual word form area (VWFA) function argue for its specific role in decoding written language, other accounts propose a more general role of VWFA in complex visual processing. However, a comprehensive examination of structural and functional VWFA circuits and their relationship to behavior has been missing. Here, using high-resolution multimodal imaging data from a large Human Connectome Project cohort (N = 313), we demonstrate robust patterns of VWFA connectivity with both canonical language and attentional networks. Brain-behavior relationships revealed a striking pattern of double dissociation: structural connectivity of VWFA with lateral temporal language network predicted language, but not visuo-spatial attention abilities, while VWFA connectivity with dorsal fronto-parietal attention network predicted visuo-spatial attention, but not language abilities. Our findings support a multiplex model of VWFA function characterized by distinct circuits for integrating language and attention, and point to connectivity-constrained cognition as a key principle of human brain organization.

More information can be found in [7].

7.2. SPARKLING: variable-density k-space filling curves for accelerated T2* -weighted MRI

Funding information Purpose: To present a new optimization-driven design of optimal k-space trajectories in the context of compressed sensing: Spreading Projection Algorithm for Rapid K-space sampLING (SPARKLING). Theory: The SPARKLING algorithm is a versatile method inspired from stippling techniques that automatically generates optimized sampling patterns compatible with MR hardware constraints on maximum gradient amplitude and slew rate. These non-Cartesian sampling curves are designed to comply with key criteria for optimal sampling: a controlled distribution of samples (e.g., variable density) and a locally uniform k-space coverage. Methods: Ex vivo and in vivo prospective $T2^\star$-weighted acquisitions were performed on a 7 Tesla scanner using the SPARKLING tra-jectories for various setups and target densities. Our method was compared to radial and variable-density spiral trajectories for high resolution imaging. Results: Combining sampling efficiency with compressed sensing, the proposed sampling patterns allowed up to 20-fold reductions in MR scan time (compared to fully-sampled Cartesian acquisitions) for two-dimensional $T2^\star$-weighted imaging without deterioration of image quality, as demonstrated by our experimental results at 7 Tesla on in vivo human brains for a high in-plane resolution of 390 um. In comparison to existing non-Cartesian sampling strategies, the proposed technique also yielded superior image quality. Conclusion: The proposed optimization-driven design of k-space trajectories is a versatile framework that is able to enhance MR sampling performance in the context of compressed sensing.

More information can be found in [14].

7.3. Benchmarking functional connectome-based predictive models for resting-state fMRI

Functional connectomes reveal biomarkers of individual psychological or clinical traits. However, there is great variability in the analytic pipelines typically used to derive them from rest-fMRI cohorts. Here, we consider a specific type of studies, using predictive models on the edge weights of functional connectomes, for which we highlight the best modeling choices. We systematically study the prediction performances of models

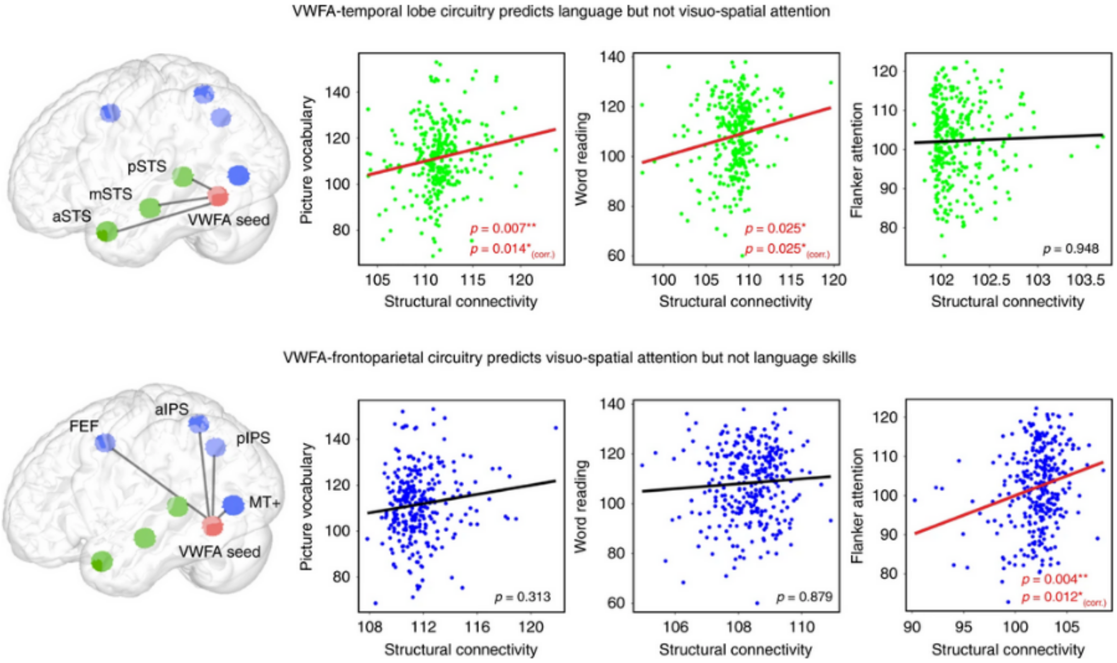

Figure 3. Structural connectivity of VWFA with STS nodes (anterior, middle, and posterior STS) was significantly correlated with individuals' performance on picture vocabulary and word reading tasks, but not on the Flanker visuo-spatial attention task. b Structural connectivity of VWFA with fronto-parietal attention network nodes (FEF, aIPS, pIPS, and MT+) was significantly correlated with individuals' performance on the Flanker attention task but not on the word reading or picture vocabulary tasks. Y-axis is age-adjusted performance scores on cognitive tasks and x-axis presents the predicted performance scores on cognitive tasks from the probability of structural connectivity of VWFA to either the language or the attention network ROIs.

in 6 different cohorts and a total of 2 000 individuals, encompassing neuro-degenerative (Alzheimer's, Post-traumatic stress disorder), neuro-psychiatric (Schizophrenia, Autism), drug impact (Cannabis use) clinical settings and psychological trait (fluid intelligence). The typical prediction procedure from rest-fMRI consists of three main steps: defining brain regions, representing the interactions, and supervised learning. For each step we benchmark typical choices: 8 different ways of defining regions –either pre-defined or generated from the rest-fMRI data– 3 measures to build functional connectomes from the extracted time-series, and 10 classification models to compare functional interactions across subjects. Our benchmarks summarize more than 240 different pipelines and outline modeling choices that show consistent prediction performances in spite of variations in the populations and sites. We find that regions defined from functional data work best; that it is beneficial to capture between-region interactions with tangent-based parametrization of covariances, a midway between correlations and partial correlation; and that simple linear predictors such as a logistic regression give the best predictions. Our work is a step forward to establishing reproducible imaging-based biomarkers for clinical settings.

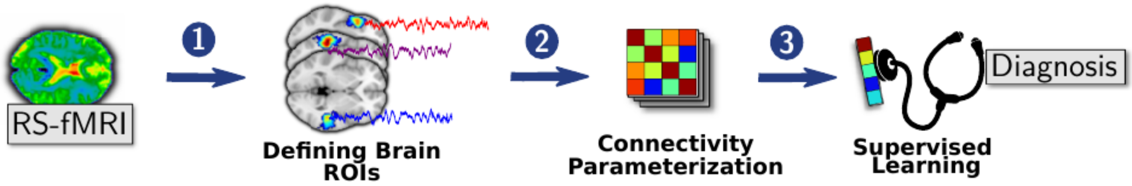

Figure 4. Functional connectome-prediction pipeline with three main steps: 1) definition of brain regions (ROIs) from rest-fMRI images or us- ing already defined reference atlases, 2) quantifying functional interactions from time series signals extracted from these ROIs and 3) comparisons of functional interactions across subjects using supervised learning.

More information can be found in [8].

7.4. Population shrinkage of covariance (PoSCE) for better individual brain functional-connectivity estimation

Estimating covariances from functional Magnetic Resonance Imaging at rest (r-fMRI) can quantify interactions between brain regions. Also known as brain functional connectivity, it reflects inter-subject variations in behavior and cognition, and characterizes neuropathologies. Yet, with noisy and short time-series, as in r-fMRI, covariance estimation is challenging and calls for penalization, as with shrinkage approaches. We introduce population shrinkage of covariance estimator (PoSCE) : a covariance estimator that integrates prior knowledge of covariance distribution over a large population, leading to a non-isotropic shrinkage. The shrinkage is tailored to the Riemannian geometry of symmetric positive definite matrices. It is coupled with a probabilistic modeling of the individual and population covariance distributions. Experiments on two large r-fMRI datasets (HCP n=815, Cam-CAN n=626) show that PoSCE has a better bias-variance trade-off than existing covariance estimates: this estimator relates better functional-connectivity measures to cognition while capturing well intra-subject functional connectivity.

More information can be found in [20].

7.5. Feature Grouping as a Stochastic Regularizer for High-Dimensional Structured Data

In many applications where collecting data is expensive , for example neuroscience or medical imaging, the sample size is typically small compared to the feature dimension. It is challenging in this setting to train

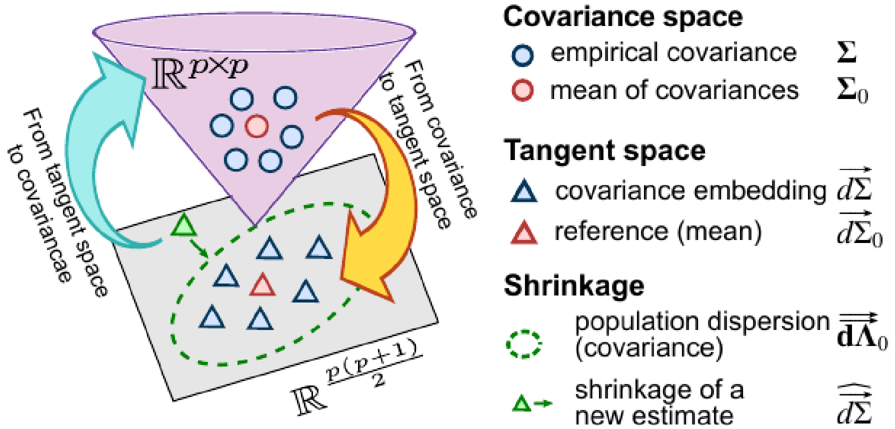

Figure 5. Tangent embedding and population prior modeling. Σ_0 is the mean covariance from a train set of covariances. It is the reference point in the tangent space. The population prior is defined as a Gaussian multivariate dis- tribution centered on $d\Sigma_0$. Λ_0 is the covariance dispersion over the population. The arrows depict the mapping between the non-Euclidean covariance space and the tangent space.

expressive, non-linear models without overfitting. These datasets call for intelligent regularization that exploits known structure, such as correlations between the features arising from the measurement device. However, existing structured regularizers need specially crafted solvers, which are difficult to apply to complex models. We propose a new regularizer specifically designed to leverage structure in the data in a way that can be applied efficiently to complex models. Our approach relies on feature grouping, using a fast clustering algorithm inside a stochas-tic gradient descent loop: given a family of feature groupings that capture feature covariations, we randomly select these groups at each iteration. We show that this approach amounts to enforcing a denoising regularizer on the solution. The method is easy to implement in many model archi-tectures, such as fully connected neural networks, and has a linear computational cost. We apply this regularizer to a real-world fMRI dataset and the Olivetti Faces datasets. Experiments on both datasets demonstrate that the proposed approach produces models that generalize better than those trained with conventional regularizers, and also improves convergence speed.

More information can be found in [25].

7.6. Manifold-regression to predict from MEG/EEG brain signals without source modeling

Magnetoencephalography and electroencephalography (M/EEG) can reveal neuronal dynamics non-invasively in real-time and are therefore appreciated methods in medicine and neuroscience. Recent advances in modeling brain-behavior relationships have highlighted the effectiveness of Riemannian geometry for summarizing the spatially correlated time-series from M/EEG in terms of their covariance. However , after artefact-suppression, M/EEG data is often rank deficient which limits the application of Riemannian concepts. In this article, we focus on the task of regression with rank-reduced covariance matrices. We study two Riemannian approaches that vectorize the M/EEG covariance between-sensors through projection into a tangent space. The Wasserstein distance readily applies to rank-reduced data but lacks affine-invariance. This can be overcome by finding a common sub-space in which the covariance matrices are full rank, enabling the affine-invariant geometric distance. We investigated the implications of these two approaches in synthetic generative models, which allowed us to control estimation bias of a linear model for prediction. We show that Wasserstein and geometric

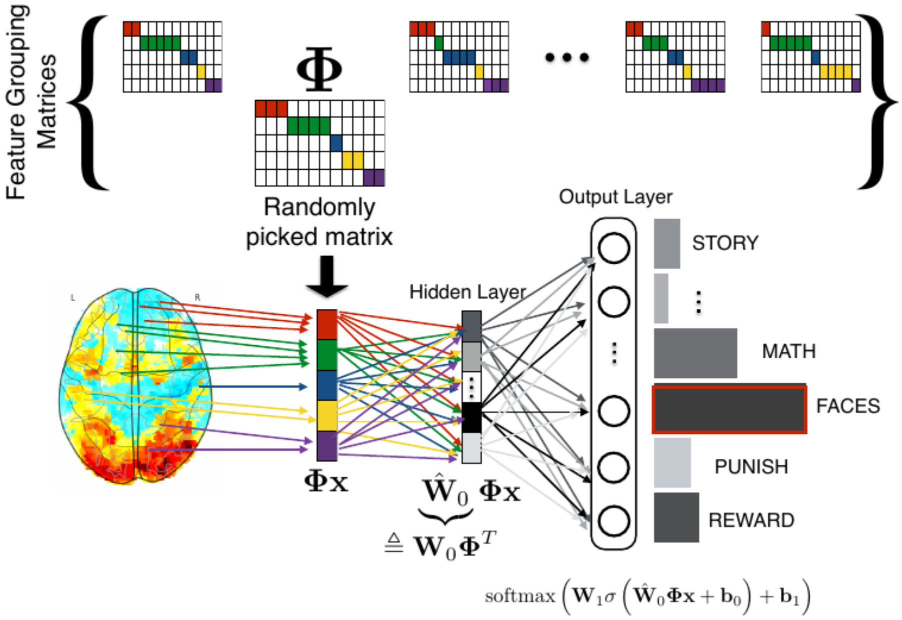

Figure 6. Illustration of the proposed approach: Forward propa- gation of a neural network with a single hidden layer using feature grouping during training. The parameters of the neural network to be estimated are $\mathbf{W}_0$, $\mathbf{b}_0$, $\mathbf{W}_1$, $\mathbf{b}1$. *A bank of feature grouping matrices are pre-generated where each matrix is calculated from a sub-sample of the training test. At each SGD iteration, a feature grouping matrix is sampled from the bank of pre-generated matri- ces. The gradient is then computed with respect to* $\widehat{\mathbf{W}}_0$ *to update* $\mathbf{W}_0$ *in backpropagation.*

distances allow perfect out-of-sample prediction on the generative models. We then evaluated the methods on real data with regard to their effectiveness in predicting age from M/EEG covariance matrices. The findings suggest that the data-driven Riemannian methods outperform different sensor-space estimators and that they get close to the performance of biophysics-driven source-localization model that requires MRI acquisitions and tedious data processing. Our study suggests that the proposed Riemannian methods can serve as fundamental building-blocks for automated large-scale analysis of M/EEG.

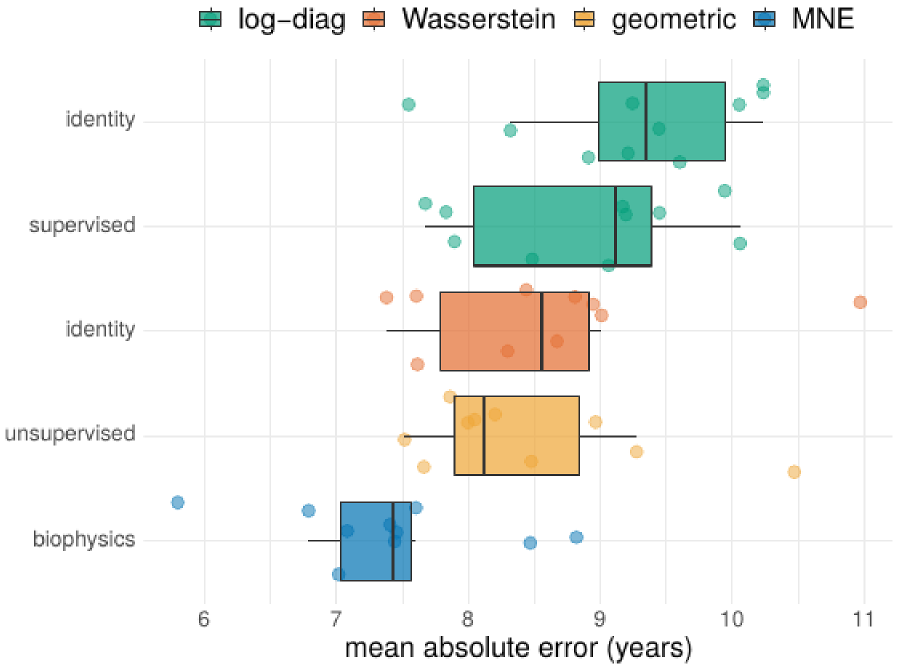

Figure 7. Age prediction on Cam-CAN MEG dataset for different methods, ordered by out-of-sample MAE. The y-axis depicts the projection method, with identity denoting the absence of projection. Colors indicate the subsequent embedding. The biophysics-driven MNE method (blue) performs best. The Riemannian methods (orange) follow closely and their performance depends little on the projection method. The non-Riemannian methods log-diag (green) perform worse, although the supervised projection clearly helps.

More information can be found in [47].

7.7. Stochastic algorithms with descent guarantees for ICA

Independent component analysis (ICA) is a widespread data exploration technique, where observed signals are modeled as linear mixtures of independent components. From a machine learning point of view, it amounts to a matrix factorization problem with a statistical independence criterion. Infomax is one of the most used ICA algorithms. It is based on a loss function which is a non-convex log-likelihood. We develop a new majorization-minimization framework adapted to this loss function. We derive an online algorithm for the streaming setting, and an incremental algorithm for the finite sum setting, with the following benefits. First, unlike most algorithms found in the literature, the proposed methods do not rely on any critical hyper-parameter like a step size, nor do they require a line-search technique. Second, the algorithm for the finite sum setting, although stochas-tic, guarantees a decrease of the loss function at each iteration. Experiments demonstrate progress on the state-of-the-art for large scale datasets, without the necessity for any manual parameter tuning.

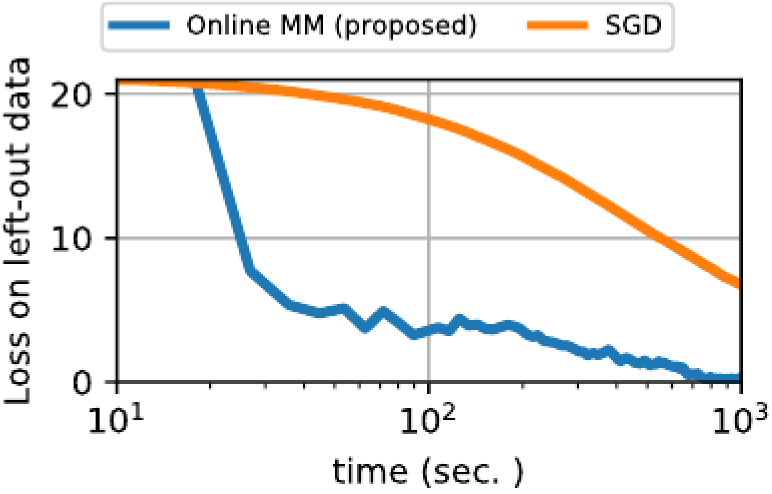

Figure 8. Online algorithms applied on a 32 GB real dataset with p = 100 and n = $4{\times}10^7$ *. Time is in logarithmic scale. Values of the loss on left out data greater than its initial value are truncated.*

More information can be found in [39].

7.8. Comparing distributions: $l1$ geometry improves kernel two-sample testing

Are two sets of observations drawn from the same distribution? This problem is a two-sample test. Kernel methods lead to many appealing properties. Indeed state-of-the-art approaches use the L2 distance between kernel-based distribution representatives to derive their test statistics. Here, we show that Lp distances (with $p \geq 1$) between these distribution representatives give metrics on the space of distributions that are well-behaved to detect differences between distributions as they metrize the weak convergence. Moreover, for analytic kernels, we show that the L1 geometry gives improved testing power for scalable computational procedures. Specifically, we derive a finite dimensional approximation of the metric given as the ℓ_1 norm of a vector which captures differences of expectations of analytic functions evaluated at spatial locations or frequencies (i.e, features). The features can be chosen to maximize the differences of the distributions and give interpretable indications of how they differs. Using an ℓ_1 norm gives better detection because differences between representatives are dense as we use analytic kernels (non-zero almost everywhere). The tests are consistent, while much faster than state-of-the-art quadratic-time kernel-based tests. Experiments on artificial and real-world problems demonstrate improved power/time tradeoff than the state of the art, based on ℓ_2 norms, and in some cases, better outright power than even the most expensive quadratic-time tests. More information can be found in [37].

7.9. Wasserstein regularization for sparse multi-task regression

We focus in this work on high-dimensional regression problems where each regressor can be associated to a location in a physical space, or more generally a generic geometric space. Such problems often employ sparse priors, which promote models using a small subset of regressors. To increase statistical power, the so-called multi-task techniques were proposed, which consist in the simultaneous estimation of several related models. Combined with sparsity assumptions, it lead to models enforcing the active regressors to be shared across models, thanks to, for instance L1 / Lq norms. We argue in this paper that these techniques fail to leverage the spatial information associated to regressors. Indeed, while sparse priors enforce that only a small subset of variables is used, the assumption that these regressors overlap across all tasks is overly simplistic given the spatial variability observed in real data. In this paper, we propose a convex reg-ularizer for multi-task regression that encodes a more flexible geometry. Our regularizer is based on unbalanced optimal transport (OT) theory, and can take into account a prior geometric knowledge on the regressor variables, without necessarily requiring overlapping supports. We derive an efficient algorithm based on a regularized formulation of OT, which iterates through applications of Sinkhorn's algorithm along with coordinate descent iterations. The performance of our model is demonstrated on regular grids with both synthetic and real datasets as well as complex triangulated geometries of the cortex with an application in neuroimaging.

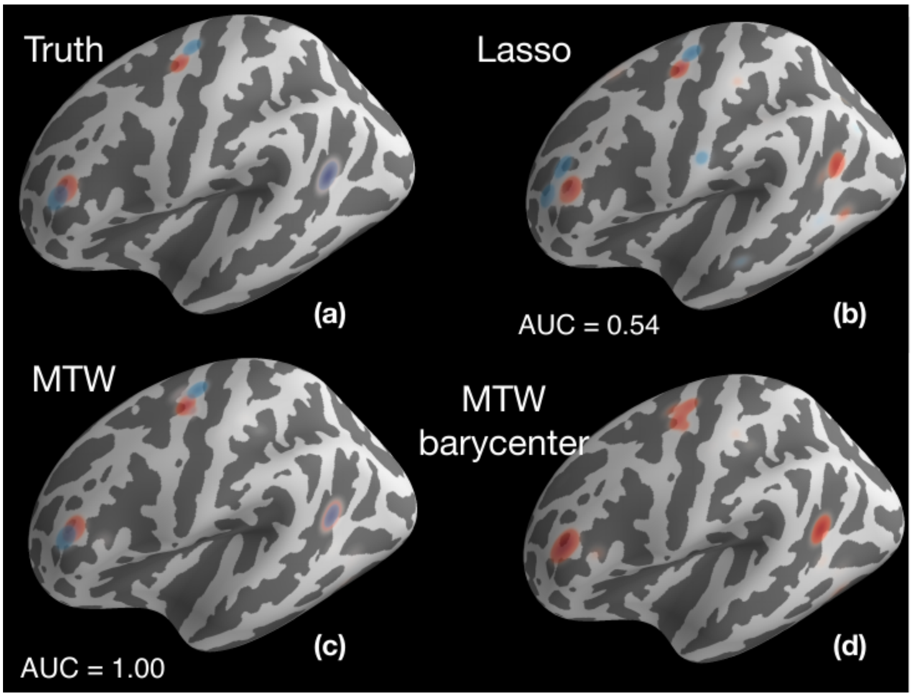

Figure 9. Each color corresponds to one of the two subjects (except for (d)). (a): True sources: one common feature (right side of the displayed hemisphere) and two non-overlapping sources. (b, c): Sources estimated by (b) Lasso and (c) MTW with the highest AUC score. (d) Shows the barycenter texttheta¯ associated with MTW model. In this figure, the displayed activations were smoothed for the sake of visibility.

More information can be found in [34].

7.10. Ensemble of Clustered Knockoffs for robust multivariate inference on MRI data

Continuous improvement in medical imaging techniques allows the acquisition of higher-resolution images. When these are used in a predictive setting, a greater number of explanatory variables are potentially related to the dependent variable (the response). Meanwhile, the number of acquisitions per experiment remains limited. In such high dimension/small sample size setting, it is desirable to find the explanatory variables that are truly related to the response while controlling the rate of false discoveries. To achieve this goal, novel multivariate inference procedures, such as knockoff inference, have been proposed recently. However, they require the feature covariance to be well-defined, which is impossible in high-dimensional settings. In this paper, we propose a new algorithm, called Ensemble of Clustered Knockoffs, that allows to select explanatory variables while controlling the false discovery rate (FDR), up to a prescribed spatial tolerance. The core idea is that knockoff-based inference can be applied on groups (clusters) of voxels, which drastically reduces the problem's dimension; an ensembling step then removes the dependence on a fixed clustering and stabilizes the results. We benchmark this algorithm and other FDR-controlling methods on brain imaging datasets and observe empirical gains in sensitivity, while the false discovery rate is controlled at the nominal level.

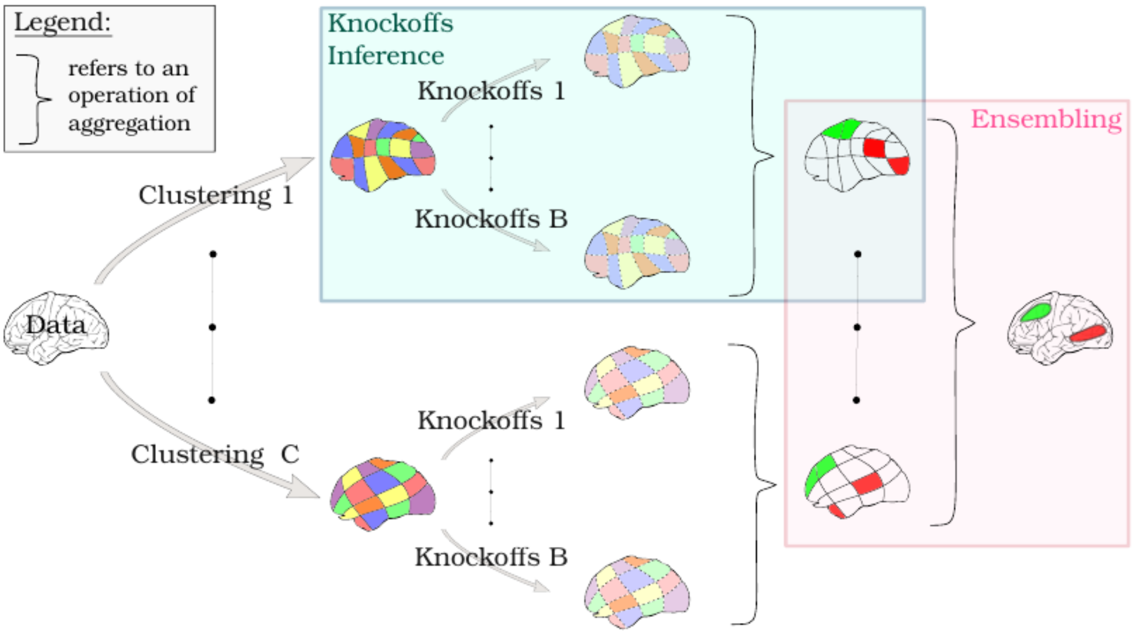

Figure 10. Representation of the ECKO algorithm. To create a stable inference result, we introduce ensembling steps both within each cluster level and at the voxel- level, across clusterings.

More information can be found in [46].

PARSIFAL Project-Team

7. New Results

7.1. Functional programming with λ-tree syntax

Participants: Ulysse Gerard, Dale Miller, Gabriel Scherer.

We have been designing a new functional programming language, MLTS, that uses the λ-*tree* syntax approach to encoding bindings that appear within data structures [20]. In this setting, bindings never become free nor escape their scope: instead, binders in data structures are permitted to *move* into binders within programs phrases. The design of MLTS—whose concrete syntax is based on that of OCaml—includes additional sites within programs that directly support this movement of bindings. Our description of MLTS includes a typing discipline that naturally extends the typing of OCaml programs.

In addition to the natural semantics for MLTS that we proposed in 2018, we also have a small-step operational semantics which gives in particular a fine-grained description of the runtime behavior of the ∇ operator in patterns. It leads in particular to a direct implementation in Lambda-Prolog (which does not contain a native ∇ operator) that allows more expressive constructs (higher-arity types) than our previous presentation.

7.2. Mechanized metatheory revisited

Participant: Dale Miller.

When proof assistants and theorem provers implement the metatheory of logical systems, they must deal with a range of syntactic expressions (e.g., types, formulas, and proofs) that involve variable bindings. Since most mature proof assistants do not have built-in methods to treat bindings, they have been extended with various packages and libraries that allow them to encode such syntax using, for example, De Bruijn numerals. In the paper, [10], Miller puts forward the argument that bindings are such an intimate aspect of the structure of expressions that they should be accounted for directly in the underlying programming language support for proof assistants and not via packages and libraries. He presents an approach to designing programming languages and proof assistants that directly supports bindings in syntax. The roots of this approach can be found in the *mobility* of binders between term-level bindings, formula-level bindings (quantifiers), and proof-level bindings (eigenvariables). In particular, the combination of Church's approach to terms and formulas (found in his Simple Theory of Types) and Gentzen's approach to proofs (found in his sequent calculus) yields a framework for the interaction of bindings with a full range of logical connectives and quantifiers. Miller also illustrates how that framework provides a direct and semantically clean treatment of computation and reasoning with syntax containing bindings.

7.3. New applications of Foundational Proof Certificates

Participants: Kaustuv Chaudhuri, Matteo Manighetti, Dale Miller.

The formal framework of *Foundational Proof Certificates* (FPC) was developed in previous years within the Parsifal team. We continue to push on their applications in a number of settings in computational logic. In 2019, we developed two such new applications.

In order to apply FPCs to the conventional setting of classical logic theorem provers, the FPC setting needed to treat proof evidence containing Skolem functions. Using FPC directly meant that we needed to do such certification without using the mathematical concepts of model-theoretic semantics (i.e., preservation of satisfiability) and choice principles (i.e., epsilon terms). Instead, our proof checking kernel is an implementation of Gentzen's sequent calculus, which directly supports quantifier alternation by using eigenvariables. In [19], we described deskolemization as a mapping from client-side terms, used in proofs generated by theorem provers, into kernel-side terms, used within our proof checking kernel. This mapping which associates skolemized terms to eigenvariables relies on using outer skolemization.

Property-based testing (PBT) is a technique for validating code against an executable specification by automatically generating test-data. In the paper [18], we presented a proof-theoretical reconstruction of this style of testing for relational specifications and employ FPCs to describe test generators. We did this by presenting certain kinds of "proof outlines" that can be used to describe various common generation strategies in the PBT literature, ranging from random to exhaustive, including their combination. We also address the shrinking of counterexamples as a first step towards their explanation. Once generation is accomplished, the testing phase boils down to a standard logic programming search. We could also we lift our techniques to treat data structures containing bindings using λ-*tree* syntax. The λProlog programming language is capable of performing both the generation and checking of tests. We validated this approach by tackling benchmarks in the metatheory of programming languages coming from related tools such as PLT-Redex Property-Based Testing via Proof Reconstruction. This work was done in collaboration with Roberto Blanco, a postdoc from Inria Paris, and Alberto Momigliano, a professor from the University of Milan.

7.4. Historical reflections on proof theory and logic programming

Participant: Dale Miller.

Miller has been working in the area of logic programming and proof theory for more than three decades. Some of his historical reflections on how these two topics influenced each other are contained in the paper [11]. While it is widely known that proof theory has been helpful in shaping the development of logic programming, particular of extensions to conventional Prolog, this paper also documents a few specific examples where logic programming influenced the development of some topics in proof theory.

7.5. Intuitionistic proofs without syntax

Participant: Lutz Straßburger.

We present Intuitionistic Combinatorial Proofs (ICPs), a concrete geometric semantics of intuitionistic logic based on the principles of classical combinatorial proofs. An ICP naturally factorizes into a linear fragment, a graphical abstraction of an IMLL proof net (an arena net), and a parallel contraction-weakening fragment (a skew fibration). ICPs relate to game semantics, and can be seen as a strategy in a Hyland-Ong arena, generalized from a tree-like to a dag-like strategy. Our first main result, Polynomial Full Completeness, is thatICPs as a semantics are complexity-aware: the translations to and from sequent calculus are size-preserving (up to a polynomial). By contrast, lambda-calculus and game semantics incur an exponential blowup. Our second main result, Local Canonicity, is that ICPs abstract fully and faithfully over the non-duplicating permutations of the sequent calculus. These results have been presented at the LICS 2019 conference [23].

7.6. Towards a combinatorial proof theory

Participants: Lutz Straßburger, Benjamin Ralph.

The main part of a classical combinatorial proof is a skew fibration, which precisely captures the behavior of weakening and contraction. Relaxing the presence of these two rules leads to certain substructural logics and substructural proof theory. We investigated what happens if we replace the skew fibration by other kinds of graph homomorphism. This leads us to new logics and proof systems that we call combinatorial. This has been presented at the TABLEAUX 2019 conference [22].

7.7. Combinatorial Proofs for Logics of Relevance and Entailment

Participants: Lutz Straßburger, Matteo Acclavio.

In this work (presented at the WoLLIC 2019 conference [16]) we characterize classical combinatorial proofs which also represent valid proofs for relevant logic with and without the mingle axiom. Moreover, we extend our syntax in order to represent combinatorial proofs for the more restrictive framework of entailment logic.

7.8. On combinatorial proofs for modal logic

Participants: Lutz Straßburger, Matteo Acclavio.

In this work [17], we extend combinatorial proofs to modal logics. The crucial ingredient for modeling the modalities is the use of a self-dual non-commutative operator that has first been observed by Retoré through pomset logic. Consequently, we had to generalize the notion of skew fibration from cographs to Guglielmi's relation webs. Our main result is a sound and complete system of combinatorial proofs for all normal and non-normal modal logics in the S4-tesseract. The proof of soundness and completeness is based on the sequent calculus with some added features from deep inference.

7.9. Deep inference and expansion trees for second-order multiplicative linear logic

Participant: Lutz Straßburger.

In this work, we introduce the notion of expansion tree for linear logic. As in Miller's original work, we have a shallow reading of an expansion tree that corresponds to the conclusion of the proof, and a deep reading which is a formula that can be proved by propositional rules. We focus our attention to MLL2, and we also present a deep inference system for that logic. This allows us to give a syntactic proof to a version of Herbrand's theorem. This has been published in an special issue of MSCS [12].

7.10. A fully labelled proof system for intuitionistic modal logics

Participants: Lutz Straßburger, Marianela Morales.

In this paper we present a labelled sequent system for intuitionistic modal logics such that there is not only one, but two relation symbols appearing in sequents: one for the accessibility relation associated with the Kripke semantics for normal modal logics and one for the preorder relation associated with the Kripke semantics for intuitionistic logic. This puts our system in close correspondence with the standard birelational Kripke semantics for intuitionistic modal logics. As a consequence it can encompass a wider range of intuitionistic modal logics than existing labelled systems. We also show an internal cut elimination proof for our system [30].

7.11. Types by Need

Participants: Beniamino Accattoli, Maico Leberle.

This joint work with Giulio Guerrieri (Post-doc at Bath University) [27] develops a multi type system for call-by-need evaluation of the -calculus. The type system is obtained by combining features by well-known systems for call-by-name and call-by-value. It characterizes termination, and, moreover, its type derivations provide precise information about the number of steps to reach the result. The novelty is that, while the systems for call-by-name and call-by-value are obtained by the linear logic interpretation of these evaluation schemes, call-by-need has no linear logic interpretation.

7.12. Sharing Equality is Linear

Participants: Beniamino Accattoli, Andrea Condoluci, Claudio Sacerdoti Coen.

This work [28] studies how to compare higher-order programs with sharing for sharing equality, that is, for equality of their unshared underlying programs. The point, of course, is to do it efficiently, without unsharing the programs, that would otherwise introduce an exponential blow-up. We develop the first algorithm linear in the size of the shared terms, by adapting the famous Patterson and Wegman algorithm for first-order unification.

7.13. Crumbling Abstract Machines

Participants: Beniamino Accattoli, Andrea Condoluci, Claudio Sacerdoti Coen.

This joint work with Giulio Guerrieri (Post-doc at Bath University) [26] studies a new compilation technique for functional programs, dubbed *crumbling* and resembling the transformation into administrative normal form of Flanagan, Sabry, Duba, and Felleisen. It is shown that it simplifies the design of abstract machines without altering the complexity of the overhead. Moreover, it smoothly scales up to open terms and it does not suffer of the slowdowns of administrative normal forms pointed out by Kennedy.

7.14. Factorization and Normalization, Essentially

Participant: Beniamino Accattoli.

This joint work with Claudia Faggian (CNRS researcher at Paris Diderot) and Giulio Guerrieri (Post-doc at Bath University) [15] refines a rewriting technique for proving factorization and normalization theorems for λ-calculi, that are theorems providing foundations to the design of functional programming languages and proof assistants. We both simplify and extend the scope of a widely used technique by Takahashi. At the concrete level, the new abstract technique is applied to four relevant case studies.

7.15. A Fresh Look at the -Calculus

Participant: Beniamino Accattoli.

This paper [25] is the trace of the invited talk given by Accattoli at FSCD 2019. More than just an abstract, the paper is a lengthy overview of the research on λ-calculus, cost models, sharing, and abstract machines pursued by Accattoli and his co-authors in the last 10 years.

7.16. Abstract Machines for Open Call-by-Value

Participant: Beniamino Accattoli.

This journal paper in collaboration with Giulio Guerrieri (Post-doc at Bath University) [4] outlines a theory of abstract machines for the call-by-value -calculus with open terms. It refines and extends the results by the same authors from 2017, which were among the selected ones from the international conference FSEN 2017 for publication in a journal.

PETRUS Project-Team

6. New Results

6.1. The Security Properties of a PDMS (Axis 1)

Participants: Nicolas Anciaux [correspondent], Luc Bouganim, Philippe Pucheral, Iulian Sandu Popa, Guillaume Scerri.

Different Personal Data Management Systems (PDMS) solutions are emerging in both academia and industry. In terms of functionality and security properties, PDMS solutions differ significantly from traditional Data Base Management Systems (DBMS). In a journal article published in Information Systems this year [3], we take stock of the functionality and security of PDMS solutions, propose five very specific security properties to be achieved and provide a preliminary architecture to meet them based on secure hardware [3]. We also presented as a tutorial at VLDB'19 [4] and a keynote at APVP'19 a review of the literature on database and security on data management issues for secure hardware and new research directions for privacy preserving management of personal data.

6.2. SEP2P and DISPERS (Axis 2)

Participants: Luc Bouganim [correspondent], Julien Loudet, Iulian Sandu Popa.

Personal Data Management Systems (PDMS) arrive at a rapid pace allowing us to integrate all our personal data in a single place and use it for our benefit and for the benefit of the community. This leads to a significant paradigm shift since personal data become massively distributed and opens an important question: how can users/applications execute queries and computations over this massively distributed data in a secure and efficient way, relying exclusively on peer-to-peer (P2P) interactions despite covert adversaries which could be executing the query? We first proposed a Secure and Efficient Peer-to-Peer protocol (SEP2P) to randomly select the nodes that will execute the query. This protocol leverages properties of distributed hash tables (DHT) to select nodes in a way that is, at the same time, secure, random and efficient. The security and randomness stem from the fact that we know, with a very high probability, that at least one honest node contributed to the creation and attestation of this list of nodes; while the efficiency stems from the fact that very few nodes are involved in this process. Building on top of SEP2P, we designed DISPERS, a protocol that applies three design rules: (D1) imposed randomness, enforced by SEP2P, (D2) knowledge dispersion, and (D3) task compartmentalization: Each user provides profile information to indexing nodes, chosen randomly thanks to the DHT (D1). Shamir secret-sharing techniques are used to avoid that any indexing node has a full knowledge of indexed nodes (D2). Then, for each query, a set of random nodes is selected (SEP2P) to coordinate the research for query targets using the indexing nodes. Each of these random nodes learns a part of the query targets IP address but does not know the query (D2, D3). Another set of random nodes is chosen to compute of the final answer based on partial local results from targets. These nodes learn part of the results but do not know the targets, thanks to proxies, nor the meaning of these results (D2, D3). These results are the core of Julien Loudet's thesis [1]. SEP2P was published at EDBT'19 [9] while a demonstration of DISPERS was published at VLDB'19 [8].Both works were also exposed/demonstrated at BDA'19 [13] [12] and APVP'19 [14] for the French research community in databases and security and privacy.

6.3. Manifest-based Framework for Secure Decentralized Queries (Axis 2)

Participants: Riad Ladjel [correspondent], Nicolas Anciaux, Philippe Pucheral, Guillaume Scerri.

The PDMS context calls for a new decentralized way of handling processing. The challenge is to allow generic treatment of large populations of PDMS, with a double objective: to preserve the mutual trust of individuals in their PDMS, and to guarantee an honest result (calculated on the right data, with the right code). To achieve this goal, our approach introduces a computational 'manifest', stipulating its execution plan and the privacy clauses (e.g., collection rules) to be guaranteed at runtime, based on trusted hardware (e.g., Intel SGX processor). Our contributions consist of (1) a protocol for randomly assigning compute tasks to participants to prevent targeted attacks, (2) a mechanism guaranteeing global compute integrity through local-only checks (without centralized trusted third party) and (3) database countermeasures limiting the impact of hidden channel attacks from corrupted participants. These contributions resulted in articles in TrustCom'19 [7] and ISD'19 [6]. Our approach guarantees confidentiality and processing integrity, it is generic and scalable, and goes far beyond existing approaches (e.g., secure multiparty computing or differential privacy).

6.4. Mobile Participatory Sensing with Strong Privacy Guarantees (Axis 2)

Participant: Iulian Sandu Popa [correspondent].

Mobile participatory sensing (MPS) could benefit many application domains. A major domain is smart transportation, with applications such as vehicular traffic monitoring, vehicle routing, or driving behavior analysis. However, MPS's success depends on finding a solution for querying large numbers of smart phones or vehicular systems, which protects user location privacy and works in real-time. This work proposes PAMPAS, a privacy-aware mobile distributed system for efficient data aggregation in MPS. In PAMPAS, mobile devices enhanced with secure hardware, called secure probes (SPs), perform distributed query processing, while preventing users from accessing other users' data. A supporting server infrastructure (SSI) coordinates the inter-SP communication and the computation tasks executed on SPs. PAMPAS ensures that SSI cannot link the location reported by SPs to the user identities even if SSI has additional background information. Moreover, an enhanced version of the protocol, named PAMPAS$^+$, makes the system robust even against advanced hardware attacks on the SPs. Hence, the risk of user location privacy leakage remains very low even for an attacker controlling the SSI and a few corrupted SPs. Our experimental results demonstrate that these protocols work efficiently on resource constrained SPs being able to collect the data, aggregate them, and share statistics or derive models in real-time. This work has been accomplished in collaboration with NJIT and DePaul University and has been recently accepted as a journal paper (an 'Online first' version is available at https://link.springer.com/article/10.1007/s10707-019-00389-4).

6.5. Empowerment and Big Data on Personal Data: from Portability to Agency (Axis 3)

Participants: Nicolas Anciaux [correspondent], Riad Ladjel, Philippe Pucheral, Guillaume Scerri.

The current highly centralised model of personal data management is based on established business practices that have led to widespread adoption, in contrast to user-centric and privacy-oriented systems such as PDMS, which therefore need to be studied in terms of technical, economic and legal feasibility and adoptability with researchers from other disciplines. In the context of the DATAIA GDP-ERE project, we are analyzing the technical and legal conditions under which individuals can exercise their right to data portability. Over the period, we have jointly studied a new notion that characterizes the true power of the individual over his or her personal data: agency. In particular, we have shown how the notion of agency, which comes from the social sciences, can be transposed and used to our context to measure the empowerment of individuals in Big Data applications. This study led to two joint publications with law researchers over the period, in particular in the journal Dalloz IP/IT [5], as well as several international panels (see in Section Popularization, e.g., panel at BDVA forum organized in Helsinky with the European Commission, at the Annual Forum of Trans Europ Expert, etc.)

6.6. OwnCare Inria Inovation Lab

Participants: Philippe Pucheral [correspondent], Nicolas Anciaux, Luc Bouganim, Laurent Schneider.

The OwnCare IILab was created in January 2018 (see section: Bilateral Contracts with Industry) and involves the Hippocad SME and the PETRUS team around the management of medical-social data at patient's home. The objective is to build a fully decentralized and highly secure personal medical-social folder based on PlugDB, and deploy it at large scale. Besides this industrial objective, the goal is also to leverage and validate the PETRUS research contributions related to secured Personal Cloud architectures. Before the creation of the OwnCare IILab initiative, PlugDB was an advanced research prototype. It is now evolving towards a transferable product. To reach this state, a considerable effort has been made in terms of development, testing platform, validation procedures and documentation. PlugDB engine is regularly registered at APP (Agence de Protection des Programmes), for both the PlugDB hardware datasheets and the code of the PlugDB-engine. The next PlugDB code registration will cover all functionalities added since the beginning of the IILab, notably: dynamic upgrade of the embedded code, TPM-based secure boot, ad-hoc embedded stored procedures, RBAC-style access control model, aggregate computation, SSL certificate management, event/error logging mechanism. Some of these developments are highly challenging considering the embedded context and the energy consumption constraints we have to face (the current device hosting PlugDB is based on two microcontrollers – MCU – powered by small batteries). Typically, we had to implement the first coupling between a TPM and a STM MCU, a lightweight version of SSL that accommodates MCU resources and energy-saving synchronization protocols between 2 MCU.

POEMS Project-Team

6. New Results

6.1. Complex ordered and disordered media

There is a need of a better understanding of wave phenomena in complex media. From a physical point of view, a *complex medium* is typically a material where the propagation of the waves may be *anisotropic* and *dispersive*. These properties are generally the effect of a microstructure, that can be ordered (in e.g. photonic crystals), or disordered (light in the atmosphere, seismic waves). From a mathematical point of view, one can take into account exactly this microstructure or, at sufficiently low frequency, use effective models justified by the *homogenization theory*.

6.1.1. Enriched homogenized model in presence of boundaries for time harmonic and time dependent wave equations

Participants: Clément Bénéteau, Sonia Fliss.

We study the wave equation set in a periodic half-space when the period is small compared to the wave length. The classical homogenization theory enables to derive an effective model which provides an approximation of the solution. However it is well known that these models are not accurate near the boundaries. In this work, we propose an enriched asymptotic expansion which enables to derive high order effective models at order 1 and 2. Let us mention that the model of order 2 is particularly relevant when one is interested in the long time behaviour of the solution of the time-dependent wave equation. Indeed, it is well-known that the classical homogenized model does not capture the long time dispersion of the exact solution. In several works, homogenized models of order 2 are proposed for the wave equation in infinite domains. Dealing with boundaries and proposing boundary conditions for these models of order 2 were open questions. Our approach enables to propose appropriate and accurate boundary conditions for these models. This work is the fruit of a long time collaboration with Xavier Claeys (LJLL, Sorbonne University) and a recent one with Timothée Pouchon (EPFL).

6.1.2. Interface homogenization

Participant: Jean-François Mercier.

In collaboration with Agnès Maurel from Institut Langevin and Kim Pham from the Department of Mechanics at ENSTA, we have developped interface effective models to describe acoustics and electromagnetic propagation through a scatterers array. The effective models are based on matched asymptotic expansions to account for the small thickness of the array. They consist of determined interface parameters involved in jump conditions for the fields.

1- In acoustics

- Perfect absorption using sparse arrays of Helmholtz resonators

Thanks to an effective model derived to describe a periodic arrangement of Helmholtz resonators, the influence of the spacing on the resonance has been inspected. The strength of the resonance is found enhanced when the array becomes sparser, which provides a degree of freedom to control the radiative damping of the array without affecting the losses within each resonator. It has been used to design a perfect absorbing wall.

- Scattering by arrays of open ended resonators

The previous study has been extended to cavities open at both ends. The effective model provides explicit expressions of the reflection and transmission coefficients, used to provide the relations required to produce zero reflection situation.

- Effective transmission conditions across a resonant bubbly metascreen

The extension to resonant obstacles has been considered with the study of the acoustic propagation through a thin bubbly screen. The analysis is conducted in the time domain and preserves the non linear response of the bubbles. It provides an effective model involving a jump of the normal velocity coupled to an equation of the Rayleigh-Plesset's type for the bubble radius.

2- In electromagnetism

- Perfect Brewster transmission by ultrathin perforated films

The scattering properties of an ultrathin perforated film, made of a material dielectric or perfectly conducting have been studied. Thanks to an asymptotic interface model, the Brewster incidence realizing perfect transmission is accurately described and is found to be significantly shifted from its classical value when the thickness of the film becomes subwavelength.

- Effective transmission conditions for an array of locally resonant inclusions

The previous study has been extended to resonant inclusions of the Mie type. Among the interface parameters involved in the effective model, one is frequency dependent and encapsulates the resonant behavior of the inclusions. Our effective model is validated by comparison with results of full wave calculations.

6.1.3. Wave equation in a weakly randomly perturbed periodic medium

Participants: Sonia Fliss, Laure Giovangigli.

The aim of this work, which is at its first stage, is to construct numerical approximations of the solution of the wave equation in weakly randomly perturbed periodic media in order to propose transparent boundary conditions. We start by studying the effects of rare random perturbations of the medium. The perturbation is weak in the sense that it happens rarely but when it happens the correction is of the order of the initial coefficient. More precisely, we consider the solution of the time harmonic wave equation in a one-dimensional periodic medium, in which each period have a probability η to have its coefficients modified, independently of the other periods. We derive an asymptotic expansion of the distribution of the solution u_η with respect to η and illustrate the convergence with numerical simulations. We also exhibit and implement approximated transparent boundary conditions for such a medium. We then extend the results to more general rare random perturbations. Currently, we are studying other random perturbations of periodic media such as a deformation by a random diffeomorphism with a stationary gradient.

6.1.4. Guided modes in a hexagonal periodic graph-like domain: the zigzag and the armchair cases

Participant: Sonia Fliss.

In this work, we study the wave propagation in hexagonal periodic media that are close to a graph domain. By using an asymptotic analysis, we exhibit situations where the introduction of lineic defects into the geometry of the domain leads to the appearance of guided modes and we show that the direction of the defect leads to very different properties of the guided modes. This work is done in collaboration with Bérangère Delourme (LAGA, Paris 13).

6.1.5. Stable perfectly matched layers for a class of anisotropic dispersive models

Participants: Eliane Bécache, Maryna Kachanovska.

We consider wave propagation in 2D anisotropic dispersive media in an unbounded domain described by Maxwell's equations with an antisymmetric dielectric permittivity tensor and scalar magnetic permeability. Bounding the computational domain is required to obtain the solution. In order to do so, we use the perfectly matched layer (PML) technique. However, the PMLs exhibit instabilities connected to the presence of backward propagating waves. This work is dedicated to stabilizing the PMLs for this case.

6.1.6. Frequency domain wave propagation in anisotropic metamaterials

Participants: Patrick Ciarlet, Maryna Kachanovska.

In this work we address the question of theoretical justification of problems arising in the wave propagation in hyperbolic metamaterials. Such phenomena are described by anisotropic, dispersive Maxwell equations, which, in the frequency domain, correspond to a problem that is hyperbolic for a range of frequencies. For a particular case of such materials (highly magnetized plasmas), we prove the well-posedness of the corresponding model in the free space, providing a suitable radiation condition, as well as study its regularity and demonstrate the limiting amplitude and limiting absorption principles.

6.1.7. On the analysis of perfectly matched layers for electromagnetic waves propagation in anisotropic media

Participants: Eliane Bécache, Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss, Maryna Kachanovska, Maria Kazakova.

This work consists of two parts. The first part is dedicated to the analysis of Cartesian Perfectly Matched Layers (PMLs) in the context of electromagnetic wave propagation in a 3D infinite anisotropic homogeneous medium with a diagonal dielectric tensor. Contrary to the 2D case some anisotropies lead to the existence of backward waves giving rise to instabilities of the PMLs in the time-domain and a lack of convergence in the frequency domain.

The second part examines the behaviour of the PMLs in the frequency domain in the case when in the time domain they give a rise to instabilities. This is the case e.g. for the 2D anisotropic wave equation. For this particular problem, we demonstrate that it is possible to choose the parameters of the PMLs (i.e. the configuration of the PML bounding box and the absorption parameter) to ensure the convergence of the PMLs in the frequency domain.

6.1.8. Maxwell's equations in presence of a conical tip with negative electromagnetic constants

Participants: Anne-Sophie Bonnet-Ben Dhia, Mahran Rihani.

This work is done in collaboration with Lucas Chesnel from CMAP at Ecole Polytechnique. We are interested in the analysis of time-harmonic Maxwell's equations in presence of a conical tip of a material with negative dielectric constants. When these constants belong to some critical range, the electromagnetic field exhibits strongly oscillating singularities at the tip which have infinite energy. In the 2D case of a wedge with critical electromagnetic constants, it has been proved for the equivalent scalar problems that well-posedness in the classical H^1 framework is lost. Well-posedness can be recovered (in a non standard framework) by working in weighted Sobolev spaces and adding in the space the outgoing propagating singularity. We have shown how to provide such functional framework for 3D Maxwell's equations, when only the dielectric permittivity (but not the magnetic permeability) takes a critical value

6.1.9. Essential spectrum related to an interface with a negative material

Participants: Christophe Hazard, Sandrine Paolantoni.

The studies carried out in recent years about the spectral effects of an interface between vacuum and a negative material (that is, a dispersive material whose electric permittivity and magnetic permeability become negative in some frequency range) have been continued in two directions. On the one hand, the previous theoretical studies only considered the non dissipative Drude model. We showed in particular that the interface is responsible for various resonance phenomena related to various components of an essential spectrum. We have extended these results to the so-called Lorentz model (dissipative or not). On the other hand, we have explored the numerical approximation of the spectrum of a cavity partially filled with a Drude material by considering a two-dimensional scalar problem. We have investigated the numerical simulation of the three resonance phenomena associated to the essential spectrum of the cavity.

6.1.10. Computation of plasmon resonances localized at corners using frequency-dependent complex scaling

Participants: Anne-Sophie Bonnet-Ben Dhia, Christophe Hazard, Florian Monteghetti.

A plasmonic device with a non-smooth boundary can exhibit strongly-oscillating surface waves whose phase velocities vanish as they reach the corners. This work investigates in the quasi-static limit the existence of corner resonances, which are analogous to scattering resonances in the sense that the local behavior at each corner plays the role of the behavior at infinity. Resonant contrasts are sought as eigenvalues of the transmission problem with complex scaling applied at corners.

6.1.11. Towards non-local interface models

Participant: Patrick Ciarlet.

Collaboration with Juan Pablo Borthagaray (DMEL, Universidad de la República, Salto, Uruguay). Consider the equation $\mathrm{div}(\sigma\nabla u) = f$ in Ω (plus boundary conditions), where the diffusivity is piecewise constant, and equals σ_i in Ω_i ($i = \{1,2\}$), with $\overline{\Omega_1} \cup \overline{\Omega_2} = \overline{\Omega}$ and $\Omega_1 \cap \Omega_2 = \varnothing$. If σ_1 and σ_2 have different sign, well-posedness in $H^1(\Omega)$ may not hold. This occurs when the ratio σ_2/σ_1 belongs to the so-called *critical interval*. When the interface has a corner, we have observed that this critical interval is shrunk if one replaces the standard H^1-bilinear forms by corresponding H^s-forms ($s \in (0,1)$). However, the expense of computing the nonlocal interactions may be prohibitive in applications. Thus, our long term goal is to confine the non-local model to a neighborhood of the interface, while keeping the standard local model in the rest of the domain. A first step in this direction consists in considering the numerical solution of the fractional Laplacian of index $s \in (1/2, 1)$ in a bounded domain Ω with homogeneous Dirichlet boundary conditions. Its solution a priori belongs to the fractional order Sobolev space $\widetilde{H}^s(\Omega)$. Under suitable assumptions on the data, its solution is also in $H^1(\Omega)$. In this case, if one uses the standard Lagrange finite element to discretize the problem, then both the exact and the computed solution belong to $H^1(\Omega)$. We show how to derive error estimates for the Lagrange finite element solutions on both quasi-uniform and graded meshes.

6.1.12. Perturbed edge finite element method for the simulation of electromagnetic waves in magnetised plasmas

Participants: Damien Chicaud, Patrick Ciarlet, Axel Modave.

Numerical simulation of electromagnetic waves in magnetised plasmas is a challenging topic. We address the finite element solution of a time-harmonic model. With the classical method, the variational formulation has a poor coercivity which leads to an ill-conditioned numerical system and numerical instabilities. We propose a perturbed formulation to improve the conditioning of the system. Promising preliminary numerical results have been obtained.

6.1.13. Resonant wave problems in plasmas

Participant: Patrick Ciarlet.

Collaboration with Martin Campos Pinto, Bruno Després and Anouk Nicolopoulos (LJLL, Sorbonne Université). The modelling of resonant waves in 2D plasma leads to the coupling of two degenerate elliptic equations. The model is set over two regions, and involves a smooth, sign-changing coefficient α. The region where $\{\alpha > 0\}$ is propagative, while the region where $\{\alpha < 0\}$ is non propagative, and elliptic. The two models are coupled through the line $\Sigma = \{\alpha = 0\}$. Generically, it is an ill-posed problem, and additional information must be introduced to get a satisfactory treatment at Σ. We define the solution by relying on the limiting absorption principle (the coefficient α is replaced by $\alpha + i0^+$) in an adapted functional setting. This approach relies on the decomposition of the solution in a regular and a singular part, which originates at Σ, and on quasi-solutions. It yields a well-posed mixed variational formulation with coupling. After the design of explicit quasi-solutions, numerical experiments can be carried out, which illustrate the nice properties of this new tool.

6.2. Towards realistic configurations : waveguides and fractals domains

To simulate realistic wave problems, devices which raise specific difficulties concerning either the modeling, the mathematical analysis or the numerical simulation. We start with propagation in *waveguides*, that is a longtime research field within our team, which has acquired an international visibility in this context. We continue with a more recent topic, propagation in *fractal* domains, motivated by a medical application (the human lung).

6.2.1. Transparent boundary conditions for periodic waveguides: analysis and extensions

Participants: Sonia Fliss, Patrick Joly.

We consider the time harmonic wave equation in perturbed periodic waveguides. We justify rigorously the construction of the transparent boundary conditions based on Dirichlet-to-Neumann map and show that the problem with these transparent boundary conditions is of Fredholm type except for a countable set of frequencies. This allows to define and compute the physical solution of the problem. This approach can be applied to deal with junctions of different periodic closed waveguides. We want now to study the extension of the method to the diffraction by locally perturbed periodic layers, surfaces or halfspaces. This work is done in collaboration with Vincent Lescarret (LSS, Centrale Supélec).

6.2.2. Invisible floating objects

Participant: Mahran Rihani.

This work is done in collaboration with Lucas Chesnel from CMAP at Ecole Polytechnique. We consider a time-harmonic water waves problem in a 2D waveguide. The geometry is symmetric with respect to an axis orthogonal to the direction of propagation of waves. Moreover, the waveguide contains two floating obstacles separated by a distance L. We study the behaviours of the scattering coefficients as L goes to ∞. From this analysis, we exhibit situations of non reflectivity or perfect invisibility.

6.2.3. A multi-trace integral equation on infinite boundaries when a global Green's function is not available

Participants: Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss, Yohanes Tjandrawidjaja.

We are interested in time-harmonic scattering problems for configurations where the Green's function is not easily computable for the exterior domain, but different Green's functions are available in several unbounded subdomains covering the whole space. This arises typically for junctions of open waveguides. For a model problem, by using integral representations of the solution in each subdomain, we propose a formulation coupling the traces and the normal traces of the solution on infinite boundaries. The system of equations is shown to have a unique solution in the dissipative case.

6.2.4. Error analysis for transparent boundary conditions in fractal trees

Participants: Patrick Joly, Maryna Kachanovska.

This work is dedicated to an efficient resolution of the wave equation in fractal trees (with application to wave propagation in a human lung). Thanks to self-similarity, it is possible to avoid computing the solution at deeper levels of the tree by using transparent boundary conditions. The corresponding DtN operator is defined by a functional equation for its symbol. in the frequency domain. In this work, we analyse an approximate transparent condition, cf. Waves 2017, based on rational approximation of the symbol. The error and complexity analysis relies on Weyl-like estimates of eigenvalues of the weighted Laplacian and related eigenfunctions.

6.3. Direct and inverse methods for imaging and identification

Imaging and identification, when involved in a real-life context, are often based on wave propagation. This is due to the fact that a substantial part of the information contained in waves can propagate across long distances without significant attenuation. This activity is partly developed in the framework of a long-term partnership with a group of CEA-List in charge of the Non Destructive Testing (NDT) of industrial structures. The aim of NDT is to detect defects inside a structure by imposing some incident waves and measuring the scattered waves caused by the presence of such defects.

6.3.1. The complex-scaled Halfspace Matching Method

Participants: Anne-Sophie Bonnet-Ben Dhia, Christophe Hazard, Sonia Fliss, Yohanes Tjandrawidjaja.

We are currently developing a method that we call the Half-Space Matching (HSM) method, to solve scattering problems in unbounded domains, when classical approaches are either not applicable or too expensive. This method is based on an explicit expression of the "outgoing" solution of the problem in half-spaces, by using Fourier, generalized Fourier or Floquet transforms when the background is respectively homogeneous (possibly anisotropic), stratified or periodic. The domain exterior to a bounded region enclosing the scatterers is recovered by a finite number of halfspaces (at least 3). The unknowns of the formulations are the restriction of the solution to the bounded region and the traces of the solution on the boundary of the halfspaces. The system of equations is derived by writing compatibility conditions between the different representations of the solution. Although the HSM method works in the non-dissipative case, the theoretical and the numerical analysis of the method has been done only in the dissipative case. In the present work, we propose, for the simple case of a homogeneous background, a new formulation of the method which is well-suited for the theoretical and numerical analysis of the non dissipative case. In the spirit of PMLs, the idea is to replace the system of equations on the traces by similar equations on exponentially decaying analytical extensions of the traces.

6.3.2. Implicit-explicit scheme for elastodynamic equations in plates

Participants: Sonia Fliss, Hajer Methenni.

Our objective is to provide an efficient simulation tool for the propagation of elastic waves in thin plates in the context of Guided Waves based Structural Health Monitoring. A naive discretization procedure based on a Leap-frog explicit scheme can be really costly because of the small thickness of the plate. By treating implicitly the operators corresponding to derivatives through the thickness, we show by a stability analysis that the time step is less restricted by the space discretization along the thickness. The price to pay is to solve at each iteration small independent linear systems, but this strategy offers an accurate and efficient discretization of the elastic fields in all dimensions. This method can be used to compute reference solutions and verify the validity of asymptotic models such as Reissner–Mindlin model and some extensions (since there exists no rigorous justifications for elastodynamic problems). Finally under some conditions on the mesh, our approach can be extended to plates with a smoothly varying thickness.

This work is done in collaboration with Sebastien Imperiale (Inria EPI M3DISIM) and Alexandre Imperiale (CEA-LIST).

6.3.3. Forward and inverse scattering in Kirchhoff plates

Participants: Laurent Bourgeois, Christophe Hazard.

A new activity has just started concerning forward and inverse scattering in thin plates governed by the simple Kirchhoff-Love model. The analysis is restricted to the purely bending case and the time-harmonic regime.

We have first considered a 2D strip, that is a waveguide which is unbounded in one direction and bounded in the other (transverse) direction. Two types of conditions on the boundary of the strip are addressed : either the strip is simply supported or the strip is clamped. The two boundary conditions are treated with two different methods. For the simply supported problem, the analysis is based on a result of Hilbert basis in the transverse section. For the clamped problem, this property does not hold. Instead we adopt the Kondratiev's approach, based on the use of the Fourier transform in the unbounded direction, together with techniques of weighted Sobolev spaces with detached asymptotics. After introducing radiation conditions, the corresponding scattering problems in the presence of a free obstacle are shown to be well-posed in the Fredholm sense. We also show that the solutions are the physical (outgoing) solutions in the sense of the limiting absorption principle. This is a joint work Lucas Chesnel, from Inria/DEFI.

We have then addressed the same kind of forward scattering problems for various impenetrable obstacles in an infinite plate. Considering four types of boundary conditions on the obstacle, well-posedness for those problems is proved with the help of a variational approach: (i) for any wave number k when the plate is clamped, simply supported or roller supported; (ii) for any k except a discrete set when the plate is free (this set is finite for convex obstacles). It is then natural to tackle the inverse problem of identifying impenetrable obstacles in a Kirchhoff-Love infinite plate from multistatic near-field data. The Linear Sampling Method is introduced in this context. We firstly prove a uniqueness result for such an inverse problem. We secondly provide the classical theoretical foundation of the Linear Sampling Method. We lastly show the feasibility of the method with the help of numerical experiments. The inverse problem is a joint work with Arnaud Recoquillay, from CEA/LIST.

6.3.4. About regularity and error estimates for the quasi-reversibility method

Participant: Laurent Bourgeois.

This work is done on collaboration with Lucas Chesnel (EPC DEFI). We are interested in the classical ill-posed Cauchy problem for the Laplace equation. One method to approximate the solution associated with compatible data consists in considering a family of regularized well-posed problems depending on a small parameter $\varepsilon > 0$. In this context, in order to prove convergence of finite elements methods, it is necessary to get regularity results of the solutions to these regularized problems which hold uniformly in ε. In the present work, we obtain these results in smooth domains and in 2D polygonal geometries. In the presence of corners, due to the particular structure of the regularized problems, classical techniques *à la* Grisvard do not work and instead, we apply the Kondratiev approach. We describe the procedure in detail to keep track of the dependence in ε in all the estimates. The main originality of this study lies in the fact that the limit problem is ill-posed in any framework.

6.3.5. Analysis of topological derivative as a means for qualitative identification

Participant: Marc Bonnet.

This work is done on collaboration with Fioralba Cakoni, Rutgers University, USA. The concept of topological derivative (TD) has proved effective as a qualitative inversion tool for a wave-based identification of finite-sized objects. Although for the most part, this approach remains based on a heuristic interpretation of the TD, a first attempt toward its mathematical justification was done in Bellis et al. (*Inverse Problems***29**:075012, 2013) for the case of isotropic media with far field data and inhomogeneous refraction index. This work extends the analysis there to the case of anisotropic scatterers and background with near field data. TD-based imaging functional is analyzed using a suitable factorization of the near fields. Our results include justification of sign heuristics for the TD in the isotropic case with jump in the main operator and for some cases of anisotropic media, as well as verifying its decaying property in the isotropic case with near field spherical measurements configuration situated far enough from the probing region.

6.3.6. Asymptotic model for elastodynamic scattering by a small surface-breaking defect

Participant: Marc Bonnet.

This work is done in collaboration with Marc Deschamps and Eric Ducasse, I2M, Bordeaux.

We establish a leading-order asymptotic model for the scattering of elastodynamic fields by small surface-breaking defects in elastic solids. The asymptotic form of the representation formula of the scattered field is written in terms of the elastodynamic Green's tensor, which is in fact available in semi-analytical form for some geometrical configurations that are of practical interest in ultrasonic NDT configurations. Preliminary numerical examples have been performed on cylindrical elastic pipes with small indentations on the outer surface.

6.3.7. Shape optimization of stokesian peristaltic pumps using boundary integral methods

Participant: Marc Bonnet.

This work is done in collaboration with with Ruowen Liu and Shravan Veerapaneni, University of Michigan, USA.

This work develops a new boundary integral approach for finding optimal shapes of peristaltic pumps that transport a viscous fluid. Formulas for computing the shape derivatives of the standard cost functionals and constraints, expressed in boundary-only form, are derived. They involve evaluating physical variables (traction, pressure, etc.) on the boundary only. By employing these formulas in conjunction with a boundary integral approach for solving forward and adjoint problems, we completely avoid the issue of volume remeshing when updating the pump shape as the optimization proceeds. This leads to significant cost savings and we demonstrate the performance on several numerical examples.

6.4. Accelerated numerical solvers for large-scale wave problems

Fast solution procedures are of critical importance for industrial applications such as non-destructive testing, electromagnetic compatibility testing and seismic risk assessment. In these examples, the wavelength is very small in comparison to the characteristic length of the problems, which leads to extremely expensive numerical procedures if standard methods are used. To address the fast numerical solution of large-scale waves problems, we work at the same time on numerical methods, algorithmic issues and implementation strategies to speed up solvers.

6.4.1. Non-overlapping Domain Decomposition Method (DDM) using non-local transmission operators for wave propagation problems.

Participants: Patrick Joly, Emile Parolin.

The research in this direction was mainly concerned by the extension to the electromagnetic setting of the linear convergence theory of non-overlapping DDM that relies on non-local transmission operators. The principal task was to propose, analyse and implement some candidate non-local operators satisfying the assumptions of the theory. There were two main propositions:

- Integral operator for the electromagnetic setting: the operator is available in closed form and its structure lead naturally to a localizable form via truncation of the kernel to limit the effective computational cost while retaining its good properties. The construction of such an operator turned out to be somewhat difficult due to the particular functional setting of Maxwell's equations.
- DtN based non-local operator: the operator is computed by solving auxiliary coercive problems in the vicinity of the transmission interface. The computational cost remains moderate as the implementation no longer involve dense matrix blocks from the integral operators but rather lead to augmented sparse linear systems. Initially developed for the electromagnetic setting, the approach is appealing as it provided a unified formalism that can be applied both to Helmholtz and Maxwell equations and proved to be efficient in numerical experiments.

Another important research direction is created by the technical and theoretical difficulty posed by junction points, which are points where three or more sub-domains abut. Xavier Claeys recently proposed a method to deal with this specific issue, based on the multi-trace formalism, which led to a joint collaboration on the subject. The main idea is to perform a global exchange operation, on the whole skeleton, rather than a local point-to-point exchange. The preliminary numerical results recently obtained are promising.

6.4.2. An efficient domain decomposition method with cross-point treatment for Helmholtz problems

Participant: Axel Modave.

This is a collaboration with X. Antoine (IECL, Nancy), A. Royer (ULiège) and C. Geuzaine (ULiège). The parallel finite-element solution of large-scale time-harmonic scattering problems is addressed with a non-overlapping domain decomposition method (DDM). It is well known that the efficiency of this method strongly depends on the transmission condition enforced on the interfaces between the subdomains. Local conditions based on high-order absorbing boundary conditions (HABCs) are well suited for configurations without cross points *(where more than two subdomains meet)*. In this work, we extend this approach to efficiently deal with cross points. Two-dimensional finite-element results are presented.

6.4.3. Modelling the fluid-structure coupling caused by a far-field underwater explosion using a convolution quadrature based fast boundary element method.

Participants: Marc Bonnet, Stéphanie Chaillat, Damien Mavaleix-Marchessoux.

This study is done in collaboration with Bruno Leblé (Naval Group). It aims at developing computational strategies for modelling the impact of a far-field underwater explosion shock wave on a structure, in deep water. An iterative fluid-structure coupling is developed to solve the problem. Two complementary methods are used: the Finite Element Method (FEM), that offers a wide range of tools to compute the structure response; and the Boundary Element Method (BEM), more suitable to deal with large surrounding fluid domains. We concentrate on developing (i) a fast transient BEM procedure and (ii) a transient FEM-BEM coupling algorithm. The fast transient BEM is based on a fast multipole-accelerated Laplace-domain BEM (implemented in the in-house code COFFEE), extended to the time domain by the Convolution Quadrature Method (CQM). In particular, using empirical approximations for the solution of integral problems involving large (complex) frequencies has been found to yield satisfactorily accurate solutions while saving significant amounts of computational work. The transient BEM-FEM coupling (under progress) will be based on a block-SOR iterative approach, for which a preliminary investigation shows the existence of relaxation parameters that ensure convergence.

6.4.4. Asymptotic based methods for very high frequency problems.

Participant: Eric Lunéville.

This research is developed in collaboration with Marc Lenoir and Daniel Bouche (CEA).

It has recently been realized that the combination of integral and asymptotic methods was a remarkable and necessary tool to solve scattering problems, in the case where the frequency is high and the geometry must be finely taken into account.

In order to implement the high-frequency approximations that we are developing as part of these hybrid HF/BF methods, we have introduced new geometric tools into the XLiFE++ library, in particular splines and B-Splines approximations as well as parameterizations to access quantities such as curvature, curvilinear abscissa, etc. We have also started to interface the OpenCascad library to the XLiFE++ library, which will eventually allow us to manage more complex geometric situations (cylinder and sphere intersection for example). In parallel, we have completed the implementation of 2D HF approximations in the shadow-light transition zone based on the Fock function. Diffraction by a 2D corner is in progress.

RANDOPT Project-Team

7. New Results

7.1. A multiobjective algorithm framework and the COMO-CMA-ES algorithm

One classical way to solve multiobjective optimization problems is to transform the multiple objective functions into a single one, also known as scalarization, and to solve multiple versions of such scalarizations to achieve multiple trade-off points. Another approach, coming from the field of evolutionary multiobjective optimization is to formulate a single-objective *set* problem via indicators: the goal here is to find the set of solutions (of a given size) that maximizes a certain quality. The hypervolume indicator has been regularly used to define the quality of the solution set because it has favorable theoretical properties.

The "classical" definition of the hypervolume indicator and how it is used in multiobjective solvers, however, has some disadvantages: (i) the resulting single-objective problem is of high dimension and the gradient of the hypervolume indicator is zero in dominated areas of the search space—not giving a solver enough information about where to search for good solutions. In [7], we discussed and visualized these disadvantages and proposed a new quality criterion which is based on the hypervolume indicator but solves the mentioned disadvantages. The implementation of this idea and its combination with the single-objective solver CMA-ES resulted in the COMO-CMA-ES which shows improved performance over several existing multiobjective solvers on a wide range of convex quadratic functions.

7.2. A mixed-integer benchmark testbed for single and multiobjective black-box optimization

We have introduced two suites of mixed-integer benchmark problems to be used for analyzing and comparing black-box optimization algorithms. They contain problems of diverse difficulties that are scalable in the number of decision variables. The bbob-mixint suite is designed by partially discretizing the established BBOB (Black-Box Optimization Benchmarking) problems. The bi-objective problems from the bbob-biobj-mixint suite are, on the other hand, constructed by using the bbob-mixint functions as their separate objectives. We explain the rationale behind our design decisions and show how to use the suites within the COCO (Comparing Continuous Optimizers) platform. Analyzing two chosen functions in more detail, we also provide some unexpected findings about their properties [8].

7.3. A large-scale optimization testbed for the COCO framework

We have finalized a large scale testbed built to model well-known difficulties in continuous optimization and to test the scaling behavior of algorithms. It contrasts with current test suites used for benchmarking solvers.

The test suite contains 24 single-objective functions in continuous domain and extends the well-known single-objective noiseless bbob test suite. A core contribution is to reduce the computational demand of the orthogonal search space transformations, that appear in the bbob test suite, while retaining some desired properties using previously introduced permuted block diagonal orthogonal matrices.

The paper discusses the implementation details, particularly the normalization and scaling to obtain backwards compatibility with the bbob test suite. Additionally, a guide for using the test suite within the COCO platform, as well as a description of the postprocessed output is presented [12].

7.4. Diagonal Acceleration for Covariance Matrix Adaptation Evolution Strategies

In [1], we have introduced an acceleration for the covariance matrix adaptation evolution strategies (CMA-ES) by means of adaptive diagonal decoding (dd-CMA). This diagonal acceleration endows the default CMA-ES with the advantages of separable CMA-ES without inheriting its drawbacks. Technically, we introduce a diagonal matrix that expresses coordinate-wise variances of the sampling distribution. The diagonal matrix can learn a rescaling of the problem in the coordinates within linear number of function evaluations. Diagonal decoding can also exploit separability of the problem, but, crucially, does not compromise the performance on non-separable problems. The latter is accomplished by modulating the learning rate for the diagonal matrix based on the condition number of the underlying correlation matrix. dd-CMA-ES not only combines the advantages of default and separable CMA-ES, but may achieve overadditive speedup: it improves the performance, and even the scaling, of the better of default and separable CMA-ES on classes of non-separable test functions that reflect, arguably, a landscape feature commonly observed in practice. The paper makes two further secondary contributions: we introduce two different approaches to guarantee positive definiteness of the covariance matrix with active CMA, which is valuable in particular with large population size; we revise the default parameter setting in CMA-ES, proposing accelerated settings in particular for large dimension. All our contributions can be viewed as independent improvements of CMA-ES, yet they are also complementary and can be seamlessly combined. In numerical experiments with dd-CMA-ES up to dimension 5120, we observe remarkable improvements over the original covariance matrix adaptation on functions with coordinate-wise ill-conditioning. The improvement is observed also for large population sizes up to about dimension squared.

7.5. A global surrogate assisted CMA-ES

In the paper [5], we have explored the arguably simplest way to build an effective surrogate fitness model in continuous search spaces. The model complexity is linear or diagonal-quadratic or full quadratic, depending on the number of available data. The model parameters are computed from the Moore-Penrose pseudoinverse. The model is used as a surrogate fitness for CMA-ES if the rank correlation between true fitness and surrogate value of recently sampled data points is high. Otherwise, further samples from the current population are successively added as data to the model. We empirically compare the IPOP scheme of the new model assisted lq-CMA-ES with a variety of previously proposed methods and with a simple portfolio algorithm using SLSQP and CMA-ES. We conclude that a global quadratic model and a simple portfolio algorithm are viable options to enhance CMA-ES. The model building code is available as part of the pycma Python module on Github and PyPI.

7.6. Benchmarking and Understanding Optimizers

Benchmarking is an important task in optimization in order to understand the working principles behind existing solvers, to find out about weaknesses of them and to finally recommend good ones. The COCO platform, developed in the Randopt team since 2007, aims at automatizing these numerical benchmarking experiments and the visual presentation of their results. We regularly use the platform to initiate workshop papers during the ACM-GECCO conference and also held a workshop this year [0].

In this context, several workshop papers have been published by members of the team and we also proposed some extensions of the platform and updated its documentation.

Two papers addressed single-objective unconstrained problems. One paper investigated the impact of the sample volume of a simple random search on the bbob test suite of COCO [2] and the other paper benchmarked all solvers available in the scipy.optimize module of Python [9], re-discovering SLSQP as a very well-performing solver for small budgets.

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[0] See numbbo.github.io/workshops/BBOB-2019/

Two additional papers addressed multiobjective problems in the context of the bbob-biobj test suite of COCO: “Benchmarking Algorithms from the platypus Framework on the Biobjective bbob-biobj Testbed” [3] compared several baseline algorithms from the literature such as NSGA-II, MOEA/D, SPEA2, and IBEA and “Benchmarking MO-CMA-ES and COMO-CMA-ES on the Bi-objective bbob-biobj Testbed” [4] compared our new COMO-CMA-ES solver with its previous version MO-CMA-ES.

As to extensions of the COCO platform, we released new test suites this year as described earlier. For the large-scale test suite of [12], 11 algorithm variants of the CMA-ES and L-BFGS solvers have been compared in the paper “Benchmarking Large Scale Variants of CMA-ES and L-BFGS-B on the bbob-largescale Testbed” [10].

Overall, we collected 54 new algorithm data sets within the COCO platform in 2019—the highest number in a single year since the release of COCO.

Finally, we updated our documentation on the biobjective test suite, we introduced in 2019. The corresponding journal paper “Using Well-Understood Single-Objective Functions in Multiobjective Black-Box Optimization Test Suites” [11] is now under revision for the Evolutionary Computation journal.

SPECFUN Project-Team

6. New Results

6.1. Becker's conjecture on Mahler functions

In 1994, Becker conjectured that if $F(z)$ is a k-regular power series, then there exists a k-regular rational function $R(z)$ such that $F(z)/R(z)$ satisfies a Mahler-type functional equation with polynomial coefficients, whose trailing coefficient (i.e., of order 0) is 1. In [2], Frédéric Chyzak and Philippe Dumas, together with Jason P. Bell (University of Waterloo, Canada) and Michael Coons (University of Newcastle, Australia) have proved Becker's conjecture in the best-possible form: they have shown that the rational function $R(z)$ can be taken to be a polynomial $z^{\gamma}Q(z)$ for some explicit non-negative integer γ and such that $1/Q(z)$ is k-regular. The article was published this year.

6.2. Fast coefficient computation for algebraic power series in positive characteristic

In [8], Alin Bostan and Philippe Dumas, together with Xavier Caruso (CNRS, Rennes) and Gilles Christol (IMJ, Paris) have studied the algorithmic question of coefficient computation of algebraic power series in positive characteristic. They revisited Christol's theorem on algebraic power series in positive characteristic and proposed another proof for it. Their new proof combines several ingredients and advantages of existing proofs, which make it very well-suited for algorithmic purposes. The construction used in the new proof was then applied to the design of a new efficient algorithm for computing the Nth coefficient of a given algebraic power series over a perfect field of characteristic p. This algorithm has several nice features: it is more general, more natural and more efficient than previous algorithms. Not only the arithmetic complexity of the new algorithm is linear in $\log N$ and quasi-linear in p, but its dependency with respect to the degree of the input is much smaller than in the previously best algorithm. Moreover, when the ground field is finite, the new approach yields an even faster algorithm, whose bit complexity is linear in $\log N$ and quasi-linear in $\sqrt{p}$.

6.3. Subresultants of $(x-\alpha)^m$ and $(x-\beta)^n$, Jacobi polynomials and complexity

A previous article described explicit expressions for the coefficients of the order-d polynomial subresultant of $(x-\alpha)^m$ and $(x-\beta)^n$ with respect to Bernstein's set of polynomials $\{(x-\alpha)^j(x-\beta)^{d-j},\ 0 \le j \le d\}$, for $0 \le d < \min\{m,n\}$. In [3], Alin Bostan, together with T. Krick, M. Valdettaro (U. Buenos Aires, Argentina) and A. Szanto (U. North Carolina, Raleigh, USA) further developed the study of these structured polynomials and showed that the coefficients of the subresultants of $(x-\alpha)^m$ and $(x-\beta)^n$ with respect to the monomial basis can be computed in *linear* arithmetic complexity, which is faster than for arbitrary polynomials. The result is obtained as a consequence of the amazing though seemingly unnoticed fact that these subresultants are scalar multiples of Jacobi polynomials up to an affine change of variables.

6.4. Least common multiple of random integers

In [4], Alin Bostan together with Kilian Raschel (CNRS, Tours) and Alexander Marynych (U. Kyiv, Ukraine) have investigated the least common multiple of random integers. Using a purely probabilistic approach, they derived a criterion for the convergence in distribution as $n \to \infty$ of $f(L_n)/n^{rk}$, for a wide class of multiplicative arithmetic functions f with polynomial growth r, where $L_n(k)$ denotes the least common multiple of k independent random integers with uniform distribution on $\{1, 2, ..., n\}$. Furthermore, they identified the limit as an infinite product of independent random variables indexed by the prime numbers. Along the way of showing the main results, they computed the (rational) generating function of a trimmed sum of independent geometric laws, which appears in the above infinite product. The latter is directly related to the generating function of a certain max-type diophantine equation, of which they solved a generalized version. The results extend theorems by Erdős and Wintner (1939), Fernández and Fernández (2013) and Hilberdink and Tóth (2016).

6.5. On sequences associated to the invariant theory of rank two simple Lie algebras

In [14], Alin Bostan together with Jordan Tirrell (Washington College, USA) Philadelphia, USA), Bruce W. Westbury (Unversity of Texas at Dallas, USA) and Yi Zhang (Xi'an Jiaotong-Liverpool University, Suzhou, China) studied two families of sequences, listed in the On-Line Encyclopedia of Integer Sequences (OEIS), which are associated to invariant theory of Lie algebras. For the first family, they proved combinatorially that the sequences A059710 and A108307 are related by a binomial transform. Based on this, they presented two independent proofs of a recurrence equation for A059710, which was conjectured by Mihailovs. Besides, they also gave a direct proof of Mihailovs' conjecture by the method of algebraic residues. As a consequence, closed formulae for the generating function of sequence A059710 were obtained in terms of classical Gaussian hypergeometric functions.

6.6. Explicit degree bounds for right factors of linear differential operators

If a linear differential operator with rational function coefficients is reducible, its factors may have coefficients with numerators and denominators of very high degree. When the base field is $\mathbb{C}$, Alin Bostan together with Bruno Salvy (Inria and ENS Lyon) and Tanguy Rivoal (CNRS and U. Grenoble) gave in [13] a completely explicit bound for the degrees of the monic right factors in terms of the degree and the order of the original operator, as well as the largest modulus of the local exponents at all its singularities. As a consequence, if a differential operator L has rational function coefficients over a number field, they obtained degree bounds for its monic right factors in terms of the degree, the order and the height of L, and of the degree of the number field.

6.7. Improved algorithms for left factorial residues

In [11], Alin Bostan together with Vladica Andrejić (University of Belgrade, Serbia) and Milos Tatarevic (CoinList, Alameda, CA) presented improved algorithms for computing the left factorial residues $!p = 0! + 1! + \cdots + (p-1)! \bmod p$. They used these algorithms for the calculation of the residues $!p \bmod p$, for all primes p up to 2^{40}. Their results confirm that Kurepa's left factorial conjecture is still an open problem, as they show that there are no odd primes $p < 2^{40}$ such that p divides $!p$. Additionally, they confirmed that there are no socialist primes p with $5 < p < 2^{40}$.

6.8. A note on gamma triangles and local gamma vectors

Alin Bostan contributed to F. Chapoton's article [5] by writing an appendix, which allowed the author to complete its article. The theme of [5] is the study of simplicial complexes in algebraic combinatorics. A basic invariant is the f-vector that counts faces according to their dimensions. A less understood invariant is the γ-vector, introduced by Gal in 2005. Also in 2005, Chapoton, motivated by the study of the combinatorics of simplicial complexes attached to cluster algebras, considered a refined version of the f-vector. The main aim of [5] is to introduce the analogue in this context of the γ-vector, and a further refinement called the Γ-triangle. The author computed explicitly the Γ-triangle for all the cluster simplicial complexes of irreducible Coxeter groups. Alin Bostan contributed to the proof of an unexpected relation between the Γ-triangles of cluster fans of type $\mathbb{B}$ and $\mathbb{D}$.

6.9. A closed-form formula for the Kullback-Leibler divergence between Cauchy distributions

In the preliminary work [16], Frédéric Chyzak and Frank Nielsen (LIX, Palaiseau and Sony Computer Science Laboratories, Tokyo, Japan) have reported on a closed-form expression for the Kullback-Leibler divergence between Cauchy distributions which involves the calculation of a parametric definite integral with 6 parameters. The formula shows that the Kullback-Leibler divergence between Cauchy densities is always finite and symmetric. This work also serves as a show-case of several methods in computer algebra to the computation of parametrized integrals.

6.10. Big prime field FFT on multi-core processors

In [9], Svyatoslav Covanov, together with Davood Mohajerani, Marc Moreno Maza, and Linxiao Wang (all from ORCCA, Canada), have worked on a multi-threaded implementation of Fast Fourier Transforms over generalized Fermat prime fields. This work extends their previous study realized on graphics processing units to multi-core processors. In this new context, they overcome the less fine control of hardware resources by successively using FFT in support of the multiplication in those fields. They obtain favorable speedup factors (up to 6.9× on a 6-core, 12 threads node, and 4.3× on a 4-core, 8 threads node) of their parallel implementation compared to the serial implementation for the overall application thanks to the low memory footprint and the sharp control of arithmetic instructions of their implementation of generalized Fermat prime fields.

6.11. Martin boundary of killed random walks on isoradial graphs

Alin Bostan contributed to an article by Cédric Boutillier and Kilian Raschel [15], devoted to the study of random walks on isoradial graphs. Contrary to the lattice case, isoradial graphs are not translation invariant, do not admit any group structure and are spatially non-homogeneous. However, Boutillier and Raschel have been able to obtain analogues of a celebrated result by Ney and Spitzer (1966) on the so-called *Martin kernel* (ratio of Green functions started at different points). Alin Bostan provided in the Appendix two different proofs of the fact that some algebraic power series arising in this context have non-negative coefficients.

6.12. Random walks in orthants and lattice path combinatorics

In the second edition of the book [39], original methods were proposed to determine the invariant measure of random walks in the quarter plane with small jumps (size 1), the general solution being obtained via reduction to boundary value problems. Among other things, an important quantity, the so-called *group of the walk*, allows to deduce theoretical features about the nature of the solutions. In particular, when the order of the group is finite and the underlying algebraic curve is of genus 0 or 1, necessary and sufficient conditions have been given for the solution to be rational, algebraic or D-finite (i.e., solution of a linear differential equation). In this framework, a number of difficult open problems related to lattice-path combinatorics are currently being explored by Alin Bostan, Frédéric Chyzak, and Guy Fayolle, both from the theoretical and computer-algebra viewpoints: concrete computation of the criteria, utilization of differential Galois theory, genus greater than 1 (i.e., when some jumps are of size ≥ 2), etc. A recent topic of future research deals with the connections between simple product-form stochastic networks (so-called *Jackson networks*) and explicit solutions of functional equations for counting lattice walks, see [17].

6.13. Quasilinear Average Complexity for Solving Polynomial Systems

How many operations do we need on the average to compute an approximate root of a random Gaussian polynomial system? Beyond Smale's 17th problem that asked whether a polynomial bound is possible, Pierre Lairez has proved in [6] a quasi-optimal bound $(inputsize)^{1+o(1)}$, which improves upon the previously known $(inputsize)^{3/2+o(1)}$ bound. His new algorithm relies on numerical continuation along *rigid continuation paths*. The central idea is to consider rigid motions of the equations rather than line segments in the linear space of all polynomial systems. This leads to a better average condition number and allows for bigger steps. He showed that on the average, one approximate root of a random Gaussian polynomial system of n equations of degree at most D in $n+1$ homogeneous variables can be computed with $O(n^5 D^2)$ continuation steps. This is a decisive improvement over previous bounds, which prove no better than $\sqrt{2}^{\min(n,D)}$ continuation steps on the average.

In 2019, the article has been accepted in the Journal of the AMS.

6.14. Computing the Volume of Compact Semi-Algebraic Sets

In [10], Pierre Lairez, Mohab Safey El Din and Marc Mezzarobba join a unique set of expertise in symbolic integration, real algebraic geometry and numerical integration to tackle a problem as old as Babylonian mathematics: the computation of volumes.

Let $S \subset R^n$ be a compact basic semi-algebraic set defined as the real solution set of multivariate polynomial inequalities with rational coefficients. They design an algorithm which takes as input a polynomial system defining S and an integer $p \geq 0$ and returns the n-dimensional volume of S at absolute precision 2^{-p}.

Their algorithm relies on the relationship between volumes of semi-algebraic sets and periods of rational integrals. It makes use of algorithms computing the Picard-Fuchs differential equation of appropriate periods, properties of critical points, and high-precision numerical integration of differential equations.

The algorithm runs in essentially linear time with respect to p. This improves upon the previous exponential bounds obtained by Monte-Carlo or moment-based methods.

6.15. Densities of Stieltjes moment sequences for pattern-avoiding permutations

A small subset of combinatorial sequences have coefficients that can be represented as moments of a nonnegative measure on $[0, \infty)$. Such sequences are known as *Stieltjes moment sequences*. They have a number of useful properties, such as log-convexity, which in turn enables one to rigorously bound their growth constant from below.

In [12], Alin Bostan together with Andrew Elvey Price, Anthony Guttmann and Jean-Marie Maillard, studied some classical sequences in enumerative combinatorics, denoted $Av(\mathcal{P})$, and counting permutations of $\{1, 2, ..., n\}$ that avoid some given pattern $\mathcal{P}$. For increasing patterns $\mathcal{P} = (12...k)$, they showed that the corresponding sequences, $Av(123...k)$, are Stieltjes moment sequences, and explicitly determined the underlying density function, either exactly or numerically, by using the Stieltjes inversion formula as a fundamental tool.

They showed that the densities for $Av(1234)$ and $Av(12345)$, correspond to an order-one linear differential operator acting on a classical modular form given as a pullback of a Gaussian ${}_2F_1$ hypergeometric function, respectively to an order-two linear differential operator acting on the square of a classical modular form given as a pullback of a ${}_2F_1$ hypergeometric function. Moreover, these density functions are closely, but non-trivially, related to the density attached to the distance traveled by a walk in the plane with $k - 1$ unit steps in random directions.

As a bonus, they studied the challenging case of the $Av(1324)$ sequence and gave compelling numerical evidence that this too is a Stieltjes moment sequence. Accepting this, they proved new lower bounds on the growth constant of this sequence, which are stronger than existing bounds. A further unproven assumption leads to even better bounds, which can be extrapolated to give a good estimate of the (unknown) growth constant.

TAU Project-Team

7. New Results

7.1. Toward Good AI

7.1.1. Causal Modeling

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag;
PhDs: Diviyan Kalainathan
Collaboration: David Lopez-Paz (Facebook).

The search for **causal models** relies on quite a few hardly testable assumptions, e.g. causal sufficiency [160]; it is a data hungry task as it has the identification of independent and conditionally independent pairs of variables at its core. A new approach investigated through the Cause-Effects Pairs (CEP) Challenge [112] formulates causality search as a supervised learning problem, considering the joint distributions of pairs of variables (e.g. (Age, Salary)) labelled with the proper causation relationship between both variables (e.g. Age "causes" Salary) and learning algorithms apt to learn from distributions have been proposed [114]. An edited book has been published [48], that somewhat summarizes the whole history of Cause-EFfect Paris research. Several chapters of this book have co-authors in TAU: *Evaluation methods of cause-effect pairs* [49], *Learning Bivariate Functional Causal Models* [47], *Discriminant Learning Machines* [51], and *Results of the Cause-Effect Pair Challenge* [50].

In D. Kalainathan's PhD [14] and O. Goudet's postdoc, the search for causal models has been tackled in the framework of generative networks [107], trained to minimize the Maximum Mean Discrepancy loss; the resulting Causal Generative Neural Network improves on the state of the art on the CEP Challenge. CGNN favorably compares with the state of the art w.r.t. usual performance indicators (AUPR, SID) on main causal benchmarks, though with a large computational cost.

An attempt to scale up causal discovery, we proposed the Structural Agnostic Model approach [14] [120]. Working directly on the observational data, this global approach implements a variant of the popular adversarial game [99] between a discriminator, attempting to distinguish actual samples from fake ones, obtained by generating each variable, given real values from all others. A sparsity L_1 penalty forces all generators to consider only a small subset of their input variables, yielding a sparse causal graph. SAM obtains state-of-the-art performances on causal benchmarks, and scales up to a few hundred variables.

An innovative usage of causal models is for educational training in sensitive domains, such as medicine, along the following line. Given a causal generative model, artificial data can be generated using a marginal distribution of causes; such data will enable students to test their diagnosis inference (with no misleading spurious correlations in principle), while forbidding to reverse-engineer the artificial data and guess the original data. Some motivating applications for causal modeling are described in section 4.1 .

7.1.2. Explainability

Participants: Isabelle Guyon, François Landes, Marc Schoenauer, Michèle Sebag
PhD: Marc Nabhan

Causal modeling is one particular method to tackle explainability, and TAU has been involved in other initiatives toward explainable AI systems. Following the LAP (Looking At People) challenges, Isabelle Guyon and co-organizers have edited a book [143] that presents a snapshot of explainable and interpretable models in the context of computer vision and machine learning. Along the same line, they propose an introduction and a complete survey of the state-of-the-art of the explainability and interpretability mechanisms in the context of first impressions analysis [57].

The team is also involved in the proposal for the IPL HyAIAI (Hybrid Approaches for Interpretable AI), coordinated by the LACODAM team (Rennes) dedicated to the design of hybrid approaches that combine state of the art numeric models (e.g., deep neural networks) with explainable symbolic models, in order to be able to integrate high level (domain) constraints in ML models, to give model designers information on ill-performing parts of the model, to provide understandable explanations on its results. Kickoff took place in September 2019, and we are still looking for good post-doc candidates.

Note also that the on-going work on the identification of the border of the failure zone in the parameter space of the autonomous vehicle simulator [37] (Section 7.1.3) also pertains to explainability.

Finally, a completely original approach to DNN explainability might arise from the study of structural glasses (7.2.3), with a parallel to Graph Neural Networks (GNNs), that could become an excellent non-trivial example for developing explainability protocols.

7.1.3. Robustness of AI Systems

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhDs: Julien Girard, Marc Nabhan, Nizham Makhoud
Collaboration: Zakarian Chihani (CEA); Hiba Hage and Yves Tourbier (Renault); Johanne Cohen (LRI-GALAC) and Christophe Labreuche (Thalès)

As said (Section 3.1.2 , TAU is considering two directions of research related to the certification of MLs. The first direction, related to formal approaches, is the topic of Julien Girard's PhD (see also Section 3.1.2). On the opposite, the second axis aims to increase the robustness of systems that can only be experimentally validated. Two paths are investigated in the team: assessing the coverage of the datasets (more particularly here, used to train an autonomous vehicle controller), topic of Marc Nabhan's CIFRE with Renault; and detecting flaws in the system by reinforcement learning, as done by Nizam Makdoud's CIFRE PhD with Thalès THERESIS.

Formal validation of Neural Networks

The topic of provable deep neural network robustness has raised considerable interest in recent years. Most research in the literature has focused on adversarial robustness, which studies the robustness of perceptive models in the neighbourhood of particular samples. However, other works have proved global properties of smaller neural networks. Yet, formally verifying perception remains uncharted. This is due notably to the lack of relevant properties to verify, as the distribution of possible inputs cannot be formally specified. With Julien Girard-Satabin's PhD thesis, we propose to take advantage of the simulators often used either to train machine learning models or to check them with statistical tests, a growing trend in industry. Our formulation [34] allows us to formally express and verify safety properties on perception units, covering all cases that could ever be generated by the simulator, to the difference of statistical tests which cover only seen examples. Along with this theoretical formulation, we provide a tool to translate deep learning models into standard logical formulae. As a proof of concept, we train a toy example mimicking an autonomous car perceptive unit, and we formally verify that it will never fail to capture the relevant information in the provided inputs.

Experimental validation of Autonomous Vehicle Command Statistical guarantees (e.g., less than 10^{-8} failure per hour of operation) are obtained by empirical tests, involving millions of kilometers of driving in all possible road, weather and traffic conditions as well as intensive simulations, the only way to full control of the driving conditions. The validation process thus involves 3 steps: i) making sure that all parts of the space of possible scenarios are covered by experiments/tests with sufficiently fine grain; ii) identify failures zones in the space of scenarios; iii) fix the controller flaws that resulted in these failures.

TAU is collaborating with Renault on step ii) within Marc Nabhan's CIFRE PhD (defense expected in Sept. 2020). The current target scenario is the insertion of a car on a motorway, the "drosophila" of autonomous car scenarios and the goal is the identification of the conditions of failures of the autonomous car controller. Only simulations are considered here, with one scenario being defined as a parameter setting of the in-house simulator SCANeR. The goal is the detection of as many failures as possible, running as few simulations as possible, and the identification of the borders of the failure zone using an as simple as possible description, thus allowing engineers to understand the reasons for the flaws. A first paper was published [37] proposing several approaches for the identification of failures. On-going work is concerned with a precise yet simple definition of the border of the failure zone.

Reinforcement Learning from Advice In the context of his CIFRE PhD with Thalès, Nizam Makdoud tests (in simulation) physical security systems using reinforcement learning to learn the best sequence of action that will break through the system. This lead him to propose an original approach called *LEarning from Advice* (LEA) that uses knowledge from several policies learned on different tasks. Whereas Learning by imitation uses the actions of the known policy, the proposed method uses the different Q-functions of the known policies. The main advantage of this strategy is its robustness to poor advice, as the policy then reverts to standard DDPG [127]. The results (submitted) demonstrate that LEA is able to learn faster than DDPG if given good-enough policies, and only slightly slower when given lousy advices.

Learning Multi-Criteria Decision Aids (Hierarchical Choquet models) In collaboration with Johanne Cohen (LRI-GALAC) and Christophe Labreuche (Thalès), the representation and data-driven elicitation of hierarchical Choquet models has been tackled. A specific neural architecture, enforcing by design the model constraints (monotonicity, additivity), and supporting the end-to-end training of the Multi-Criteria Decision aid, has been proposed in Roman Bresson's PhD. Under mild assumptions, an identifiability result (existence and unicity of the sought model in the neural space) is obtained. The approach is empirically validated and successfully compared to the state of the art.

7.2. Learning to Learn

7.2.1. Auto-*

Participants: Guillaume Charpiat, Isabelle Guyon, Marc Schoenauer, Michèle Sebag

PhDs: Léonard Blier, Guillaume Doquet, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun, Pierre Wolinski

Collaboration: Vincent Renault (SME Artelys); Yann Ollivier (Facebook)

Auto-☆ studies at TAU investigate several research directions.

As mentioned in Section 3.3 , a popular approach for algorithm selection is collaborative filtering. In Lisheng Sun's PhD [15], active learning was used on top of the CofiRank algorithm for matrix factorization [164], improving the results and the time to solution of the recommendation algorithm. Furthermore, most real-world domains evolve with time, and an important issue in real-world applications is that of life-long learning, as static models can rapidly become obsolete. Another contribution in Lisheng's PhD is an extension of AutoSklearn that detects concept drifts and corrects the current model accordingly.

An original approach to Auto-☆, explored in Herilalaina Rakotoarison's PhD, extends and adapts Monte-Carlo Tree Search to explore the structured space of pre-processing + learning algorithm configurations, and gradually determine the best pipeline [40]; the resulting MOSAIC algorithm performs on par with AutoSklearn, the winner of Auto-☆ international competitions in the last few years.

Auto-☆ would be much easier if appropriate and affordable meta-features (describing datasets) were available. Taking inspiration from equivariant learning [144] and learning from distributions [130], on-going work aims to learn such meta-features, based on the OpenML archive [161].

A key building block in Auto-☆ lies in the data preparation and specifically variable selection. Guillaume Doquet's PhD [13] addresses the problem of agnostic feature selection, independently of any target variable. The point d'orgue of his work is Agnos [32] (Best Paper Award at ECML 2019), that combines an AutoEncoder with structural regularizations to sidestep the combinatorial optimization problem at the core of feature selection. The extensive experimental validation of AgnoS on the scikit-feature benchmark suite demonstrates its ability compared to the state of the art, both in terms of supervised learning and data compression.
Several works have focused on the adjustment of specific hyper-parameters for neural nets. Pierre Wolinski's PhD (to be defended in January 2020, publication submitted) studies three such hyper-parameters: i) network width (number of neurons in each layer); ii) regularizer importance in the objective function to minimize (factor balancing data term and regularizer); and iii) learning rate. Regarding the network width, it is adjusted during training thanks to a criterion quantifying each neuron's importance, naturally leading to a sparsification effect (as for L1 norm minimization). This study is actually extendable to not only layers' widths but also layers' connectivity (e.g., in modern networks where each layer may be connected to any other layer with 'skip' connections). Regarding the regularizer weight, it is formulated as a probabilistic prior from a Bayesian perspective, which leads to a particular value that the regularizer weight should have in order the network to satisfy some property. Regarding the learning rate, Pierre Wolinski and Leonard Blier [27] proposed to attach fixed learning rates to each neuron (picked randomly) and calibrate this learning rate distribution in such a way that neurons are sequentially active, learning in an optimally agile manner during a first learning phase, and being stable in later phases. This remove the need to tune the learning rate.
A last direction of investigation concerns the design of challenges, that contribute to the collective advance of research in the Auto-☆ direction. The team has been very active in the series of AutoML challenges [154], and steadily contributes to the organization of new challenges (Section 7.6).

7.2.2. Deep Learning: Practical and Theoretical Insights

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, Corentin Tallec
Collaboration: Yann Ollivier (Facebook AI Research, Paris), the Altschuler and Wu lab. (UCSF, USA), Y. Tarabalka (Inria Titane)

Although a comprehensive mathematical theory of deep learning is yet to come, theoretical insights from information theory or from dynamical systems can deliver principled improvements to deep learning and/or explain the empirical successes of some architectures compared to others.

In his PhD [16], Corentin Tallec presents several contributions along these lines:

- In [158], it is shown that the LSTM structure can be understood from axiomatic principles, enforcing the *robustness of the learned model to temporal deformation (warpings) in the data*. The complex LSTM architecture, introduced in the 90's, has become the currently dominant architecture for modeling temporal sequences (such as text) in deep learning. It is shown that this complex LSTM architecture necessarily arises if one wants the model to be able to handle time warpings in the data (such as arbitrary accelerations or decelerations in the signal), and their complex equations can be derived axiomatically.
- In [132] (oral presentation at ICML 2018) the issue of mode dropping in adversarial generative models is tackled using information theory. The adversary (discriminator) task is set to predict the proportion of true and fake images in a set of images, via an information theory criterion, thus working at the level of the *overall distribution* of images. The discriminator is thus mande more able to detect statistical imbalances between the modes created by the generator, thereby reducing the mode dopping phenomenon. The proposed architecture, inspired from equivariant approaches, is provably able to detect all permutation-invariant statistics in a set of images.
- In [159], the problem of recurrent network training is tackled via the theory of dynamical systems by proposing a simple fully online solution avoiding the "time rewind" step, based on real-time, noisy but unbiased approximations of model gradients, which can be implemented easily in a black-box fashion on top of any recurrent model, and which is well-justified mathematically. The price to pay is an increase of variance.

- In [42], we identify sensitivity to time discretization of Deep RL in near continuous-time environments as a critical factor. Empirically, we find that Q-learning-based approaches collapse with small time steps. Formally, we prove that Q-learning does not exist in continuous time. We detail a principled way to build an off-policy RL algorithm that yields similar performances over a wide range of time discretizations, and confirm this robustness empirically.

Several other directions have been investigated: In [41], we introduce a multi-domain adversarial learning algorithm in the semi-supervised setting. We extend the single source H-divergence theory for domain adaptation to the case of multiple domains, and obtain bounds on the average- and worst-domain risk in multi-domain learning. This leads to a new loss to accommodate semi-supervised multi-domain learning and domain adaptation. We obtain state-of-the-art results on two standard image benchmarks, and propose as a new benchmark a novel bioimage dataset, CELL, in the domain of automated microscopy data, where cultured cells are imaged after being exposed to known and unknown chemical perturbations, and in which each dataset displays significant experimental bias.

Another direction regards the topology induced by a trained neural net, and how similar are two samples in the NN perspective. The definition proposed in [29] relies on varying the NN parameters and examining whether the impacts of this variation on both samples are aligned. The mathematical properties of this similarity measure are investigated and the similarity is shown to define a kernel on the input space. This kernel can be used to tractably estimate the sample density, and it leads to new directions for the statistical learning analysis of NN, e.g. in terms of additional loss (requiring that similar examples have a similar latent representation in the above sense) or in terms of resistance to noise. Specifically, a multimodal image registration task is presented where almost perfect accuracy is reached, despite a high label noise (see Section 7.5.2). Such an impressive self-denoising phenomenon can be explained and quantified as a noise averaging effect over the labels of similar examples.

7.2.3. Analyzing and Learning Complex Systems

Participants: Cyril Furtlehner, Aurélien Decelle, François Landes
PhDs: Giancarlo Fissore
Collaboration: Jacopo Rocchi (LPTMS Paris Sud); the Simons team: Rahul Chako (post-doc), Andrea Liu (UPenn), David Reichman (Columbia), Giulio Biroli (ENS), Olivier Dauchot (ESPCI).; Clément Vignax (EPFL); Yufei Han (Symantec).

The information content of a trained restricted Boltzmann machine (RBM) can be analyzed by comparing the singular values/vectors of its weight matrix, referred to as modes, to that of a random RBM (typically following a Marchenko-Pastur distribution) [83]. The analysis of a single learning trajectory is replaced by analyzing the distribution of a well chosen ensemble of models. In G. Fissore's PhD, the learning trajectory of an RBM is shown to start with a linear phase recovering the dominant modes of the data, followed by a non-linear regime where the interaction among the modes is characterized [84]. Although simplifying assumptions are required for a mean-field analysis in closed form of the above distribution, it nevertheless delivers some simple heuristics to speed up the learning convergence and to simplify the models.

This analysis will be extended along two directions: handling missing data [58]; and considering exactly solvable RBM (non-linear RBM for which the contrastive divergence can be computed in closed forms, e.g. using a spherical model) [54]. W.r.t. missing data, state of the art results have been obtained on semi-supervised tasks in the context of Internet-of-Things security, considering a high rate of missing inputs and labels). On the theoretical side exact generic RBM learning trajectories have been characterized, showing intriguing connections based on Bose-Einstein condensation mechanism associated to information storing. Our collaboration with J. Rocchi(LPTMS, Univ. Paris Sud) aims to characterize the landscape of RBMs learned from different initial conditions, and to relate this landscape to the number of parameters (hidden nodes) of the system.

An emerging research topic, concerns the interpretation of deep learning by means of Gaussian processes and associated neural tangent limit kernel in the thermodynamical limit obtained by letting layer's width go to infinity [118]. Various things are planned to be investigated on the basis of this theoretical tool in particular how this translate to RBM or DBM setting, and whether a double dip behaviour is to be expected as well for generative models.

As mentioned earlier, the use of ML to address fundamental physics problems is quickly growing. This leads to some methodological mistakes from newcomers, that have been investigated by Rémi Perrier (2 month internship). One example is the domain of glasses (how the structure of glasses is related to their dynamics), which is one of the major problems in modern theoretical physics. The idea is to let ML models automatically find the hidden structures (features) that control the flowing or non-flowing state of matter, discriminating liquid from solid states. These models can then help identifying "computational order parameters", that would advance the understanding of physical phenomena [19], on the one hand, and support the development of more complex models, on the other hand. More generally, attacking the problem of amorphous condensed matter by novel Graph Neural Networks (GNN) architectures is a very promising lead, regardless of the precise quantity one may want to predict. Currently GNNs are engineered to deal with molecular systems and/or crystals, but not to deal with amorphous matter. This second axis is currently being attacked in collaboration with Clément Vignac (PhD Student at EPFL), using GNNs. Furthermore, this problem is new to the ML community and it provides an original non-trivial example for engineering, testing and benchmarking explainability protocols.

7.3. Computational Social Sciences

Computational Social Sciences (CSS) is making significant progress in the study of social and economic phenomena thank to the combination of social science theories and new insight from data science. While the simultaneous advent of massive data and unprecedented computational power has opened exciting new avenues, it has also raised new questions and challenges.

Several studies are being conducted in TAU, about labor (labor markets, platform "micro-work", quality of life and economic performance), about nutrition (health, food, and socio-demographic issues), around Cartolabe, a platform for scientific information system and visual querying and around GAMA, a multi-agent based simulation platform.

7.3.1. Labor Studies

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag, Paola Tubaro
PhDs: Diviyan Kalainathan, Guillaume Bied, Armand Lacombe
Post-Docs: Saumya Jetley
Engineers: Raphael Jaiswal, Victor Alfonso Naya
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Antonio Casilli, Ulrich Laitenberger (Telecom Paris); Odile Chagny (IRES); Alessandro Delfanti (University of Toronto)

A first area of activity of TAU in Computational Social Sciences is the study of labor, from the functioning of the job market, to the rise of new, atypical forms of work in the networked society of internet platforms, and the quality of life at work.
Job markets Two projects deal with the domain of job markets and machine learning. The DATAIA project Vadore, in collaboration with ENSAE and Pôle Emploi, has two goals. First, to improve the recommendation of jobs for applicants (and the recommendation of applicants to job offers). The main originalities in this project are: i) to use both machine learning and optimal transport to improve the recommendation by learning a matching function for past hiring, and then to apply optimal transport-like bias to tackle market congestion (e.g. to avoid assigning many applicants to a same job offer); ii) to use randomized test on micro-markets (AB testing) in collaboration with Pôle Emploi to test the global impact of the algorithms.

The JobAgile project, BPI-PIA contract, coll. EHESS, Dataiku and Qapa, deals with low salary interim job recommendations. A main difference with the Vadore project relies on the high reactivity of the Qapa and Dataiku startups: i) to actually implement AB-testing; ii) to explore related functionalities, typically the recommendation of formations; iii) to propose a visual querying of the job market, using the Cartolabe framework (below).

The platform economy and digital labor

Another topic concerns the digital economy and the transformations of labor that accompany it. One part of the platform economy carries promises of social, not only techno-economic, innovation. If enthusiasms for a new "sharing economy" or "collaborative economy" have progressively faded away, values of decentralization, autonomy, and flatter coordination are still commonly associated to platforms. A conference paper by P. Tubaro studies how events constitute places where actors of the platform economy negotiate values and collectively drive forms of social change [43].

The platform economy and its effects on labor are also linked to the current developments of AI [22]. In collaboration with A.A. Casilli (Telecom ParisTech), P. Tubaro has received funding from the Union Force Ouvrière, from France Stratégie (a Prime Minister's service), and from MSH Paris-Saclay, to map "micro-work" in France (DiPLab project). The term micro-work refers to small, data-related tasks that are performed online against low remunerations, such as tagging objects in images, transcribing bits of text, and recording utterances aloud. Specialized platforms such as Amazon Mechanical Turk, Clickworker and Microworkers recruit online providers to execute these tasks for their clients, mostly for data-intensive production processes. In addition to poor working conditions and low pay, micro-work raises issues in terms of privacy and data protection, insofar as outside providers are entrusted with data that may include personal information [23].

The results of the DiPLab study were published in a report that attracted significant media attention [52], and presented as part of a large event on micro-work at the headquarters of France Stratégie in June 2019. Two articles relying on DiPlab results, one of which was first published as a working paper [62], [61], are now under review.

A joint franco-Canadian grant obtained by P. Tubaro and A. Delfanti (University of Toronto) enabled the creation of an "International Network on Digital Labor", aiming to bring together scholars interested in various forms of digital platform labor. Inauguration of the network involved the organization of two workshops, one in Paris (June 2019) and the other in Toronto (October 2019).

Further research on how digital platforms transform labor practices and affect the very definition of professions is being undertaken by P. Tubaro as part of a two-year (2018-2020) grant from DARES (French Ministry of Labor), in collaboration with O. Chagny of IRES, a union-funded think-tank), and A.A. Casilli (Telecom ParisTech).

A newly-obtained grant from ANR (with A.A. Casilli and U. Laitenberger, Telecom ParisTech) will enable P. Tubaro to further explore the global production networks that link AI developers and producers to data-related work across national boundaries, following outsourcing chains that extend from France to French-speaking African countries, and from Spain and the USA to parts of Latin America. This new project, entitled "The HUman Supply cHain behind smart technologies" (HUSH), will start in January 2020.

7.3.2. Health, food, and socio-demographic relationships

Participants: Philippe Caillou, Michèle Sebag, Paola Tubaro
Post-doc: Ksenia Gasnikova
Collaboration: Louis-Georges Soler, Olivier Allais (INRA)

Another area of activity concerns the relationships between eating practices, socio-demographic features and health.

The Nutriperso project (IRS Univ. Paris-Saclay, coll. INRA, CEA, CNRS, INSERM, Telecom ParisTech and Univ. Paris-Sud) aims to: i) determine the impact of food items on health (e.g., related to T2 diabetes); ii) identify alternative food items, admissible in terms of taste and budget, and better in terms of health; iii) emit personalized food recommendations> One project motivation is the fact that general recommendations (e.g., *Eat 5 fruit and vegetable per day*) are hardly effective on populations at risk. Based on the Kantar database, reporting the food habits of 20,000 households over 20 years, our challenge is to analyze the food purchases at an unprecedented fine-grained scale (at the barcode level), and to investigate the relationship between diets, socio-demographic features, and body mass index (BMI). The challenge also regards the direction of causality; while some diets are strongly correlated to high BMI, the question is to determine whether, e.g., sugar-free sodas are a cause of obesity, or a consequence thereof, or both a cause and a consequence. A main difficulty is the lack of control populations to assess a diet impact. Such a control population could be approximated in the case of the organic diet, showing a statistically significant impact of this diet on the BMI distribution. The question of finding confounders (e.g. based on wealth or education) or "backdoor" variables in under study.

7.3.3. Scientific Information System and Visual Querying

Participants: Philippe Caillou, Michèle Sebag
Engineers: Anne-Catherine Letournel, Jonas Renault
Collaboration: Jean-Daniel Fekete (AVIZ, Inria Saclay)

A third area of activity concerns the 2D visualisation and querying of a corpus of documents. Its initial motivation was related to scientific organisms, institutes or Universities, using their scientific production (set of articles, authors, title, abstract) as corpus. The Cartolabe project started as an Inria ADT (coll. TAO and AVIZ, 2015-2017). It received a grant from CNRS (coll. TAU, AVIZ and HCC-LRI, 2018-2019). Further extensions, as an open-source platform, are under submission at the time of writing.

The originality of the approach is to rely on the content of the documents (as opposed to, e.g. the graph of co-authoring and citations). This specificity allowed to extend Cartolabe to various corpora, such as Wikipedia, Bibliotheque Nationale de France, or the Software Heritage. Cartolabe was also applied in 2019 to the *Grand Debat* dataset: to support the interactive exploration of the 3 million propositions; and to check the consistency of the official results of the *Grand Debat* with the data.

Among its intended functionalities are: the visual assessment of a domain and its structuration (who is expert in a scientific domain, how related are the domains); the coverage of an institute expertise relatively to the general expertise; the evolution of domains along time (identification of rising topics). A round of interviews with beta-user scientists is under way since end 2019. Cartolabe usage raises questions at the crossroad of human-centered computing, data visualization and machine learning: i) how to deal with stressed items (the 2D projection of the item similarities poorly reflects their similarities in the high dimensional document space; ii) how to customize the similarity and exploit the users' feedback about relevant neighborhoods.

7.3.4. Multi-Agent based simulation framework for social science

Participants: Philippe Caillou
Collaboration: Patrick Taillandier (INRA), Alexis Drogoul and Nicolas Marilleau (IRD), Arnaud Grignard (MediaLab, MIT), Benoit Gaudou (Université Toulouse 1)

Since 2008, P. Caillou contributes to the development of the GAMA platform, a multi-agent based simulation framework. Its evolution is driven by the research projects using it, which makes it very well suited for social sciences studies and simulations.

The focus of the development team in 2019 was on the stability of the platform and on the documentation to provide a stable and well documented framework to the users.

7.4. Energy Management

7.4.1. Power Grids Daily Management

Participants: Isabelle Guyon, Marc Schoenauer

PhDs: Benjamin Donnot, Balthazar Donon
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Olivier Teytaud (Facebook)

Benjamin Donnot's CIFRE PhD with RTE [12] dealt with Power Grid safety: The goal is to assess in real time the so-called "(n-1) safety" (see Section 4.2) of possible recovery actions modifying the topology of the grid after some problem occurred somewhere on the grid. However, the HADES simulator, that allows to compute the power flows in the whole network, is far too slow to simulate in real time all n-1 possible failures of a tentative topology. A simplified simulator is also available, but its accuracy is too poor to give good results. Deep surrogate models can be trained off-line for a given topology, based on the results of the slow simulator, with high-enough accuracy, but training as many models as possible failures (i.e., n-1) obviously doesn't scale up: the topology of the grid must be an input of the learned model, allowing to instantly compute the power flows at least for grid configurations close to the usual running state of the grid. A standard approach is the one-hot encoding of the topology, where n additional boolean inputs are added to the neural network, encoding the presence or absence of each line. Nevertheless, this approach poorly generalize to topologies outside the distribution of the ones used for training.

An original "guided dropout" approach was first proposed [87], in which the topology directly acts on the connections of the deep network: a missing line suppresses some connections. Whereas the standard dropout method disconnect random connections for every batch, in order to improve the generalization capacity of the network, the "guided dropout" method removes some connections based on the actual topology of the network. This approach is experimentally validated against the one-hot encoding on small subsets of the French grid (up to 308 lines). Interestingly, and rather surprisingly, even though only examples with a single disconnected line are used in the training set, the learned model is able of some additive generalization, and predictions are also accurate enough in the case 2 lines are disconnected. The guided dropout approach was later robustified [86] by learning to rapidly rank higher order contingencies including all pairs of disconnected lines, in order to prioritize the cases where the slow simulator is run: Another neural network is trained to rank all (n-1) and (n-2) contingencies in decreasing order of presumed severity.

The guided dropout approach has been further extended and generalized with the LEAP (Latent Encoding of Atypical Perturbation) architecture [30], [17], by crossing-out connections between the encoder and the decoder parts of the ResNet architecture. LEAP then performs transfer learning over spaces of distributions of topology perturbations, allowing to better handle more complex actions on the tolology, going beyond (n-1) and (n-2) perturbations by also including node-split, a current action in the real world. The LEAP approach was theoretically studied in the case of additive perturbations, and experimentally validated on an actual sub-grid of the French grid with 46 consumption nodes, 122 production nodes, 387lines and 192 substations.

LEAP is also the firs part of Balthazar Donon's on-going PhD, that currently develops using a completely different approach to approximate the power flows on a grid, i.e. that of Graph Neural Networks (GNNs). From a Power Grid perspective, GNNs can be viewed as including the topology in the very structure of the neural network, and learning some generic transfer function amongst nodes that will perform well on any topology. First results [31] use a loss based on a large dataset of actual power flows computed using the slow HADES simulator. The results indeed generalize to very different topologies than the ones used for training, in particular very different sizes of power grids. On-going work [56] removes the need to run HADES thanks to a loss that directly aims to minimize Kirshoff's law on all lines.

7.4.2. Local Grids Optimization, and the Modeling of Worst-case Scenarios

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Victor Berger, Herilalaina Rakotoarison; **Post-doc**: Berna Batu
Collaboration: Vincent Renaut (Artelys)

One of the goals of the ADEME Next project, in collaboration with SME Artelys (see also Section 4.2), is the sizing and capacity design of regional power grids. Though smaller than the national grid, regional and urban grids nevertheless raise scaling issues, in particular because many more fine-grained information must be taken into account for their design and predictive growth.

Regarding the design of such grids, and provided accurate predictions of consumption are available (see below), off-the-shelf graph optimization algorithms can be used. Berna Batu is gathering different approaches. Herilalaina Rakotoarison's PhD tackles the automatic tuning of their parameters (see Section 7.2.1); while the Mosaic algorithm is validated on standard AutoML benchmarks [40], its application to Artelys' home optimizer at large Knitro is on-going, and compared to the state-of-the-art in parameter tuning (confidential deliverable).

In order to get accurate consumption predictions, V. Berger's PhD tackles the identification of the peak of energy consumption, defined as the level of consumption that is reached during at least a given duration with a given probability, depending on consumers (profiles and contracts) and weather conditions. The peak identification problem is currently tackled using Monte-Carlo simulations based on consumer profile- and weather-dependent individual models, at a high computational cost. The challenge is to exploit individual models to train a generative model, aimed to sampling the collective consumption distribution in the quantiles with highest peak consumption. The concept of *Compositional Variational Auto-Encoder* was proposed: it is amenable to multi-ensemblist operations (addition or subtraction of elements in the composition), enabled by the invariance and generality of the whole framework w.r.t. respectively, the order and number of the elements. It has been first tested on synthetic problems [26].

7.5. Data-driven Numerical Modelling

7.5.1. High Energy Physics

Participants: Cécile Germain, Isabelle Guyon
PhD: Victor Estrade, Adrian Pol
Collaboration: D. Rousseau (LAL), M. Pierini (CERN)

The role and limits of simulation in discovery is the subject of V. Estrade's PhD, specifically uncertainty quantification and calibration, that is how to handle the systematic errors, arising from the differences ("known unknowns") between simulation and reality, coming from uncertainty in the so-called nuisance parameters. In the specific context of HEP analysis, where relatively numerous labelled data are available, the problem is at the crosspoint of domain adaptation and representation learning. We have investigated how to directly enforce the invariance w.r.t. the nuisance in the sought embedding through the learning criterion (tangent back-propagation) or an adversarial approach (pivotal representation). The results [93] contrast the superior performance of incorporating a priori knowledge on a well separated classes problem (MNIST data) with a real case setting in HEP, in relation with the Higgs Boson Machine Learning challenge [68] and the TRrackML challenge [46]. More indirect approaches based on either incorporating variance reduction for the parameter of interest or constraining the representation in a variational auto-encoder farmework are currently considered.

Anomaly detection (AD) is the subject of A. Pol's PhD. Reliable data quality monitoring is a key asset in delivering collision data suitable for physics analysis in any modern large-scale high energy physics experiment. [21] focuses on supervised and semi-supervised methods addressing the identification of anomalies in the data collected by the CMS muon detectors. The combination of DNN classifiers capable of detecting the known anomalous behaviors, and convolutional autoencoders addressing unforeseen failure modes has shown unprecedented efficiency. The result has been included in the production suite of the CMS experiment at CERN. Recent work has focused on improving AD for the trigger system, which is the first stage of event selection process in most experiments at the LHC at CERN. The hierarchical structure of the trigger process called for exploiting the advances in modeling complex structured representations that perform probabilistic inference effectively, and specifically variational autoencoders. Previous works argued that training VAE models only with inliers is insufficient and the framework should be significantly modified in order to discriminate the anomalous instances. In this work, we exploit the deep conditional variational autoencoder (CVAE) and we define an original loss function together with a metric that targets hierarchically structured data AD [39], [64]. This results in an effective, yet easily trainable and maintainable model.

The highly visible TrackML challenge [46] is described in section 7.6 .

7.5.2. Remote Sensing Imagery

Participants: Guillaume Charpiat
Collaboration: Yuliya Tarabalka, Armand Zampieri, Nicolas Girard, Pierre Alliez (Titane team, Inria Sophia-Antipolis)

The analysis of satellite or aerial images has been a long-time ongoing topic of research, but the remote sensing community moved only very recently to a principled vision of the tasks in a machine learning perspective, with sufficiently large benchmarks for validation. The main topics are the segmentation of (possibly multispectral) remote sensing images into objects of interests, such as buildings, roads, forests, etc., and the detection of changes between two images of the same place taken at different moments. The main differences with classical computer vision is that images are large (covering whole countries, typically cut into 5000×5000 pixels tiles), containing many small, potentially similar objects (and not one big object per image), that every pixel needs to be annotated (w.r.t. assigning a single label to a full image), and that the ground truth is often not reliable (spatially mis-registered, missing new constructions).

These last years, deep learning techniques took over classical approaches in most labs, adapting neural network architectures to the specifics of the tasks. This is due notably to the creation of several large scale benchmarks (including one by us [133] and, soon after, larger ones by GAFAM).

This year, we continued the work started in [167] about the registration of remote sensing images (RGB pictures) with cadastral maps (made of polygons indicating buildings and roads). We extended it in [33] to the case of real datasets, i.e. to noisy data. Indeed, in remote sensing, datasets are often large but of poor ground truth annotation quality. It turns out that, when training on datasets with noisy labels, one can still obtain accuracy scores far better than the noise variance in the training set, due to averaging effects over the labels of similar examples. To properly explain this, a theoretical study was conducted (cf. Section 7.2.2). Given any already trained neural network and its noisy training set, without knowing the real ground truth, we were then able to quantify this noise averaging effect [29].

We also tackled the problem of pansharpening, i.e. the one of producing a high-resolution color image, given a low-resolution color image and a high-resolution greyscale one [35], with deep convolutional neural networks as well.

7.5.3. Space Weather Forecasting

Participants: Cyril Furtlehner, Michèle Sebag
PhD: Mandar Chandorkar
Collaboration: Enrico Camporeale (CWI)

Space Weather is broadly defined as the study of the relationships between the variable conditions on the Sun and the space environment surrounding Earth. Aside from its scientific interest from the point of view of fundamental space physics phenomena, Space Weather plays an increasingly important role on our technology-dependent society. In particular, it focuses on events that can affect the performance and reliability of space-borne and ground-based technological systems, such as satellite and electric networks that can be damaged by an enhanced flux of energetic particles interacting with electronic circuits.[0]

Since 2016, in the context of the Inria-CWI partnership, a collaboration between TAU and the Multiscale Dynamics Group of CWI aims to long-term Space Weather forecasting. The goal is to take advantage of the data produced everyday by satellites surveying the sun and the magnetosphere, and more particularly to relate solar images and the quantities (e.g., electron flux, proton flux, solar wind speed) measured on the L1 libration point between the Earth and the Sun (about 1,500,000 km and 1 hour time forward of Earth). A challenge is to formulate such goals in terms of supervised learning problem, while the "labels" associated to solar images are recorded at L1 (thus with a varying and unknown time lag). In essence, while typical ML models aim to answer the question *What*, our goal here is to answer both questions *What* and *When*. This project has been articulated around Mandar Chandorkar's Phd thesis[11] which has been defended this year in Eindhoven. One

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[0] After a recent survey conducted by the insurance company Lloyd's, an extreme Space Weather event could produce up to $2.6 trillion in financial damage.

of the main result that has been obtained concerns the prediction of solar wind impacting earth magnetosphere from solar images. In this context we encountered an interesting sub-problem related to the non deterministic travel time of a solar eruption to earth's magnetosphere. We have formalized it as the joint regression task of predicting the magnitude of signals as well as the time delay with respect to their driving phenomena. We have provided in[28] an approach to this problem combining deep learning and an original Bayesian forward attention mechanism. A theoretical analysis based on linear stability has been proposed to put this algorithm on firm ground. From the practical point of view, encouraging tests have been performed both on synthetic data and real data with results slightly better than those present in the specialized literature on a small dataset. Various extension of the method, of the experimental tests and of the theoretical analysis are planned.

7.5.4. Genomic Data and Population Genetics

Participants: Guillaume Charpiat, Flora Jay, Aurélien Decelle, Cyril Furtlehner
PhD: Théophile Sanchez – **PostDoc**: Jean Cury
Collaboration: Bioinfo Team (LRI), Estonian Biocentre (Institute of Genomics, Tartu, Estonia), Pasteur Institute (Paris), TIMC-IMAG (Grenoble)

Thanks to the constant improvement of DNA sequencing technology, large quantities of genetic data should greatly enhance our knowledge about evolution and in particular the past history of a population. This history can be reconstructed over the past thousands of years, by inference from present-day individuals: by comparing their DNA, identifying shared genetic mutations or motifs, their frequency, and their correlations at different genomic scales. Still, the best way to extract information from large genomic data remains an open problem; currently, it mostly relies on drastic dimensionality reduction, considering a few well-studied population genetics features.

We developed an approach that extracts features from genomic data using deep neural networks and combines them with a Bayesian framework to approximate the posterior distribution of demographic parameters. The key difficulty is to build flexible problem-dependent architectures, supporting transfer learning and in particular handling data with variable size. We designed new generic architectures, that take into account DNA specificities for the joint analysis of a group of individuals, including its variable data size aspects and compared their performances to state-of-the-art approaches [148]. In the short-term these architectures can be used for demographic inference or selection inference in bacterial populations (ongoing work with a postdoctoral researcher, J Cury, and the Pasteur Institute); the longer-term goal is to integrate them in various systems handling genetic data or other biological sequence data.

In collaboration with the Institute of Genomics of Tartu (Estonia; B Yelmen, 3-month visitor at LRI), we leveraged two types of generative neural networks (Generative Adversarial Networks and Restricted Boltzmann Machines) to learn the high dimensional distributions of real genomic datasets and create artificial genomes [66]. These artificial genomes retain important characteristics of the real genomes (genetic allele frequencies and linkage, hidden population structure, ...) without copying them and have the potential to be valuable assets in future genetic studies by providing anonymous substitutes for private databases (such as the ones hold by companies or public institutes like the Institute of Genomics of Tartu). Yet, ensuring anonymity is a challenging point and we measured the privacy loss by using and extending the Adversarial Accuracy score developed by the team for synthetic medical data [44].

In collaboration with TIMC-IMAG, we proposed a new factor analysis approach that process genetic data of multiple individuals from present-day and ancient populations to visualize population structure and estimate admixture coefficients (that is, the probability that an individual belongs to different groups given the genetic data). This method corrects the traditionally-used PCA by accounting for time heterogeneity and enables a more accurate dimension reduction of paleogenomic data [59].

7.5.5. Sampling molecular conformations

Participants: Guillaume Charpiat
PhD: Loris Felardos
Collaboration: Jérôme Hénin (IBPC), Bruno Raffin (InriAlpes)

Numerical simulations on massively parallel architectures, routinely used to study the dynamics of biomolecules at the atomic scale, produce large amounts of data representing the time trajectories of molecular configurations, with the goal of exploring and sampling all possible configuration basins of given molecules. The configuration space is high-dimensional (10,000+), hindering the use of standard data analytics approaches. The use of advanced data analytics to identify intrinsic configuration patterns could be transformative for the field.

The high-dimensional data produced by molecular simulations live on low-dimensional manifolds; the extraction of these manifolds will enable to drive detailed large-scale simulations further in the configuration space. This year, we studied how to bypass simulations by directly predicting, given a molecule formula, its possible configurations. This is done using Graph Neural Networks [89] in a generative way, producing 3D configurations. The goal is to sample all possible configurations, and with the right probability.

7.5.6. Storm trajectory prediction

Participants: Guillaume Charpiat
Collaboration: Sophie Giffard-Roisin (IRD), Claire Monteleoni (Boulder University), Balazs Kegl (LAL)

Cyclones, hurricanes or typhoons all designate a rare and complex event characterized by strong winds surrounding a low pressure area. Their trajectory and intensity forecast, crucial for the protection of persons and goods, depends on many factors at different scales and altitudes. Additionally storms have been more numerous since the 1990s, leading to both more representative and more consistent error statistics.

Currently, track and intensity forecasts are provided by numerous guidance models. Dynamical models solve the physical equations governing motions in the atmosphere. While they can provide precise results, they are computationally demanding. Statistical models are based on historical relationships between storm behavior and other parameters [82]. Current national forecasts are typically driven by consensus methods able to combine different dynamical models.

Statistical models perform poorly compared to dynamical models, although they rely on steadily increasing data resources. ML methods have scarcely been considered, despite their successes in related forecasting problems [169]. A main difficulty is to exploit spatio-temporal patterns. Another difficulty is to select and merge data coming from heterogeneous sensors. For instance, temperature and pressure are real values on a 3D spatial grid, while sea surface temperature or land indication rely on a 2D grid, wind is a 2D vector field, while many indicators such as geographical location (ocean, hemisphere...) are just real values (not fields), and displacement history is a 1D vector (time). An underlying question regards the *innate* vs *acquired* issue, and how to best combine physical models with trained models. The continuation of the work started last year [101] shows that with deep learning one can outperform the state-of-the-art in many cases [18].

7.6. Challenges

Participants: Cécile Germain, Isabelle Guyon, Adrien Pavao, Anne-Catherine Letournel, Michèle Sebag
PhD: Zhengying Liu, Lisheng Sun, Balthazar Donon
Collaborations: D. Rousseau (LAL), André Elisseeff (Google Zurich), Jean-Roch Vilmant (CERN), Antoine Marot and Benjamin Donnot (RTE), Kristin Bennett (RPI), Magali Richard (Université de Grenoble).

The TAUgroup uses challenges (scientific competitions) as a means of stimulating research in machine learning and engage a diverse community of engineers, researchers, and students to learn and contribute advancing the state-of-the-art. The TAUgroup is community lead of the open-source **Codalab** platform, hosted by Université Paris-Saclay. The project had grown in 2019 and includes now an engineer dedicated full time to administering the platform and developing challenges (Adrien Pavao), financed by a new project just starting with the Région Ile-de-France. This project will also receive the support of the Chaire Nationale d'Intelligence Artificielle of Isabelle Guyon for the next four years.

Following the highly successful ChaLearn **AutoML** Challenges (NIPS 2015 – ICML 2016 [111] – PKDD 2018 [113]), a series of challenges on the theme of **AutoDL** [129] was run in 2019 (see http://autodl.chalearn.org, addressing the problem of tuning the hyperparameters of Deep Neural Networks, including the topology of the network itself. Co-sponsored by Google Zurich, it required participants to upload their code on the Codalab platform. The series included two challenges in computer vision called **AutoCV** and **AutoCV2**, to promote automatic machine learning for image and video processing, in collaboration with University of Barcelona [45]. It also included challenges in speech processing (**AutoSpeech**), text processing (**AutoNLP**), weakly supervised learning (**AutoWeakly**) and times series (**AutoSeries**), co-organized with 4Paradigm. It culminated with launching the **AutoDL** challenge combining multiple modalities (presently on-going). The winners of each challenge open-sourced their code. GPU cloud resources were donated by Google. AutoDL was an official NeurIPS 2020 competition.

Part of the High Energy Physics activities of the team, **TrackML** [79], [80] first phase was run and co-sponsored by Kaggle, until September 2018. The second phase has been run on Codalab until March 2019, requiring code submission; algorithms were then ranked by combining accuracy and speed. The best submissions largely outperform the existing solutions. The challenge has been presented at NeurIPS [46], and at a CERN workshop[0]. I. Guyon and C. Germain are in the organizing committee, and M. Schoenauer is member of the Advisory Committee. The TAU team, in collaboration with CERN, has taken a leading role in stimulating both the ML and HEP communities to address the combinatorial complexity explosion created by the next generation of particle detectors.

A new challenge series in Reinforcement Learning was started with the company RTE France, one the theme "Learning to run a power network" [134] (**L2RPN**, http://l2rpn.chalearn.org). The goal is to test the potential of Reinforcement Learning to solve a real world problem of great practical importance: controlling electricity transportation in smart grids while keeping people and equipment safe. The first edition was run in Spring 2019 and was part of the official selection of the IJCNN 2019 conference. It ran on the Codalab platform coupled with the open source PyPower simulator of power grids interfaced with the Opengym RL framework, developed by OpenAI. In this gamified environment, the participants had to create a proper controller of a small grid of 14 nodes. Not all of them used RL, but some combinations of RL and human expertise proved to be competitive. In 2020, we will launch a new edition of the challenge with a more powerful simulator rendering the grid more realistic and capable of simulating a 118-node grid within our computational constraints. This competition was already accepted as part of the official program of IJCNN 2020.

The **HADACA** project (EIT Health) aims to run a series of challenges to promote and encourage innovations in data analysis and personalized medicine. Université de Grenoble organized a challenge on matrix factorization (https://www.medinfo-lyon.org/en/matrixen) using Codalab. The challenge gathered transdisciplinary instructors (researchers and professors), students, and health professionals (clinicians). The HADACA project contributed to create a large dataset to assess tumor heterogeneity in cancer research as well as developing innovative pedagogical methods to sensitize students to big data analysis in health. One of the products of HADACA is the ChaGrade platform (https://chagrade.lri.fr/), a tool allowing instructors to easily use challenges in the classroom, grading them as homework, and monitoring submissions and progress. HADACA will be pursued in 2020 by a sequel project also funded by EIT Health, called COMETH. The objective of COMETH will be to create an environment to conduct systematic benchmarks, based on Codalab. As a synergistic activity, TAU is also engaged in a collaboration with the Rensselaer Polytechnic Institute (RPI, New-York, USA) to use challenges in the classroom, as part of their health-informatics curriculum.

It is important to introduce **challenges in ML teaching**. This has been done (and is on-going) in I. Guyon's Licence and Master courses [38] : some assignments to Master students are to design small challenges, which are then given to Licence students in labs, and both types of students seem to love it. Codalab has also been used to implement reinforcement learning homework in the form of challenges by Victor Berger and Heri Rakotoarison for the class of Michèle Sebag. Along similar line, F. Landes proposed a challenge in the context of S. Mallat's course, at Collège de France. Finally, in collaboration with aiforgood.org, and Heri Rakotoarison has put in place a hackathon for the conference Data Science Africa (https://codalab.lri.fr/competitions/522)

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[0] https://indico.cern.ch/event/813759/

In terms of dissemination, four books were published in 2019 in the Springer series on challenges in machine learning, see http://www.chalearn.org/books.html.

TOCCATA Project-Team

7. New Results

7.1. Foundations and Spreading of Deductive Program Verification

A Why3 Framework for Reflection Proofs and its Application to GMP's Algorithms Earlier works using Why3 showed that automatically verifying the algorithms of the arbitrary-precision integer library GMP exceeds the current capabilities of automatic solvers. To complete this verification, numerous cut indications had to be supplied by the user, slowing the project to a crawl. G. Melquiond and R. Rieu-Helft extended Why3 with a framework for proofs by reflection, with minimal impact on the trusted computing base. This framework makes it easy to write dedicated decision procedures that make full use of Why3's imperative features and are formally verified. This approach opens the way to efficiently tackling the further verification of GMP's algorithms [33].

GOSPEL - Providing OCaml with a Formal Specification Language In the context of the ANR project "VOCaL" (see Sec. 9.2.2), which aims at building a formally verified OCaml library of data structures and algorithms, a specification language for OCaml is designed and implemented. It is called GOSPEL, for Generic Ocaml SPEcification Language. During his post-doc in the Toccata team, from September 2018 to August 2019, C. Lourenço implemented a parser and type checker for GOSPEL. The work on the GOSPEL language has been presented at FM'19 [23]. J.-C. Filliâtre was keynote speaker at iFM 2019 and he gave a talk on the on-going work in the VOCaL project, including GOSPEL [17].

Program Verification Competition VerifyThis 2018 VerifyThis 2018 took place on April 14 and 15, 2018 in Thessaloniki, Greece, as a satellite event of ETAPS 2018. It was the sixth edition in the VerifyThis annual competition series. Typical challenges in the VerifyThis competitions are small but intricate algorithms given in pseudo-code with an informal specification in natural language. Participants have to formalize the requirements, implement a solution, and formally verify the implementation for adherence to the specification. There are no restrictions on the programming language and verification technology used. The time frame to solve each challenge is limited to 90 minutes. Submissions are judged for correctness, completeness, and elegance. The focus includes the usability of the tools, their facilities for formalizing the properties and providing helpful output.

VerifyThis 2018 consisted of three increasingly difficult verification challenges, selected to showcase various aspects of software verification. Eleven teams (one or two participants) took part in the competition. A full report on the VerifyThis 2018 event [39] provides a presentation of the competing teams, a description of the challenges, a high-level overview of the solutions, and the results of the competition.

Proof automation with the Coq proof assistant Proof assistants based on Type Theory, such as Coq, allow the implementation of effective automatic tactics based on computational reflection. These are usually limited to a particular mathematical domain (such as linear arithmetic or ring theory). In contrast, SMTCoq is a modular and extensible tool, using external provers, which generalizes these computational approaches to combine the reasoning from multiple domains. For this, it is based on a high-level interface, which offers greater expressiveness, at the cost of more complex automation. Q. Garchery and his co-authors [22] focused on two improvements: the ability to use quantified lemmas, and the ability to use multiple representations of the same data structure. They realized a new automatic tactic, based on SMTCoq, that is expressive while keeping the modularity and the efficiency of the latter. Such a tactic thus enable scalable, low-cost automation of new domains supported by state-of-the-art automatic provers.

Certificates for Logic Transformations In a context of formal program verification, using automatic provers, the trusted code base of verification environments is typically very broad. An environment such as Why3 implements many complex procedures: generation of verification conditions, logical transformations of proof tasks, and interactions with external provers. Considering only the logical transformations of Why3, their implementation already amounts to more than 17,000 lines of OCaml code. In order to increase our confidence in the correction of such a verification tool, Garchery, Keller, Marché and Paskevich present [32] proposed a mechanism of certifying transformations, producing certificates that can be validated by an external tool, according to the *skeptical* approach. They explored two methods to validate certificates: one based on a dedicated verifier developed in OCaml, the other based on the universal proof checker Dedukti. A specificity of their certificates is to be "small grains" and composable, which makes the approach incremental, allowing to gradually add new certifying transformations.

Reasoning About Universal Cubes in MCMT The Model Checking Modulo Theories (MCMT) framework is a powerful model checking technique for verifying safety properties of parameterized transition systems. In MCMT, logical formulas are used to represent both transitions and sets of states and safety properties are verified by an SMT-based backward reachability analysis. To be fully automated, the class of formulas handled in MCMT is restricted to cubes, i.e. existentially quantified conjunction of literals. While being very expressive, cubes cannot define properties with a global termination condition, usually described by a universally quantified formula. In this work, S. Conchon and M. Roux describe BRWP, an extension of the backward reachability of MCMT for reasoning about validity properties expressed as universal cubes, that is formulas of the form $\exists i \forall j. C(i,j)$, where $C(i,j)$ is a conjunction of literals. Their approach consists in a tight cooperation between the backward reachability loop and a deductive verification engine based on weakest-precondition calculus (WP). To provide evidence for the applicability of this new algorithm, they show how to make the model checker Cubicle cooperate with Why3 [25].

A Generalized Program Verification Workflow Based on Loop Elimination and SA Form. C. Lourenço, together with Maria Frade and Jorge Sousa Pinto from Universidade do Minho, developed a minimal model of the functioning of program verification and property checking tools based on (i) the encoding of loops as non-iterating programs, either conservatively, making use of invariants and assume/assert commands, or in a bounded way; and (ii) the use of an intermediate single-assignment (SA) form. The model captures the basic workflow of tools like Boogie, Why3, or CBMC, building on a clear distinction between operational and axiomatic semantics. This allows one to consider separately the soundness of program annotation, loop encoding, translation into SA form, and verification condition (VC) generation, as well as appropriate notions of completeness for each of these processes. To the best of our knowledge, this is the first formalization of a bounded model checking of software technique, including soundness and completeness proofs using Hoare logic; they also give the first completeness proof of a deductive verification technique based on a conservative encoding of invariant-annotated loops with assume/assert in SA form, as well as the first soundness proof based on a program logic. [21]

7.2. Reasoning on mutable memory in program verification

Certified Symbolic Execution Engine using Ghost Code Symbolic execution amounts to representing sets of concrete program states as a logical formula relating the program variables, and interpreting sets of executions as a transformation of that formula. B. Becker and C. Marché formalised the correctness of a symbolic interpreter engine, expressed by an over-approximation property stating that symbolic execution covers all concrete executions, and an under-approximation property stating that no useless symbolic states are generated. This formalisation is tailored for automated verification, that is the automated discharge of verification conditions to SMT solvers. To achieve this level of automation, they appropriately annotated the code of the symbolic interpreter with an original use of both ghost data and ghost statements [20].

Ghost Monitors M. Clochard, C. Marché and A. Paskevich proposed a new approach to deductive program verification based on auxiliary programs called *ghost monitors*. This technique is useful when the syntactic structure of the target program is not well suited for verification, for example, when an essentially recursive algorithm is implemented in an iterative fashion. This new approach consists in implementing, specifying, and verifying an auxiliary program that monitors the execution of the target program, in such a way that the correctness of the monitor entails the correctness of the target. The ghost monitor maintains the necessary data and invariants to facilitate the proof. It can be implemented and verified in any suitable framework, which does not have to be related to the language of the target programs. This technique is also applicable when one wants to establish relational properties between two target programs written in different languages and having different syntactic structure.

Ghost monitors can be used to specify and prove fine-grained properties about the *infinite behaviors* of target programs. Since this cannot be easily done using existing verification frameworks, this work introduces a dedicated language for ghost monitors, with an original construction to *catch* and handle divergent executions. The soundness of the underlying program logic is established using a particular flavor of transfinite games. This language and its soundness are formalized and mechanically checked. [24]

7.3. Verification of Computer Arithmetic

Formal Verification of a State-of-the-Art Integer Square Root Even though some programs only use integer operations, the best way to understand and verify them might be to view them as fixed-point arithmetic algorithm. This is the case of the function from the GMP library that computes the square root of a 64-bit integer. The C code is short but intricate, as it implements Newton's method and it relies on magic constants and intentional arithmetic overflows. G. Melquiond and R. Rieu-Helft have verified this algorithm using the Why3 tool and automated solvers such as Gappa [28].

Round-off error and exceptional behavior analysis of explicit Runge-Kutta methods S. Boldo, F. Faissole, and A. Chapoutot developed a new fine-grained analysis of round-off errors in explicit Runge-Kutta integration methods, taking into account exceptional behaviors, such as underflow and overflow [12]. First steps towards the formalization has been done by F. Faissole [34].

Optimal Inverse Projection of Floating-Point Addition In a setting where we have intervals for the values of floating-point variables x, a, and b, we are interested in improving these intervals when the floating-point equality $x \oplus a = b$ holds. This problem is common in constraint propagation, and called the inverse projection of the addition. D. Gallois-Wong, S. Boldo, and P. Cuoq proposed floating-point theorems that provide optimal bounds for all the intervals [13].

Emulating round-to-nearest-ties-to-zero "augmented" floating- point operations using round-to-nearest-ties-to-even ari The 2019 version of the IEEE 754 Standard for Floating-Point Arithmetic recommends that new "augmented" operations should be provided for the binary formats. These operations use a new "rounding direction": round to nearest *ties-to-zero*. S. Boldo, C. Lauter, and J.-M. Muller show how they can be implemented using the currently available operations, using round-to-nearest *ties-to-even* with a partial formal proof of correctness [42].

LTI filters Several developments were made towards the efficency and accuracy of the implementation of LTI (linear time-invariant) numerical filters: a word-length optimization problem under accuracy constraints [26] by T. Hilaire, H. Ouzia, and B. Lopez, and a tight worst-case error analysis [16] by A. Volkova, T. Hilaire, and C. Lauter.

7.4. Spreading Formal Proofs

7.4.1. Real Analysis

- **Formally Verified Approximations of Definite Integrals** The CoqInterval library provides some tactics for computing and formally verifying numerical approximations of real-valued expressions inside the Coq system. In particular, it is able to compute reliable bounds on proper definite integrals [64]. A. Mahboubi, G. Melquiond, and T. Sibut-Pinote extended these algorithms to also cover some improper integrals, e.g., those with an unbounded integration domain [14]. This makes CoqInterval one of the very few tools able to produce reliable results for improper integrals, be they formally verified or not.
- **Coq Formalization of algorithms for numerical filters** D. Gallois-Wong developed a Coq formalization of a generic representation of numerical filters, called SIF [31] in order to encompass all other representations of filters, and prove useful theorems only once.
- **Complexity theory and constructive analysis** E. Neumann and F. Steinberg extended the framework for complexity of operators in analysis devised by Kawamura and Cook (2012) to allow for the treatment of a wider class of representations and applied it to the study of interval computation [15]. A. Kawamura, F. Steinberg, and H. Thies put forward a complexity class of type-two linear-time [27].

  F. Steinberg, L. Théry, and H. Thies give a number of formal proofs of theorems from the field of computable analysis. Results include that the algebraic operations and the efficient limit operator on the reals are computable, that certain countably infinite products are isomorphic to spaces of functions, compatibility of the enumeration representation of subsets of natural numbers with the abstract definition of the space of open subsets of the natural numbers, and that continuous realizability implies sequential continuity [46] [29]. F. Steinberg and H. Thies formalized proofs about Baire spaces and the isomorphy of the concrete and abstract spaces of open sets [45].

7.4.2. Formal Analysis of Debian packages

Several new results were produced in the context of the CoLiS project for the formal analysis of Debian packages. A first important step is the version 2 of the design of the CoLiS language done by B. Becker, C. Marché and other co-authors [38], that includes a modified formal syntax, a extended formal semantics, together with the design of concrete and symbolic interpreters. Those interpreters are specified and implemented in Why3, proved correct (following the initial approach for the concrete interpreter published in 2018 [60] and the recent approach for symbolic interpretation mentioned above [20]), and finally extracted to OCaml code.

To make the extracted code effective, it must be linked together with a library that implements a solver for feature constraints [61], and also a library that formally specifies the behavior of basic UNIX utilities. The latter library is documented in details in a research report [40].

A third result is a large verification campaign running the CoLiS toolbox on all the packages of the current Debian distribution. The results of this campaign were reported in another article [41] that will be presented at TACAS conference in 2020. The most visible side effect of this experiment is the discovery of bugs: more than 150 bugs report have been filled against various Debian packages.

7.4.3. Miscellaneous

- **Functional Programming.** J.-C. Filliâtre was invited speaker at JFLA 2019, as part of a session celebrating the 30 years of JFLA (a French-speaking national conference related to functional programming). He talked about 25 years of programming with OCaml [18]. At JFLA 2020, J.-C. Filliâtre will give a talk related to the elimination of non-tail calls [30].
- **Formal Verification of “ParcourSup” algorithms.** In May–July 2019, Léo Andrès (M1 student at Paris Sud) did a three month internship on the verification of the first algorithm of Parcoursup using Why3. Most of the expected properties, taken from the public description of Parcoursup’s algorithms, have been verified. Léo Andrès’s report (in French), is available on-line [37]. In June-December 2019, Benedikt Becker worked on the verification of the Java source code of ParcourSup. The findings and lessons learnt are described in a report under preparation.

Formalizing loop-carried dependencies in Coq for high-level synthesis. F. Faissole, G. Constantinides, and D. Thomas developed Coq formalizations in order to improve high-level synthesis for FPGAs [44].

TRIBE Project-Team

6. New Results

6.1. Human Mobility completion of Sparse Call Detail Records

Participants: Guangshuo Chen [Inria], Aline Carneiro Viana, Marco Fiore [CNR], Carlos Sarraute [Gran-Data].

Mobile phone data are a popular source of positioning information in many recent studies that have largely improved our understanding of human mobility. These data consist of time-stamped and geo-referenced communication events recorded by network operators, on a per-subscriber basis. They allow for unprecedented tracking of populations of millions of individuals over long time periods that span months. Nevertheless, due to the uneven processes that govern mobile communications, the sampling of user locations provided by mobile phone data tends to be sparse and irregular in time, leading to substantial gaps in the resulting trajectory information. In this work, we illustrate the severity of the problem through an empirical study of a large-scale Call Detail Records (CDR) dataset. We then propose two novel and effective techniques to reduce temporal sparsity in CDR that outperform existing ones. the fist technique performs completion (1) at nightime by identifying temporal home boundary and (2) at daytime by inferring temporal boundaries of users, i.e., the time span of the cell position associated with each communication activity. The second technique, named Context-enhanced Trajectory Reconstruction, complete individual CDR-based trajectories that hinges on tensor factorization as a core method by leveraging regularity in human movement patterns.

Our approach lets us revisit seminal works in the light of complete mobility data, unveiling potential biases that incomplete trajectories obtained from legacy CDR induce on key results about human mobility laws, trajectory uniqueness, and movement predictability. In addition, the CTR solution infers missing locations with a median displacement within two network cells from the actual position of the user, on a hourly basis and even when as little as 1% of her original mobility is known.

These works have been published at two journals: EPJ Data Science in 2019 and at Computer Communication Elsevier in 2018.

6.2. Adaptive sampling frequency of human mobility

Participants: Panagiota Katsikouli [AGORA], Aline Carneiro Viana, Marco Fiore [CNR], Diego Madariaga.

In recent years, mobile device tracking technologies based on various positioning systems have made location data collection a ubiquitous practice. Applications running on smartphones record location samples at different frequencies for varied purposes.The frequency at which location samples are recorded is usually pre-defined and fixed but can differ across applications; this naturally results in big location datasets of various resolutions. What is more, continuous recording of locations results usually in redundant information, as humans tend to spend significant amount of their time either static or in routine trips, and drains the battery of the recording device.

In this work, we aim at answering the question *"at what frequency should one sample individual human movements so that they can be reconstructed from the collected samples with minimum loss of information?"*. Our first analyses on fine-grained GPS trajectories from users around the world unveil *(i)* seemingly universal spectral properties of human mobility, and *(ii)* a linear scaling law of the localization error with respect to the sampling interval. Such results were published at a paper at IEEE Globecom 2017.

Building on these results, we challenge the idea of a fixed sampling frequency and present a lightweight mobility aware adaptive location sampling mechanism. This is an on-going work with Panagiota Katsikouli, who spent 5 months in our team working as an internship in 2017, and Diego Madariaga who spent 3 months in 2018 in our team working as an internship and has started a PhD in co-tutelle with Aline C. Viana and Javier Bustos (NIC/Univ. of Chile).

Our mechanism can serve as a standalone application for *adaptive location sampling*, or as complimentary tool alongside auxiliary sensors (such as accelerometer and gyroscope). In this work, we implemented our mechanism as an application for mobile devices and tested it on mobile users worldwide. Our experiments show that our method adjusts the sampling frequency to the mobility habits of the tracked users, it reliably tracks a mobile user incurring acceptable approximation errors and significantly reduces the energy consumption of the mobile device.

A journal paper is being prepared for submission.

6.3. Inference of human personality from mobile phones datasets

Participants: Adriano Di Luzio [Sapienza U. di Rome], Aline Carneiro Viana, Julinda Stefa [Sapienza U. di Rome], Katia Jaffres-Runser [U. of Toulouse], Alessandro Mei [Sapienza U. di Rome].

Related to human behavioral studies, personality prediction research has enjoyed a strong resurgence over the past decade. Due to the recognition that personality is predictive of a wide range of behavioral and social outcomes, the human migration to the digital environment renders also possible to base prediction of individual personality traits on digital records (i.e., datasets) mirroring human behaviors. In psychology, one of the most commonly used personality model is the Big5, based on five crucial traits and commonly abbreviated as OCEAN: Openness (O), Conscientiousness (C), Extroversion (E), Agreeableness (A), and Neuroticism (N). They are relatively stable over time, differ across individuals, and, most importantly, guide our emotions and our reactions to life circumstances. It is so for social and work situations, and even for things as simple as the way we use our smartphone. For instance, a person that is curious and open to new experiences will tend to look continuously for new places to visit and thrills to experience.

This work brings the deepest investigation in the literature on the prediction of human personality (*i.e.,* captured by the Big5 traits) from smartphone data describing daily routines and habits of individuals. This work shows that human personality can be accurately predicted by looking at the data generated by our smartphones. GPS location, calls, battery usage and charging, networking context like bluetooth devices and WiFi access points in proximity, and more give enough information about individual habits, reactions, and idiosyncrasies to make it possible to infer the psychological traits of the user. We demonstrate this by using machine learning techniques on a dataset of 55 volunteers who took a psychological test and allowed continuous collection of data from their smartphones for a time span of up to three years. Openness, Conscientiousness, Extroversion, Agreeableness, and Neuroticism (the so called Big5 personality traits) can be predicted with good accuracy even by using just a handful of features. The possible applications of our findings go from network optimization, to personal advertising, and to the detection of mental instability and social hardship in cities and neighborhoods. We also discuss the ethical concerns of our work, its privacy implications, and ways to tradeoff privacy and benefits.

A paper describing this work is under submission at ACM Transactions on Data Science (TDS) , but a technical report is also registered under the name hal-01954733.

6.4. Data offloading decision via mobile crowdsensing

Participants: Emanuel Lima [U. of Porto], Aline Carneiro Viana, Ana Aguiar [U. of Porto], Paulo Carvalho [Univ. Do Minho].

According to Cisco forecasts, mobile data traffic will grow at a compound annual growth rate of 47 % from 2016 to 2021 with smartphones surpassing four-fifths of mobile data traffic. It is known that mobile network operators are struggling to keep up with such traffic demand, and part of the solution is to offload communications to WiFi networks. Mobile data offloading systems can assist mobile devices in the decision making of when and what to offload to WiFi networks. However, due to the limited coverage of a WiFi AP, the expected offloading performance of such a system is linked with the users mobility. Unveiling and understanding human mobility patterns is a crucial issue in supporting decisions and prediction activities for mobile data offloading.

Several studies on the analysis of human mobility patterns have been carried out focusing on the identification and characterization of important locations in users' life in general. We extended these works by studying human mobility from the perspective of mobile data offloading. In our study, offloading zones are identified and characterized from individual GPS trajectories when small offloading time windows are considered. The characterization is performed in terms availability, sojourn, transition time; type and spatial characteristics. We then evaluate the offloading opportunities provided to users while they are travelling in terms of availability, time window to offload and offloading delay. We also study the mobility predictability in an offloading scenario through the theoretical and practical evaluation of several mobility predictors. The results show that (i) attending to users mobility, ten seconds is the minimum offloading time window that can be considered; (ii) offloading predictive methods can have variable performance according to the period of the day; and (iii) per-user opportunistic decision models can determine offloading system design and performance.

This work was published at ACM CHANTS 2018 and its extension will be submitted to WoWMON 2020. This is an on-going work with the the PhD Emanuel Lima (one of my co-supervision), who spent 4 months as an intern in our team in 2018, and his advisors.

6.5. Identifying how places impact each other by means of user mobility

Participants: Lucas Santos de Oliveira [EMBRACE], Pedro Olmo Stancioli [Federal U. of Minas Gerais], Aline Carneiro Viana.

The way in which city neighborhoods become popular and how people trajectory impacts the number of visitation is a fundamental area of study in traditional urban studies literature. Many works address this problem by means of user mobility prediction and POI recommendation. In a different approach, other works address the human mobility in terms of social influence which refers to the case when individuals change their behaviors persuaded by others. Nevertheless, fewer works measure influence of POI based on human mobility data.

Different from previous literature, in this work, we are interested in understanding how the neighborhood POI affect each other by means of human mobility using location-based social networks (LBSNs) data source. Key location identification in cities is a central in human mobility investigation as well as for societal problem comprehension. In this context, we propose a methodology to quantify the power of point-of-interests (POIs) in their vicinity, in terms of impact and independence – the first work in the literature (to the best of our knowledge). Different from literature, we consider the flow of people in our analysis, instead of the number of neighbor POIs or their structural locations in the city. Thus, we first modeled POI's visits using the multiflow graph model where each POI is a node and the transitions of users among POIs are a weighted direct edge. Using this multiflow graph model, we compute the attract, support and independence powers. The attract power and support power measure how many visits a POI gather from and disseminate over its neighborhood, respectively. Moreover, the independence power captures the capacity of POI to receive visitors independently from other POIs. Using a dataset describing the mobility of individuals in the Dartmouth College campus, we identify a slight dependence among buildings as well as the tendency of people to be mostly stationary in few buildings with short transit periods among them.

This work was published in ACM MobiWac 2019 [14] and an extended version is being prepared. Lucas is doing an internship in our team from Nov. 2019 to Jan. 2020.

6.6. Infering friends in the crowd in Device-to-Device communication

Participants: Rafael Lima Da Costa [CAPES], Aline Carneiro Viana, Leobino Sampaio [Federal U. of Bahia], Artur Ziviani [LNCC].

The next generation of mobile phone networks (5G) will have to deal with spectrum bottleneck and other major challenges to serve more users with high-demanding requirements. Among those are higher scalability and data rates, lower latencies and energy consumption plus reliable ubiquitous connectivity. Thus, there is a need for a better spectrum reuse and data offloading in cellular networks while meeting user expectations. According to literature, one of the 10 key enabling technologies for 5G is device-to-device (D2D) communications, an approach based on direct user involvement. Nowadays, mobile devices are attached to human daily life activities, and therefore communication architectures using context and human behavior information are promising for the future. User-centric communication arose as an alternative to increase capillarity and to offload data traffic in cellular networks through opportunistic connections among users. Although having the user as main concern, solutions in the user-centric communication/networking area still do not see the user as an individual, but as a network active element. Hence, these solutions tend to only consider user features that can be measured from the network point of view, ignoring the ones that are intrinsic from human activity (e.g., daily routines, personality traits, etc).

In this work, we first introduce the Tactful Networking paradigm, whose goal is to add perceptive senses to the network, by assigning it with human-like capabilities of observation, interpretation, and reaction to daily-life features and involved entities. To achieve this, knowledge extracted from human inherent behavior (routines, personality, interactions, preferences, among others) is leveraged, empowering user-needs learning and prediction to improve QoE while respecting privacy. We survey the area, propose a framework for enhancing human raw data to assist networking solutions and discuss the tactful networking impact through representative examples. Finally, we outline challenges and opportunities for future research. This tutorial paper is under submittion to ACM Computing and Surveys and a technical report is registered as hal-01675445.

Besides, we investigate how human-aspects and behavior can be useful to leverage future device-to-device communication. We have designed a strategy to select next-hops in a D2D communication that will be human-aware: i.e., that will consider not only available physical resources at the mobile device of a wireless neighbor, her mobility features and restrictions but also any information allowing to infer how much sharing willing she is. Such forwarders nodes will be then used at the offloading of content data through Device-to-Device (D2D) communication, from devices to the closest Mobile Edge Computing infrastructure, transforming mobile phone neighbors in service providers. The selection of next hops based on mobility behavior, resource capability as well as collaboration constitute the novelty we plan to exploit. A conference paper is under preparation and a Brazilian paper under submission to SBRC 2020.

6.7. Deciphering Predictability Limits in Human Mobility

Participants: Douglas Do Couto Teixiera, Aline Carneiro Viana, Jussara Almeida [Federal U. of Minas Gerais], Mario S. Alvim [Federal U. of Minas Gerais].

Human mobility has been studied from different perspectives. One approach addresses predictability, deriving theoretical limits on the accuracy that any prediction model can achieve in a given dataset. Measuring the predictability of any phenomenon is a very useful, but hard task, and especially so in the case of human behavior. Such complexity is due to the uncertain and heterogeneous behavior of humans, as well as to the variability of parameters influencing such behavior. Predictability is concerned with the maximum theoretical accuracy that an ideal prediction model could achieve in a scenario expressed by a given dataset. As such, unlike particular comparisons of alternative prediction models on different datasets, it does not depend on a specific prediction strategy but rather on human behavior, as captured by the available data. Besides, it does not rely on the tuning of a multitude of sensible parameters, providing instead a parameter-free view of how predictable human mobility can be (as expressed in the data).

This approach focuses on the inherent nature and fundamental patterns of human behavior captured in the dataset, filtering out factors that depend on the specificities of the prediction method adopted. In this work, we revisit the state-of-the-art method for estimating the predictability of a person's mobility, which, despite being widely adopted, suffers from low interpretability and disregards external factors that have been suggested to improve predictability estimation, notably the use of contextual information (e.g., weather, day of the week, and time of the day). We propose a new measure, *regularity*, which together with *stationarity*, helps us understand what makes a person's mobility trajectory more or less predictable, as captured by Song et al.'s technique. We show that these two simple measures are complementary and jointly are able to explain most of the variation in Song et al.'s predictability. As such, we here use them as proxies of that technique to analyze how one's mobility predictability varies.

Additionally, we investigate strategies to incorporate different types of contextual information into predictability estimates. In particular, we were the first to quantify the impact of different types of contextual information on predictability in human mobility, for different prediction tasks and datasets. Our results show that, for the next place prediction problem, the use of contextual information plays a larger role than one's history of visited locations in estimating their predictability. Finally, we propose and evaluate alternative estimates of predictability which, while being much easier to interpret, provide comparable results to the state-of-the-art. We show that these estimators, while being more interpretable, provide comparable results in terms of predictability.

This paper was published at ACM SIGSPATIAL 2019, a A+-ranked conference in our domain, and was indicated as a top-six best paper candidate. An extended version is being prepared for submission to a journal.

6.8. Identifying and profiling novelty-seeking behavior in human mobility

Participants: Licia Amichi, Aline Carneiro Viana, Mark Corvella [Boston Univ.], Antonio F. Loureiro [Federal U. of Minas Gerais].

The prediction of individuals' dynamics has attracted significant community attention and has implication for many fields: e.g. epidemic spreading, urban planning, recommendation systems. Current prediction models, however, are unable to capture uncertainties in the mobility behavior of individuals, and consequently, suffer from *the inability to predict visits to new places*. This is due to the fact that current models are oblivious to the exploration aspect of human behavior.

Many prediction models have been proposed to forecast individuals trajectories. However, they all show limited bounded predictive performance. Regardless of the applied methods (e.g., Markov chains, Naive Bayes, neural networks), the type of prediction (i.e., next-cell or next place) or the used data sets (e.g., GPS, CDR, surveys), accuracy of prediction never reaches the coveted 100%. The reasons for such limitations in the accuracy are manyfold: the lack of ground truth data, human beings' complex nature and behavior, as well the exploration phenomenon (i.e., visits to never seen before places). In this work, we focus on the exploration problem, which has rarely been tackled in the literature but indeed, represents a real issue. By construction, most prediction models attempt to forecast future locations from the set of known places, which hinders predicting new unseen places and by consequence, reduces the predictive performance.

Thus, when considering the exploration problem, previous studies either did not provide any consideration of the exploration factors of individuals, or divided the population based on properties that are not always consistent, or assumed that all individuals have the same propensity to explore. Our main goal in this work is to understand the exploration phenomenon and answer the following question: *What type of visits characterize the mobility of individuals?* Using newly designed metrics capturing spatiotemporal properties of human mobility – i.e., known/new and recurrent/intermittent visits – our strategy identifies three groups of individuals according to their degree of exploration: scouters, routineers, and regulars. In the future, we plan to deeply investigate the mobility behavior of individuals in each profile and to assign to each individual an *exploration factor* describing her susceptibility to explore.

This work was published at the Student workshop of ACM CONEXT 2019 [9]. An extended version is being prepared for submission to an int. conference.

6.9. How Geo-indistinguishability Affects Utility in Mobility-based Geographic Datasets

Participants: Adriano Di Luzio [Inria], Aline Carneiro Viana, Catuscia Palamidessi [Comete – Inria], Konstantinos Chatzikokolakis [Comete – Inria], Georgi Dikov [Comete – Inria], Julinda Stefa [Sapienza University].

Many of the scientific challenges that we face today deal with improving the quality of our everyday lives. They aim at making the cities around us smarter, more efficient, and more sustainable (e.g., how to schedule public transport during peak hours or what is the most efficient path for waste disposal). All these challenges share a common ground. They rely on datasets gathered from the real world that depict the mobility of hundreds of thousands individuals and picture, with great detail, the whereabouts of their lives—where they live, work, shop for groceries, and hangout with friends. At the same time, however, the collection of personal data also endangers the privacy of the users that to whom these data belong. To protect the privacy of the users, it is necessary to sanitize these datasets before releasing them to the public.

When we sanitize the datasets we trade the accuracy of the information they contain to protect the privacy of their users. The task of this work is to shed light on the effects of the trade-off between privacy and utility in mobility-based geographic datasets. We aim at finding out whether it is possible to protect the privacy of the users in a dataset while, at the same time, maintaining intact the utility of the information that it contains. In particular, we focus on geo-indistinguishability as a privacy-preserving sanitization methodology, and we evaluate its effects on the utility of the Geolife dataset. We test the sanitized dataset in two real world scenarios: (1) Deploying an infrastructure of WiFi hotspots to offload the mobile traffic of users living, working, or commuting in a wide geographic area; (2) Simulating the spreading of a gossip-based epidemic as the outcome of a device-to-device communication protocol. We show the extent to which the current geo-indistinguishability techniques trade privacy for utility in real world applications and we focus on their effects at the levels of the population as a whole and of single individuals.

This paper was published at the LocalRec 2019 workshop, jointly with ACM SIGSPATIAL [12].

6.10. General-purpose Low-power Secure Firmware Updates for Constrained IoT Devices

Participants: Koen Zandberg [Inria / Freie Universität Berlin], Kaspar Schleiser [Inria / Freie Universität Berlin], Francisco Acosta [Inria], Hannes Tschofenig [Arm Ltd., Cambridge, U.K], Emmanuel Baccelli.

While the IoT deployments multiply in a wide variety of verticals, the most IoT devices lack a built-in secure firmware update mechanism. Without such a mechanism, however, critical security vulnerabilities cannot be fixed, and the IoT devices can become a permanent liability, as demonstrated by recent large-scale attacks. In this paper, we survey open standards and open source libraries that provide useful building blocks for secure firmware updates for the constrained IoT devices–by which we mean low-power, microcontroller-based devices such as networked sensors/actuators with a small amount of memory,among other constraints. We design and implement a prototype that leverages these building blocks and assess the security properties of this prototype. We present experimental results including first experiments with SUIT, a new IETF standard for secure IoT firmware updates. We evaluate the performance of our implementation on a variety of commercial off-the-shelf constrained IoT devices. We conclude that it is possible to create a secure, standards-compliant firmware update solution that uses the state-of-the-art security for the IoT devices with less than 32 kB of RAM and 128 kB of flash memory. Moreover, our prototype is general-purpose, in that it works out-of-the-box or with minimal adaptation on 80% of the hardware supported by RIOT (i.e. approximately 100 different types of IoT devices). As such, this work paves the way towards generic and secure low-power IoT firmware updates.

This paper was published in the IEEE journal IEEE Access [8].

6.11. LoRa-MAB: A Flexible Simulator for Decentralized Learning Resource Allocation in IoT Networks

Participants: Duc-Tuyen Ta [LRI and Inria], Kinda Khawam [UVSQ], Samer Lahoud [ESIB], Cédric Adjih, Steven Martin [LRI, Université Paris-Saclay].

LoRaWAN is a media access control (MAC) protocol for wide area networks. It is designed to allow low-powered devices to communicate with Internet-connected applications over long-range wireless connections. The targeted dense deployment will inevitably cause a shortage of radio resources. Hence, autonomous and lightweight radio resource management is crucial to offer ultra-long battery lifetime for LoRa devices. One of the most promising solutions to such a challenge is the use of artificial intelligence. This will enable LoRa devices to use innovative and inherently distributed learning techniques, thus freeing them from draining their limited energy by constantly communicating with a centralized controller.Before proceeding with the deployment of self-managing solutions on top of a LoRaWAN application, it is sensible to conduct simulation-based studies to optimize the design of learning-based algorithms as well as the application under consideration. Unfortunately, a network simulator for such a context is not fully considered or lacks real deployment parameters. In order to address this shortcoming, we have developed an event-based simulator for resource allocation in LoRaWAN. To demonstrate the usefulness of our simulator, extensive simulations were run in a realistic environment taking into account physical phenomenon in LoRaWAN such as the capture effect and inter-spreading factor interference. The simulation results show that the proposed simulator provides a flexible and efficient environment to evaluate various network design parameters and self-management solutions as well as verify the effectiveness of distributed reinforcement-based learning algorithms for resource allocation problems in LoRaWAN.

This paper was published at the conference WCNC 2019 [15].

6.12. A Survey of Recent Extended Variants of the Traveling Salesman and Vehicle Routing Problems for Unmanned Aerial Vehicles

Participants: Ines Khoufi [Telecom SudParis], Anis Laouiti [Telecom SudParis], Cédric Adjih.

The use of Unmanned Aerial Vehicles (UAVs) is rapidly growing in popularity. Initially introduced for military purposes, over the past few years, UAVs and related technologies have successfully transitioned to a whole new range of civilian applications such as delivery, logistics, surveillance, entertainment, and so forth. They have opened new possibilities such as allowing operation in otherwise difficult or hazardous areas, for instance. For all applications, one foremost concern is the selection of the paths and trajectories of UAVs, and at the same time, UAVs control comes with many challenges, as they have limited energy, limited load capacity and are vulnerable to difficult weather conditions. Generally, efficiently operating a drone can be mathematically formalized as a path optimization problem under some constraints. This shares some commonalities with similar problems that have been extensively studied in the context of urban vehicles and it is only natural that the recent literature has extended the latter to fit aerial vehicle constraints. The knowledge of such problems, their formulation, the resolution methods proposed—through the variants induced specifically by UAVs features—are of interest for practitioners for any UAV application. Hence, in this study, we propose a review of existing literature devoted to such UAV path optimization problems, focusing specifically on the sub-class of problems that consider the mobility on a macroscopic scale. These are related to the two existing general classic ones—the Traveling Salesman Problem and the Vehicle Routing Problem. We analyze the recent literature that adapted the problems to the UAV context, provide an extensive classification and taxonomy of their problems and their formulation and also give a synthetic overview of the resolution techniques, performance metrics and obtained numerical results.

This paper was published in the journal "Drones" 2019, 3(3), 66 [5].

6.13. LoRa-MAB: Toward an Intelligent Resources Allocation Approach for LoRaWAN Networks

Participants: Duc-Tuyen Ta [LRI and Inria], Kinda Khawam [UVSQ], Samer Lahoud [ESIB], Cédric Adjih, Steven Martin [LRI, Université Paris-Saclay].

For a seamless deployment of the Internet of Things (IoT), self-managing solutions are needed to overcome the challenges of IoT, including massively dense networks and careful management of constrained resources in terms of calculation, memory, and battery. Leveraging on artificial intelligence will enable IoT devices to operate autonomously by using inherently distributed learning techniques. Fully distributed resource management will free devices from draining their limited energy by constantly communicating with a centralized controller. The present work is devoted to a specific IoT context, that of LoRaWAN, where devices communicate with the access network via ALOHA-type access and spread spectrum technology. Concurrent transmissions on different spreading factors increase the network capacity. However, the bottleneck is inevitable with the expected massive deployment of LoRa devices. To address this issue, we resort to the popular EXP3 (Exponential Weights for Exploration and Exploitation) algorithm to steer autonomously the decision of LoRa devices towards the least solicited spreading factors. Furthermore, the spreading factor selection is cast as a proportional fair optimization problem used as a benchmark for the learning-based algorithm. Extensive simulations were run in a realistic environment taking into account physical phenomena in LoRaWAN such as the capture effect and inter-spreading factor collision, as well as non-uniform device distribution. In such a realistic setting, we evaluate the performances of the EXP3.S algorithm, an efficient variant of the EXP3 algorithm, and show its relevance against the fair centralized solution and basic heuristics.

This paper was published at the conference GLOBECOM 2019 [16].

6.14. An IoT-Blockchain Architecture Based on Hyperledger Framework for Healthcare Monitoring Application

Participants: Oumaima Attia, Ines Khoufi [Telecom SudParis], Anis Laouiti [Telecom SudParis], Cédric Adjih.

Blockchains are one of the most promising technologies in the domain of the Internet of Things (IoT). At the same time, healthcare monitoring is one of IoT applications where many devices are connected, and collect data that need to be stored in a highly secure way. In this context, we focus on IoT Blockchain architectures for healthcare monitoring applications. We start our study by exploring both IoT and blockchain technologies and identify how Fabric Hyperledger is a blockchain framework that fits our application needs. In this paper, we propose a security architecture based on this framework. We validate our approach first at a design level through concrete examples, then by showing some implemented functionalities.

This paper was published at the conference NTMS 2019 [10].

TROPICAL Project-Team

7. New Results

7.1. Optimal control and zero-sum games

7.1.1. Fixed points of order preserving homogeneous maps and zero-sum games

Participants: Marianne Akian, Stéphane Gaubert.

In a series of joint works with Antoine Hochart, applied methods of non-linear fixed point theory to zero-sum games.

A key issue is the solvability of the ergodic equation associated to a zero-sum game with finite state space, i.e., given a dynamic programming operator T associated to an undiscounted problem, one looks for a vector u, called the bias, and for a scalar λ, the ergodic constant, such that $T(u) = \lambda e + u$. The bias vector is of interest as it allows to determine optimal stationnary strategies.

In [41], we studied zero-sum games with perfect information and finite action spaces, and showed that the set of payments for which the bias vector is not unique (up to an additive constant) coincides with the union of lower dimensional cells of a polyhedral complex, in particular, the bias vector is unique, generically. We provided an application to perturbation schemes in policy iteration.

In [14], we apply game theory methods to the study of the nonlinear eigenproblem for homogeneous order preserving self maps of the interior of the cone. We show that the existence and uniqueness of an eigenvector is governed by combinatorial conditions, involving dominions (sets of states “controlled” by one of the two players). In this way, we characterize the situation in which the existence of an eigenvector holds independently of perturbations, and we solve an open problem raised in [77].

7.1.2. Nonlinear fixed point methods to compute joint spectral raddi of nonnegative matrices

Participant: Stéphane Gaubert.

In [21], we introduce a non-linear fixed point method to approximate the joint spectral radius of a finite set of nonnegative matrices. We show in particular that the joint spectral radius is the limit of the eigenvalues of a family of non-linear risk-sensitive type dynamic programming operators. We develop a projective version of Krasnoselskii-Mann iteration to solve these eigenproblems, and report experimental results on large scale instances (several matrices in dimensions of order 1000 within a minute).

7.1.3. Probabilistic and max-plus approximation of Hamilton-Jacobi-Bellman equations

Participant: Marianne Akian.

We consider fully nonlinear Hamilton-Jacobi-Bellman equations associated to diffusion control problems with finite horizon involving a finite set-valued (or switching) control and possibly a continuum-valued control. In [36], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [92], [98] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [70] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [37] and [27], we improved the method of Fahim, Touzi and Warin by introducing probabilistic schemes which are monotone without any restrictive condition, allowing one to solve fully nonlinear parabolic partial differential equations with general volatilities. We studied the convergence and obtain error estimates when the parameters and the value function are bounded.

7.1.4. Tropical-SDDP algorithms for stochastic control problems involving a switching control

Participants: Marianne Akian, Duy Nghi Benoît Tran.

The PhD thesis of Benoît Tran, supervised by Jean-Philippe Chancelier (ENPC) and Marianne Akian concerns the numerical solution of the dynamic programming equation of discrete time stochastic control problems.

Several methods have been proposed in the litterature to bypass the curse of dimensionality difficulty of such an equation, by assuming a certain structure of the problem. Examples are the max-plus based method of McEneaney [99], [100], the stochastic max-plus scheme proposed by Zheng Qu [108], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [105], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [55], the probabilistic numerical method of Fahim, Touzi and Warin [70]. We propose to associate and compare these methods in order to solve more general structures.

In a first work [35], see also [24], we build a common framework for both the SDDP and a discrete time and finite horizon version of Zheng Qu's algorithm for deterministic problems involving a finite set-valued (or switching) control and a continuum-valued control. We propose an algorithm that generates monotone approximations of the value function as a pointwise supremum, or infimum, of basic (affine or quadratic for example) functions which are randomly selected. We give sufficient conditions that ensure almost sure convergence of the approximations to the value function. More recently, we study generalizations of these algorithms to the case of stochastic optimal control problems.

In a recent work, we introduce and study an entropic relaxation of the Nested Distance introduced by Pflug [106].

7.1.5. A variance reduction deflated value iteration algorithm to solve ergodic games

Participants: Marianne Akian, Stéphane Gaubert, Omar Saadi.

Recently, Sidford et al. introduced in [116] a variance reduced value iteration algorithm to solve discounted Markov decision processes. In [25], in a joint work work with Zheng Qu (Hong Kong University), we extended this algorithm to the ergodic (mean payoff) case, and also to the two-player case, exploiting techniques from non-linear spectral theory [39] and variational analysis. The deterministic version of this algorithm also yields a new method (alternative to relative value iteration) to solve ergodic problems.

7.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

7.2.1. Order isomorphisms and antimorphisms on cones

Participant: Cormac Walsh.

We have been studying non-linear operators on ordered vector spaces that preserve or reverse the order structure. A bijective map that preserves the order in both directions is called an order isomorphism, and one that reverse the order in both directions is called an order antimorphism. These maps are closely related to the isometries of the Hilbert and Thompson metrics on the interior of the cone of positive elements.

The study of the order isomorphisms of an ordered vector space goes back to Alexandrov and Zeeman, who considered maps preserving the light cone that arises in special relativity. This work was extended to more general cones by Rothaus; Noll and Schäffer; and Artstein-Avidan and Slomka. It was shown, in the finite-dimensional case, that all isomorphisms are affine if the cone has no one-dimensional factors. There are also some results in infinite dimension—however these are unsatisfactory because of the strong assumptions that must be made in order to get the finite-dimensional techniques to work. For example, a typical assumption is that the positive cone is the convex hull of its extreme rays, which is overly restrictive in infinite dimension.

In a recent preprint [34], we broaden the scope of these results, requiring only very mild assumptions, namely that the spaces involved are *complete order unit spaces*. These are ordered vector spaces whose cone of positive elements is Archimedean, and that have an order unit, such that the norm induced by this order unit is complete. We show that the existence of an order isomorphism between two such spaces implies that they are in fact linearly isomorphic as ordered vector spaces.

In addition, we introduce a necessary and sufficient criterion for all order isomorphisms on a complete order-unit space to be affine. This criterion is in terms of the geometry of the dual cone. In the current setting, the dual cone has a cross-section called the state space, whose extreme points are called pure states. The closure of the set of pure states is known as the pure state space. The criterion is then that the union of the supports of the affine dependencies supported by the pure state space is dense in the pure state space.

7.2.2. Generalization of the Hellinger distance

Participant: Stéphane Gaubert.

In [58] (joint work with Rajendra Bhatia of Ashoka University and Tanvi Jain, Indian Statistic Institute, New Delhi), we study some generalizations of the Hellinger distance to the space of positive definite matrices.

7.2.3. Spectral inequalities for nonnegative tensors and their tropical analogues

Participant: Stéphane Gaubert.

In [30] (joint work with Shmuel Friedland, University of Illinois at Chicago) we extend some characterizations and inequalities for the eigenvalues of nonnegative matrices, such as Donsker-Varadhan, Friedland-Karlin, Karlin-Ost inequalities, to nonnegative tensors. These inequalities are related to a correspondence between nonnegative tensors and ergodic control: the logarithm of the spectral radius of a tensor is given by the value of an ergodic problem in which instantaneous payments are given by a relative entropy. Some of these inequalities involve the tropical spectral radius, a limit of the spectral radius which we characterize combinatorially as the value of an ergodic Markov decision process.

7.3. Tropical algebra and convex geometry

7.3.1. Formalizing convex polyhedra in Coq

Participant: Xavier Allamigeon.

This work is joint with Ricardo Katz (Conicet, Argentina) and Pierre-Yves Strub (LIX, Ecole Polytechnique).

In [54], we have made the first steps of a formalization of the theory of convex polyhedra in the proof assistant Coq. The originality of our approach lies in the fact that our formalization is carried out in an effective way, in the sense that the basic predicates over polyhedra (emptiness, boundedness, membership, etc) are defined by means of Coq programs. All these predicates are then proven to correspond to the usual logical statements. The latter take the form of the existence of certificates: for instance, the emptiness of a polyhedron is shown to be equivalent to the existence of a certificate *a la* Farkas. This equivalence between Boolean predicates and formulas living in the kind `Prop` is implemented by using the boolean reflection methodology, and the supporting tools provided by the Mathematical Components library and its tactic language. The benefit of the effective nature of our approach is demonstrated by the fact that we easily arrive at the proof of important results on polyhedra, such as several versions of Farkas Lemma, duality theorem of linear programming, separation from convex hulls, Minkowski Theorem, etc.

Our effective approach is made possible by implementing the simplex method inside Coq, and proving its correctness and termination. Two difficulties need to be overcome to formalize it. On the one hand, we need to deal with its termination. More precisely, the simplex method iterates over the so-called bases. Its termination depends on the specification of a pivoting rule, whose aim is to determine, at each iteration, the next basis. In this work, we have focused on proving that the lexicographic rule ensures termination. On the other hand, the simplex method is actually composed of two parts. The part that we previously described, called Phase II, requires an initial basis to start with. Finding such a basis is the purpose of Phase I. It consists in building an extended problem (having a trivial initial basis), and applying to it Phase II. Both phases need to be formalized to obtain a fully functional algorithm.

The most recent advances on the project are described in the software section.

7.3.2. Tropical totally positive matrices and planar networks

Participant: Stéphane Gaubert.

In [79] (joint work with Adi Niv) we characterized the tropical analogues of totally positive and totally non-negative matrices, i.e, the images by the valuation of the corresponding classes of matrices over a non-archimedean field. We showed in particular that tropical totally positive matrices essentially coincide with the Monge matrices (defined by the positivity of 2×2 tropical minors), arising in optimal transport, and compare the set of tropical totally positive matrices with the tropicalization of the totally positive Grassmannian. A fundamental property of classical totally positive matrices is their representation as weight matrices of planar network; in the recent work [31], we studied the tropical analogue of this property.

7.3.3. Linear algebra over systems

Participants: Marianne Akian, Stéphane Gaubert.

In a joint work with Louis Rowen (Univ. Bar Ilan), we study linear algebra and convexity properties over “systems”. The latter provide a general setting encompassing extensions of the tropical semifields and hyperfields. A first account of this work was presented by Marianne Akian and Louis Rowen at the SIAM conference on applied algebraic geometry, in Bern.

7.3.4. Ambitropical convexity and Shapley retracts

Participants: Marianne Akian, Stéphane Gaubert.

Closed tropical convex cones are the most basic examples of modules over the tropical semifield. They coincide with sub-fixed-point sets of Shapley operators – dynamic programming operators of zero-sum games. We study a larger class of cones, which we call “ambitropical” as it includes both tropical cones and their duals. Ambitropical cones can be defined as lattices in the order induced by Rn. Closed ambitropical cones are precisely the fixedpoint sets of Shapley operators. They are characterized by a property of best co-approximation arising from the theory of nonexpansive retracts of normed spaces. Finitely generated ambitropical cones arise when considering Shapley operators of deterministic games with finite action spaces. Finitely generated ambitropical cones are special polyhedral complexes whose cells are alcoved poyhedra, and locally, they are in bijection with order preserving retracts of the Boolean cube This is a joint work with Sara Vannucci (invited PhD student from Salerno university). A first account of this work was presented by Stéphane Gaubert at the JAMI Workshop, Riemann-Roch theorem in characteristic one and related topics, in Baltimore.

7.3.5. Volume and integer points of tropical polytopes

Participant: Stéphane Gaubert.

We investigate in [20] (joint work with Marie McCaig) the volume of tropical polytopes, as well as the number of integer points contained in integer polytopes. We proved that even approximating these values for a tropical polytope given by its vertices is hard, with no approximation algorithm with factor $2^{\mathrm{poly}(m,n)}$ existing unless $\mathrm{P} = \mathrm{NP}$.

7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

7.4.1. Tropicalization of semidefinite programming and its relation with stochastic games

Participants: Xavier Allamigeon, Stéphane Gaubert.

Semidefinite programming consists in optimizing a linear function over a spectrahedron. The latter is a subset of $\mathbb{R}^n$ defined by linear matrix inequalities, i.e., a set of the form

$$\left\{x \in \mathbb{R}^n : Q^{(0)} + x_1 Q^{(1)} + \cdots + x_n Q^{(n)} \succeq 0\right\}$$

where the $Q^{(k)}$ are symmetric matrices of order m, and $\succeq$ denotes the Loewner order on the space of symmetric matrices. By definition, $X \succeq Y$ if and only if $X - Y$ is positive semidefinite.

Semidefinite programming is a fundamental tool in convex optimization. It is used to solve various applications from engineering sciences, and also to obtain approximate solutions or bounds for hard problems arising in combinatorial optimization and semialgebraic optimization.

A general issue in computational optimization is to develop combinatorial algorithms for semidefinite programming. Indeed, semidefinite programs are usually solved via interior point methods. However, the latter provide an approximate solution in a polynomial number of iterations, provided that a strictly feasible initial solution. Semidefinite programming becomes a much harder matter if one requires an exact solution. The feasibility problem belongs to $\mathsf{NP}_{\mathbb{R}} \cap \mathsf{coNP}_{\mathbb{R}}$, where the subscript $\mathbb{R}$ refers to the BSS model of computation. It is not known to be in NP in the bit model.

The PhD thesis of Mateusz Skomra [118] dealt about semidefinite programming, in the case where the field $\mathbb{R}$ is replaced by a nonarchimedean field, like the field of Puiseux series. In this case, methods from tropical geometry can be applied and are expected to allow one, in generic situations, to reduce semialgebraic problems to combinatorial problems, involving only the nonarchimedean valuations (leading exponents) of the coefficients of the input.

To this purpose, we studied tropical spectrahedra, which are defined as the images by the valuation of nonarchimedean spectrahedra. We establish that they are closed semilinear sets, and that, under a genericity condition, they are described by explicit inequalities expressing the nonnegativity of tropical minors of order 1 and 2. These results are presented in the preprint [52] (now accepted for publication in Disc. Comp. Geom), with further results in the PhD thesis [118].

We showed in [53] that the feasibility problem for a generic tropical spectrahedron is equivalent to solving a stochastic mean payoff game (with perfect information). The complexity of these games is a long-standing open problem. They are not known to be polynomial, however they belong to the class $\mathsf{NP} \cap \mathsf{coNP}$, and they can be solved efficiently in practice. This allows to apply stochastic game algorithms to solve nonarchimedean semidefinite feasibility problems. We obtain in this way both theoretical bounds and a practicable method which solves some large scale instances.

A long-standing problem is to characterize the convex semialgebraic sets that are SDP representable, meaning that they can be represented as the image of a spectrahedron by a (linear) projector. Helton and Nie conjectured that every convex semialgebraic set over the field of real numbers are SDP representable. Recently, [114] disproved this conjecture. In [15], we show, however, that the following result, which may be thought of as a tropical analogue of this conjecture, is true: over a real closed nonarchimedean field of Puiseux series, the convex semialgebraic sets and the projections of spectrahedra have precisely the same images by the nonarchimedean valuation. The proof relies on game theory methods and on our previous results [52] and [53].

In [50] and [118], we exploited the tropical geometry approach to introduce a condition number for stochastic mean payoff games (with perfect information). This condition number is defined as the maximal radius of a ball in Hilbert's projective metric, contained in a primal or dual feasible set. We show that the convergence time of value iteration is governed by this condition number, and derive fixed parameter tractability results.

7.4.2. Tropical polynomial systems and colorful interior of convex bodies

Participants: Marianne Akian, Marin Boyet, Xavier Allamigeon, Stéphane Gaubert.

We studied tropical polynomial systems, with motivations from call center performance evaluation (see Section 7.6.1). We introduced a notion of colorful interior of a family of convex bodies, and showed that the solution of such a polynomial system reduces to linear programming if one knows a vector in the colorful interior of an associated family of Newton polytopes. Further properties of colorful interiors were investigated, as well as the relation between tropical colorful interiors and support vector machines. These results were presented by M. Boyet at the SIAM AG conference in Bern.

7.4.3. Universal approximation theorems by log-sum-exp neural networks

Participant: Stéphane Gaubert.

This is a joint work with Giuseppe Calafiore and Corrado Possieri (Torino).

We establish universal properties of functions by neural networks with log-sum-exp activation functions, first for convex functions [19], and then in general [29]. Some consequences, including approximation by subtraction free rational expressions, are derived.

7.5. Tropical algebra, number theory and directed algebraic topology

7.5.1. An arithmetic site of Connes-Consani type for number fields with narrow class number 1

Participant: Aurélien Sagnier.

In 1995, A. Connes ([65]) gave a spectral interpretation of the zeroes of the Riemann zeta function involving the action of $\mathbb{R}_+^*$ on the sector $X = \mathbb{Q}_+^\times \backslash \mathbb{A}_\mathbb{Q} / \widehat{\mathbb{Z}}^\times$ of the adele class space $\mathbb{A}_\mathbb{Q}/\mathbb{Q}^*$ of the field of rational numbers. In [66], [68], the action of $\mathbb{R}_+^*$ on this sector X was shown to have a natural interpretation in algebraic geometry. This interpretation requires the use of topos theory as well as of the key ingredient of characteristic one namely the semifield $\mathbb{R}_{\max}$ familiar in tropical geometry. The automorphism group of this semifield is naturally isomorphic to $\mathbb{R}_+^*$ and plays the role of the Frobenius. As it turns out, its action on the points of a natural semiringed topos corresponds canonically to the above action on X. This semiringed topos is called the arithmetic site. In my PhD, I extended the construction of the arithmetic site, replacing the field of rational numbers by certain number fields. I considered the simplest complex case, namely that of imaginary quadratic fields on which we assume that the units are not reduced to ± 1 that is when K is either $\mathbb{Q}(\imath)$ or $\mathbb{Q}(\imath\sqrt{3})$. In particular, during this year, we showed that the semiring of convex polygons introduced for those cases satisfies a sublte arithmetical universal property. These results are presented in the accepted in *Journal of Number Theory* article [111]. In a further work, developed this year, I extended this construction, dealing now with number fields K with narrow class number 1, this generalization will rely on the universal property discovered this year and on the extensive use of Shintani's unit theorem. Here again tropical algebra play a crucial role in the geometrical constructions.

7.5.2. Duality between tropical modules and congruences

Participants: Stéphane Gaubert, Aurélien Sagnier.

In a joint work with Éric Goubault (LIX, École polytechnique), we establish a duality theorem between congruences and modules over tropical semifields.

7.5.3. Directed topological complexity and control

Participant: Aurélien Sagnier.

This is a joint work with Michael Farber and Eric Goubault.

The view we are taking here is that of topological complexity, as defined in [71], adapted to directed topological spaces.

Let us briefly motivate the interest of a directed topological complexity notion. It has been observed that the very important planification problem in robotics boils down to, mathematically speaking, finding a section to the path space fibration $\chi \ : \ PX = X^I \to X \times X$ with $\chi(p) = (p(0), p(1))$. If this section is continuous, then the complexity is the lowest possible (equal to one), otherwise, the minimal number of discontinuities that would encode such a section would be what is called the topological complexity of X. This topological complexity is both understandable algorithmically, and topologically, e.g. as s having a continuous section is equivalent to X being contractible. More generally speaking, the topological complexity is defined as the Schwartz genus of the path space fibration, i.e. is the minimal cardinal of partitions of $X \times X$ into "nice" subspaces F_i such that $s_{F_i} \ : \ F_i \to PX$ is continuous.

This definition perfectly fits the planification problem in robotics where there are no constraints on the actual control that can be applied to the physical apparatus that is supposed to be moved from point a to point b. In many applications, a physical apparatus may have dynamics that can be described as an ordinary differential equation in the state variables $x \in \mathbb{R}^n$ and in time t, parameterized by control parameters $u \in \mathbb{R}^p$, $\dot{x}(t) = f(t, x(t))$. These parameters are generally bounded within some set U, and, not knowing the precise control law (i.e. parameters u as a function of time t) to be applied, the way the controlled system can evolve is as one of the solutions of the differential inclusion $\dot{x}(t) \in F(t, x(t))$ where $F(t, x(t))$ is the set of all $f(t, x(t), u)$ with $u \in U$. Under some classical conditions, this differential inclusion can be proven to have solutions on at least a small interval of time, but we will not discuss this further here. Under the same conditions, the set of solutions of this differential inclusion naturally generates a dspace (a very general structure of directed space, where a preferred subset of paths is singled out, called directed paths, see e.g. [83]). Now, the planification problem in the presence of control constraints equates to finding sections to the analogues to the path space fibration (That would most probably not qualify for being called a fibration in the directed setting) taking a dipath to its end points. This notion is developed in this article, and we introduce a notion of directed homotopy equivalence that has precisely, and in a certain non technical sense, minimally, the right properties with respect to this directed version of topological complexity.

This notion of directed topological complexity also has applications in informatics where a directed space can be used to model the space of all possible executions of a concurrent process (ie when several running programs must share common limited ressources).

In the article [22], after defining the notion of directed topological complexity,this invariant (directed topological complexity) is studied for directed spheres and directed graphs.

7.6. Applications

7.6.1. Performance evaluation of emergency call centers

Participants: Xavier Allamigeon, Marin Boyet, Baptiste Colin, Stéphane Gaubert.

Since 2014, we have been collaborating with Préfecture de Police (Régis Reboul and LcL Stéphane Raclot), more specifically with Brigade de Sapeurs de Pompiers de Paris (BSPP) and Direction de Sécurité de Proximité de l'agglomération parisienne (DSPAP), on the performance evaluation of the new organization (PFAU, “Plate forme d'appels d'urgence”) to handle emergency calls to firemen and policemen in the Paris area. We developed analytical models, based on Petri nets with priorities, and fluid limits, see [46], [47], [59]. In 2019, with four students of École polytechnique, Céline Moucer, Julia Escribe, Skandère Sahli and Alban Zammit, we performed case studies, showing the improvement brought by the two level filtering procedure.

Moreover, in 2019, this work was extended to encompass the handling of health emergency calls, with a new collaboration, involving responsibles from the four services of medical emergency aid of Assistance Publique – Hôpitaux de Paris (APHP), i.e., with SAMU75, 92, 93, 94, in the framework of a project led by Dr. Christophe Leroy from APHP. As part of his PhD work, Marin Boyet developed Petri net models capturing the characteristic of the centers (CRRA) handling emergency calls the SAMU, in order to make dimensioning recommendations.

7.6.2. Game theory and optimization methods for decentralized electric systems

Participants: Stéphane Gaubert, Paulin Jacquot.

This work is in collaboration with Nadia Oudjane, Olivier Beaude and Cheng Wan (EDF Lab).

The PhD work of Paulin Jacquot concerns the application of game theory and distributed optimization techniques to the operation of decentralized electric systems, and in particlar to the management of distributed electric consumption flexibilities. We start by adopting the point of view of a centralized operator in charge of the management of flexibilities for several agents. We provide a distributed and privacy-preserving algorithm to compute consumption profiles for agents that are optimal for the operator. In the proposed method, the individual constraints as well as the individual consumption profile of each agent are never revealed to the operator or the other agents [33] [28]. A patent related to this method has been submitted [89].

Then, in a second model, we adopt a more decentralized vision and consider a game theoretic framework for the management of consumption flexibilities. This approach enables, in particular, to take into account the strategic behavior of consumers. Individual objectives are determined by dynamic billing mechanisms, which is motivated by the modeling of congestion effects occurring on time periods receiving a high electricity load from consumers. A relevant class of games in this framework is given by atomic splittable congestion games. We obtain several theoretical results on Nash equilibria for this class of games, and we quantify the efficiency of those equilibria by providing bounds on the price of anarchy. We address the question of the decentralized computation of equilibria in this context by studying the conditions and rates of convergence of the best response and projected gradients algorithms [91], [88].

A fruitful collaboration with Cheng Wan (EDF Lab) led to the third part of this PhD thesis. In this part, we consider an operator dealing with a very large number of players, for which evaluating the equilibria in a congestion game will be difficult. To address this issue, we give approximation results on the equilibria in congestion and aggregative games with a very large number of players, in the presence of coupling constraints. These results, obtained in the framework of variational inequalities and under some monotonicity conditions, can be used to compute an approximate equilibrium, solution of a small dimension problem [32]. In line with the idea of modeling large populations, we consider nonatomic congestion games with coupling constraints, with an infinity of heterogeneous players: these games arise when the characteristics of a population are described by a parametric density function. Under monotonicity hypotheses, we prove that Wardrop equilibria of such games, given as solutions of an infinite dimensional variational inequality, can be approximated by symmetric Wardrop equilibria of auxiliary games, solutions of low dimension variational inequalities. Again, those results can be the basis of tractable methods to compute an approximate Wardrop equilibrium in a nonatomic infinite-type congestion game [33]. Last, in a collaboration with Hélène Le Cadre, Cheng Wan and Clémence Alasseur, we consider a game model for the study of decentralized peer-to-peer energy exchanges between a community of consumers with renewable production sources. We study the generalized equilibria in this game, which characterize the possible energy trades and associated individual consumptions. We compare the equilibria with the centralized solution minimizing the social cost, and evaluate the efficiency of equilibria through the price of anarchy [23].

Paulin Jacquot defended his PhD on December 5, 2019 at Ecole polytechnique [90].

XPOP Project-Team

7. New Results

7.1. Modelling inheritance and variability of kinetic gene expression parameters in microbial cells

Modern experimental technologies enable monitoring of gene expression dynamics in individual cells and quantification of its variability in isogenic microbial populations. Among the sources of this variability is the randomness that affects inheritance of gene expression factors at cell division. Known parental relationships among individually observed cells provide invaluable information for the characterization of this extrinsic source of gene expression noise. Despite this fact, most existing methods to infer stochastic gene expression models from single-cell data dedicate little attention to the reconstruction of mother-daughter inheritance dynamics. Starting from a transcription and translation model of gene expression, we proposed a stochastic model for the evolution of gene expression dynamics in a population of dividing cells. Based on this model, we developed a method for the direct quantification of inheritance and variability of kinetic gene expression parameters from single-cell gene expression and lineage data. We demonstrated that our approach provides unbiased estimates of mother-daughter inheritance parameters, whereas indirect approaches using lineage information only in the post-processing of individual-cell parameters underestimate inheritance. Finally, we have shown on yeast osmotic shock response data that daughter cell parameters are largely determined by the mother, thus confirming the relevance of our method for the correct assessment of the onset of gene expression variability and the study of the transmission of regulatory factors [9].

7.2. Main effects and interactions in mixed and incomplete data frames

A mixed data frame (MDF) is a table collecting categorical, numerical and count observations. The use of MDF is widespread in statistics and the applications are numerous from abundance data in ecology to recommender systems. In many cases, an MDF exhibits simultaneously main effects, such as row, column or group effects and interactions, for which a low-rank model has often been suggested. Although the literature on low-rank approximations is very substantial, with few exceptions, existing methods do not allow to incorporate main effects and interactions while providing statistical guarantees. We proposed a new method that fills this gap [11], [3].

7.3. Quantification of gemcitabine intravenous drugs

This aim of this study was to assess the ability of Raman spectroscopy to quantify antineoplastic drugs directly in the finished product in plastic bags using a handled Raman spectrometer. Gemcitabine diluted in 0.9% sodium chloride was analyzed at various concentrations ranging from 1 to 20mg/mL directly through plastic bags using a handled 785nm Raman spectrometer.In accordance with EMA guidelines, quantitative models were developed to predict gemcitabine concentration in bag using partial least squares (PLS) regression. In order to evaluate the transposability of the developed Raman method and the routine method (flow injection analysis with UV detection), independent samples were analyzed using both techniques. The impact of the plastic bag was also evaluated by analysis samples through two different bags.The best model was obtained after standard normal variates preprocessing (SNV) for 15 latent variables. This model presented an excellent correlation between predicted and theoretical concentration values (R^2 of 0.9938 from the calibration set), a low limit of quantification (LLOQ) of 3.68mg/mL and acceptable repeatability and intermediate precision lower than the expected acceptance limit of 5% over the entire concentration range tested (except for the average concentration of 5.73mg/mL). For the 48 preparations higher than the LLOQ, the Bland-Altman approach showed the interchangeability of the wo methods with a difference bias of 2%. Moreover, no significant difference of predicted concentrations between the two containers tested ($p = 0.189$) was observed.Despite some limitations for low concentrations, this study clearly shows promising results for real-time monitoring of gemcitabine infusion preparations without removing samples. The non-invasive nature of this method should ensure the correct dose before administration to patients and with heightened safety for operators [8].

7.4. Low-rank model with covariates for count data analysis

Count data are collected in many scientific and engineering tasks including image processing, single-cell RNA sequencing and ecological studies. Such data sets often contain missing values, for example because some ecological sites cannot be reached in a certain year. In addition, in many instances, side information is also available, for example covariates about ecological sites or species. Low-rank methods are popular to denoise and impute count data, and benefit from a substantial theoretical background. Extensions accounting for covariates have been proposed, but to the best of our knowledge their theoretical and empirical properties have not been thoroughly studied, and few softwares are available for practitioners. We propose a complete methodology called LORI (Low-Rank Interaction), including a Poisson model, an algorithm, and automatic selection of the regularization parameter, to analyze count tables with covariates. We also derive an upper bound on the estimation error. We provide a simulation study with synthetic data, revealing empirically that LORI improves on state of the art methods in terms of estimation and imputation of the missing values. We illustrate how the method can be interpreted through visual displays with the analysis of a well-know plant abundance data set, and show that the LORI outputs are consistent with known results. Finally we demonstrate the relevance of the methodology by analyzing a waterbirds abundance table from the French national agency for wildlife and hunting management (ONCFS). The method is available in the R package lori on the Comprehensive Archive Network (CRAN), [10].

7.5. Imputation and low-rank estimation with Missing Non At Random data

Missing values challenge data analysis because many supervised and unsupervised learning methods cannot be applied directly to incomplete data. Matrix completion based on low-rank assumptions are very powerful solution for dealing with missing values. However, existing methods do not consider the case of informative missing values which are widely encountered in practice. We propose matrix completion methods to recover Missing Not At Random (MNAR) data. Our first contribution is to suggest a model-based estimation strategy by modelling the missing mechanism distribution. An EM algorithm is then implemented, involving a Fast Iterative Soft-Thresholding Algorithm (FISTA). Our second contribution is to suggest a computationally efficient surrogate estimation by implicitly taking into account the joint distribution of the data and the missing mechanism: the data matrix is concatenated with the mask coding for the missing values ; a low-rank structure for exponential family is assumed on this new matrix, in order to encode links between variables and missing mechanisms. The methodology that has the great advantage of handling different missing value mechanisms is robust to model specification errors, [22].

7.6. A mathematical model to predict BNP levels in hemodialysis patients

Clinical interpretation of B-Type Natriuretic Peptide (BNP) levels in hemodialysis patients (HD) for fluid management remains elusive. We conducted a retrospective observational monocentric study. We built a mathematical model to predict BNP levels, using multiple linear regressions, [12].

7.7. Analysis of the global convergence of (fast) incremental EM methods

The EM algorithm is one of the most popular algorithm for inference in latent data models. The original formulation of the EM algorithm does not scale to large data set, because the whole data set is required at each iteration of the algorithm. To alleviate this problem, Neal and Hinton (1998) have proposed an incremental version of the EM (iEM) in which at each iteration the conditional expectation of the latent data (E-step) is updated only for a mini-batch of observations. Another approach has been proposed by Cappé and Moulines (2009) in which the E-step is replaced by a stochastic approximation step, closely related to stochastic gradient.

In this study, we analyzed incremental and stochastic version of the EM algorithm in a common unifying framework. We also introduced a new version incremental version, inspired by the SAGA algorithm by Defazio et al. (2014). We established non-asymptotic convergence bounds for global convergence, [15].

7.8. Efficient Metropolis-Hastings sampling for nonlinear mixed effects models

The ability to generate samples of the random effects from their conditional distributions is fundamental for inference in mixed effects models. Random walk Metropolis is widely used to conduct such sampling, but such a method can converge slowly for high dimension problems, or when the joint structure of the distributions to sample is complex. We proposed a Metropolis-Hastings (MH) algorithm based on a multidimensional Gaussian proposal that takes into account the joint conditional distribution of the random effects and does not require any tuning, in contrast with more sophisticated samplers such as the Metropolis Adjusted Langevin Algorithm or the No-U-Turn Sampler that involve costly tuning runs or intensive computation. Indeed, this distribution is automatically obtained thanks to a Laplace approximation of the original model. We have shown that such approximation is equivalent to linearizing the model in the case of continuous data, [14], [2].