RESEARCH CENTER
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FIELD

Activity Report 2018

Section New Results

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COMETE Project-Team

6. New Results

6.1. Foundations of information hiding

Information hiding refers to the problem of protecting private information while performing certain tasks or interactions, and trying to avoid that an adversary can infer such information. This is one of the main areas of research in Comète; we are exploring several topics, described below.

6.1.1. Secure Information Flow and Game Theory

In the inference attacks studied in Quantitative Information Flow (QIF), the attacker typically tries to interfere with the system in the attempt to increase its leakage of secret information. The defender, on the other hand, typically tries to decrease leakage by introducing some controlled noise. This noise introduction can be modeled as a type of protocol composition, i.e., a probabilistic choice among different protocols, and its effect on the amount of leakage depends heavily on whether or not this choice is visible to the attacker. In [21], [11], we considered operators for modeling visible and hidden choice in protocol composition, and we studied their algebraic properties. We then formalized the interplay between defender and attacker in a game-theoretic framework adapted to the specific issues of QIF, where the payoff is information leakage. We considered various kinds of leakage games, depending on whether players act simultaneously or sequentially, and on whether or not the choices of the defender are visible to the attacker. In the case of sequential games, the choice of the second player is generally a function of the choice of the first player, and his/her probabilistic choice can be either over the possible functions (mixed strategy) or it can be on the result of the function (behavioral strategy). We showed that when the attacker moves first in a sequential game with a hidden choice, then behavioral strategies are more advantageous for the defender than mixed strategies. This contrasts with the standard game theory, where the two types of strategies are equivalent. Finally, we established a hierarchy of these games in terms of their information leakage and provide methods for finding optimal strategies (at the points of equilibrium) for both attacker and defender in the various cases.

6.1.2. The additive capacity problem for Quantitative Information Flow

Preventing information leakage is a fundamental goal in achieving confidentiality. In many practical scenarios, however, eliminating such leaks is impossible. It becomes then desirable to quantify the severity of such leaks and establish bounds on the threat they impose. Aiming at developing measures that are robust wrt a variety of operational conditions, a theory of channel capacity for the g-leakage model was developed in [25], providing solutions for several scenarios in both the multiplicative and the additive setting. In [16] we continued this line of work by providing substantial improvements over the results of [25] for additive leakage. The main idea of employing the Kantorovich distance remains, but it is now applied to quasimetrics, and in particular the novel "convex-separation" quasimetric. The benefits were threefold: first, it allowed to maximize leakage over a larger class of gain functions, most notably including the one of Shannon. Second, a solution was obtained to the problem of maximizing leakage over both priors and gain functions, left open in [25]. Third, it allowed to establish an additive variant of the " Miracle " theorem from [26].

6.1.3. Local Differential Privacy and Statistical Utility

Local differential privacy (LDP) is a variant of differential privacy (DP) where the noise is added directly on the individual records, before being collected. The main advantage with respect to DP is that we do not need a trusted third party to collect and sanitise the sensitive data of the user. 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 sanitised data it is necessary to have access to a huge collection of them. In [22], we focused on the problem of estimating the counting queries on numerical data, and we proposed a variant of LDP based on the addition of geometric noise. Such noise function is known to have appealing properties in the case of counting queries. In particular, it is universally optimal for DP, i.e., it provides the best utility for a given level of DP, regardless of the side knowledge of the attacker. We explored the properties of geometric noise for counting queries in the LDP setting, and we conjectured an optimality property, similar to the one that holds in the DP setting. In [15] we proposed a variant of LDP suitable for metric spaces, such as location data or energy consumption data, and we showed that it provides a better utility, for the same level of privacy, then the other known LPD mechanisms.

6.1.4. Information-Theoretic Methods for Feature Selection in Machine Learning

The identification of the "best" features for classification is a problem of increasing importance in machine learning. The size of available datasets is becoming larger and larger, both in terms of samples and in terms of features of the samples, and keeping the dimensionality of the data under control is necessary for avoiding an explosion of the training complexity and for the accuracy of the classification. The known methods for reducing the dimensionality can be divided in two categories: those which transform the feature space by reshaping the original features into new ones (feature extraction), and those which select a subset of the features (feature selection). Several proposals for feature selection have successfully applied concepts and techniques from information theory. In [19] we proposed a new information-theoretic algorithm for ordering the features according to their relevance for classification. The novelty of our proposal consisted in adopting Rényi min-entropy instead of the commonly used Shannon entropy. In particular, we adopted a notion of conditional min-entropy that has been recently proposed in the field of security and privacy, and that avoids the anomalies of previously-attempted information-theoretic definitions. This notion is strictly related to the Bayes error, which is a promising property for achieving accuracy in the classification. We evaluated our method on various classifiers and datasets, and we showed that it compares favorably to the corresponding one based on Shannon entropy.

6.1.5. A Logical Characterization of Differential Privacy via Behavioral Metrics

Differential privacy (DP) is a formal definition of privacy ensuring that sensitive information relative to individuals cannot be inferred by querying a database. In [18], we exploited a modeling of this framework via labeled Markov Chains (LMCs) to provide a logical characterization of differential privacy: we considered a probabilistic variant of the Hennessy-Milner logic and we defined a syntactical distance on formulae in it measuring their syntactic disparities. Then, we defined a trace distance on LMCs in terms of the syntactic distance between the sets of formulae satisfied by them. We proved that such distance corresponds to the level of privacy of the LMCs. Moreover, we used the distance on formulae to define a real-valued semantics for them, from which we 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 focused on bisimulation semantics on nondeterministic probabilistic processes and we provide 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 showed that the generalized bisimulation distance on processes is equal to the syntactic distance on their mimicking formulae. Moreover, we used the distance on mimicking formulae to obtain bounds on differential privacy.

6.1.6. Probability and Nondeterminism in Process Calculi from a Logical Perspective

Behavioral equivalences and modal logics have been successfully employed for the specification and verification of communicating concurrent systems, henceforth processes. The former ones, in particular the family of bisimulations, provide a simple and elegant tool for the comparison of the observable behavior of processes. The latter ones allow for an immediate expression of the desired properties of processes. Since the work on the Hennessy-Milner logic (HML), these two approaches are connected by means of logical characterizations of behavioral equivalences: two processes are behaviorally equivalent if and only if they satisfy the same formulae in the logic. Hence, the characterization of an equivalence subsumes both the fact that the logic is as expressive as the equivalence and the fact that the equivalence preserves the logical properties of processes.

However, the connection between behavioral equivalences and modal logics goes even further: modal decomposition of formulae exploits the characterization of an equivalence to derive its compositional properties. Roughly speaking, the definition of the semantic behavior of processes by means of the Structural Operational Semantics (SOS) framework allowed for decomposing the satisfaction problem of a formula for a process into the verification of the satisfaction problem of certain formulae for its subprocesses. In [12] we extended the SOS-driven decomposition approach to processes in which the nondeterministic behavior coexists with probability. To deal with the probabilistic behavior of processes, and thus with the decomposition of formulae characterizing it, we introduced a SOS-like machinery allowing for the specification of the behavior of open distribution terms. By our decomposition, we obtained (pre)congruence formats for probabilistic bisimilarity, ready similarity and similarity.

The combination of nondeterminism and probability in concurrent systems leads to different interpretations of process behavior. If we restrict our attention to linear properties only, we can identify three main approaches to trace and testing semantics: the trace distributions, the trace-by-trace and the extremal probabilities approaches. In [17] we proposed novel notions of behavioral metrics that are based on the three classic approaches above, and that can be used to measure the disparities in the linear behavior of processes wrt. trace and testing semantics. We studied the properties of these metrics, like non-expansiveness, and we compare their expressive powers.

6.2. Foundations of Concurrency

Distributed systems have changed substantially in the recent past with the advent of phenomena like social networks and cloud computing. In the previous incarnation of distributed computing the emphasis was on consistency, fault tolerance, resource management and related topics; these were all characterized by *interaction between processes*. Research proceeded along two lines: the algorithmic side which dominated the Principles Of Distributed Computing conferences and the more process algebraic approach epitomized by CONCUR where the emphasis was on developing compositional reasoning principles. What marks the new era of distributed systems is an emphasis on managing access to information to a much greater degree than before.

6.2.1. Real-time Rewriting Logic Semantics for Spatial Concurrent Constraint Programming

In [20] we used rewriting logic for specifying and analyzing a calculus for concurrent constraint programming (ccp) processes combining spatial and real-time behavior. These processes can run processes in different computational spaces (e.g., containers) while subject to real-time requirements (e.g., upper bounds in the execution time of a given operation), which can be specified with both discrete and dense linear time. The real-time rewriting logic semantics is fully executable in Maude with the help of rewriting modulo SMT: partial information (i.e., constraints) in the specification is represented by quantifier-free formulas on the shared variables of the system that are under the control of SMT decision procedures. The approach is used to symbolically analyze existential real-time reachability properties of process calculi in the presence of spatial hierarchies for sharing information and knowledge.

6.2.2. Characterizing Right Inverses for Spatial Constraint Systems with Applications to Modal Logic

In [14] spatial constraint systems are used to give an abstract characterization of the notion of normality in modal logic and to derive right inverse/reverse operators for modal languages. In particular, a necessary and sufficient condition for the existence of right inverses is identified and the abstract notion of normality is shown to correspond to the preservation of finite suprema. Furthermore, a taxonomy of normal right inverses is provided, identifying the greatest normal right inverse as well as the complete family of minimal right inverses. These results were applied to existing modal languages such as the weakest normal modal logic, Hennessy-Milner logic, and linear-time temporal logic. Some implications of these results were also discussed in the context of modal concepts such as bisimilarity and inconsistency invariance.

6.2.3. Observational and Behavioural Equivalences for Soft Concurrent Constraint Programming

In [13] we presented a labelled semantics for Soft Concurrent Constraint Programming (SCCP), a meta-language where concurrent agents may synchronise on a shared store by either posting or checking the satisfaction of (soft) constraints. SCCP generalises the classical formalism by parametrising the constraint system over an order-enriched monoid, thus abstractly representing the store with an element of the monoid, and the standard unlabelled semantics just observes store updates. The novel operational rules were shown to offer a sound and complete co-inductive technique to prove the original equivalence over the unlabelled semantics. Based on this characterisation, we provided an axiomatisation for finite agents.

DATASHAPE Project-Team

7. New Results

7.1. Algorithmic aspects of topological and geometric data analysis

7.1.1. DTM-based filtrations

Participants: Frédéric Chazal, Marc Glisse, Raphaël Tinarrage.

In collaboration with H. Anai, Y. Ike, H. Inakoshi and Y. Umeda of Fujitsu.

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 this paper [33], 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.

7.1.2. Persistent Homology with Dimensionality Reduction: k-Distance vs Gaussian Kernels

Participants: Shreya Arya, Jean-Daniel Boissonnat, Kunal Dutta.

We investigate the effectiveness of dimensionality reduction for computing the persistent homology for both k-distance and kernel distance [34]. For k-distance, we show that the standard Johnson-Lindenstrauss reduction preserves the k-distance, which preserves the persistent homology upto a $(1-\varepsilon)^{-1}$ factor with target dimension $O(k\log n/\varepsilon^2)$. We also prove a concentration inequality for sums of dependent chi-squared random variables, which, under some conditions, allows the persistent homology to be preserved in $O(\log n/\varepsilon^2)$ dimensions. This answers an open question of Sheehy. For Gaussian kernels, we show that the standard Johnson-Lindenstrauss reduction preserves the persistent homology up to an $4(1-\epsilon)^{-1}$ factor.

7.1.3. Computing Persistent Homology of Flag Complexes via Strong Collapses

Participants: Jean-Daniel Boissonnat, Siddharth Pritam.

In collaboration with Divyansh Pareek (Indian Institute of Technology Bombay, India)

We introduce a fast and memory efficient approach to compute the persistent homology (PH) of a sequence of simplicial complexes. The basic idea is to simplify the complexes of the input sequence by using strong collapses, as introduced by J. Barmak and E. Miniam [DCG (2012)], and to compute the PH of an induced sequence of reduced simplicial complexes that has the same PH as the initial one. Our approach has several salient features that distinguishes it from previous work. It is not limited to filtrations (i.e. sequences of nested simplicial subcomplexes) but works for other types of sequences like towers and zigzags. To strong collapse a simplicial complex, we only need to store the maximal simplices of the complex, not the full set of all its simplices, which saves a lot of space and time. Moreover, the complexes in the sequence can be strong collapsed independently and in parallel. Finally, we can compromize between precision and time by choosing the number of simplicial complexes of the sequence we strong collapse. As a result and as demonstrated by numerous experiments on publicly available data sets, our approach is extremely fast and memory efficient in practice [27].

7.1.4. Strong Collapse for Persistence

Participants: Jean-Daniel Boissonnat, Siddharth Pritam.

In this paper, we build on the initial success of and show that further decisive progress can be obtained if one restricts the family of simplicial complexes to flag complexes. Flag complexes are fully characterized by their graph (or 1-skeleton), the other faces being obtained by computing the cliques of the graph. Hence, a flag complex can be represented by its graph, which is a very compact representation. Flag complexes are very popular and, in particular, Vietoris-Rips complexes are by far the most widely simplicial complexes used in Topological Data Analysis. It has been shown in that the persistent homology of Vietoris-Rips filtrations can be computed very efficiently using strong collapses. However, most of the time was devoted to computing the maximal cliques of the complex prior to their strong collapse. In this paper [37], we observe that the reduced complex obtained by strong collapsing a flag complex is itself a flag complex. Moreover, this reduced complex can be computed using only the 1-skeleton (or graph) of the complex, not the set of its maximal cliques. Finally, we show how to compute the equivalent filtration of the sequence of reduced flag simplicial complexes using again only 1-skeletons. x On the theory side, we show that strong collapses of flag complexes can be computed in time $O(v^2k^2)$ where v is the number of vertices of the complex and k the maximal degree of its graph. The algorithm described in this paper has been implemented and the code will be soon released in the Gudhi library. Numerous experiments show that our method outperforms previous methods, e.g. Ripser.

7.1.5. Triangulating submanifolds: An elementary and quantified version of Whitney's method

Participants: Jean-Daniel Boissonnat, Siargey Kachanovich, Mathijs Wintraecken.

We quantize Whitney's construction to prove the existence of a triangulation for any C^2 manifold, so that we get an algorithm with explicit bounds. We also give a new elementary proof, which is completely geometric [36].

7.1.6. Randomized incremental construction of Delaunay triangulations of nice point sets

Participants: Jean-Daniel Boissonnat, Kunal Dutta, Marc Glisse.

In collaboration with Olivier Devillers (Inria, CNRS, Loria, Université de Lorraine).

Randomized incremental construction (RIC) is one of the most important paradigms for building geometric data structures. Clarkson and Shor developed a general theory that led to numerous algorithms that are both simple and efficient in theory and in practice.

Randomized incremental constructions are most of the time space and time optimal in the worst-case, as exemplified by the construction of convex hulls, Delaunay triangulations and arrangements of line segments.

However, the worst-case scenario occurs rarely in practice and we would like to understand how RIC behaves when the input is nice in the sense that the associated output is significantly smaller than in the worst-case. For example, it is known that the Delaunay triangulations of nicely distributed points in $\mathbb{R}^d$ or on polyhedral surfaces in $\mathbb{R}^3$ has linear complexity, as opposed to a worst-case complexity of $\Theta(n^{\lfloor d/2 \rfloor})$ in the first case and quadratic in the second. The standard analysis does not provide accurate bounds on the complexity of such cases and we aim at establishing such bounds in this paper [35]. More precisely, we will show that, in the two cases above and variants of them, the complexity of the usual RIC is $O(n \log n)$, which is optimal. In other words, without any modification, RIC nicely adapts to good cases of practical value.

Along the way, we prove a probabilistic lemma for sampling without replacement, which may be of independent interest.

7.1.7. Approximate Polytope Membership Queries

Participant: Guilherme Da Fonseca.

In collaboration with Sunil Arya (Hong Kong University of Science and Technology) and David Mount (University of Maryland).

In the polytope membership problem, a convex polytope K in $\mathbb{R}^d$ is given, and the objective is to preprocess K into a data structure so that, given any query point $q \in \mathbb{R}^d$, it is possible to determine efficiently whether $q \in K$. We consider this problem in an approximate setting. Given an approximation parameter ϵ, the query can be answered either way if the distance from q to K's boundary is at most ϵ times K's diameter. We assume that the dimension d is fixed, and K is presented as the intersection of n halfspaces. Previous solutions to approximate polytope membership were based on straightforward applications of classic polytope approximation techniques by Dudley (1974) and Bentley et al. (1982). The former is optimal in the worst-case with respect to space, and the latter is optimal with respect to query time. We present four main results. First, we show how to combine the two above techniques to obtain a simple space-time trade-off. Second, we present an algorithm that dramatically improves this trade-off. In particular, for any constant $\alpha \geq 4$, this data structure achieves query time roughly $O(1/\epsilon^{(d-1)/\alpha})$ and space roughly $O(1/\epsilon^{(d-1)(1-\Omega(\log \alpha))/\alpha})$. We do not know whether this space bound is tight, but our third result shows that there is a convex body such that our algorithm achieves a space of at least $\Omega(1/\epsilon^{(d-1)(1-O(\sqrt{\alpha}))/\alpha})$. Our fourth result shows that it is possible to reduce approximate Euclidean nearest neighbor searching to approximate polytope membership queries. Combined with the above results, this provides significant improvements to the best known space-time trade-offs for approximate nearest neighbor searching in $\mathbb{R}^d$. For example, we show that it is possible to achieve a query time of roughly $O(\log n + 1/\epsilon^{d/4})$ with space roughly $O(n/\epsilon^{d/4})$, thus reducing by half the exponent in the space bound [11].

7.1.8. Approximate Convex Intersection Detection with Applications to Width and Minkowski Sums

Participant: Guilherme Da Fonseca.

In collaboration with Sunil Arya (Hong Kong University of Science and Technology) and David Mount (University of Maryland).

Approximation problems involving a single convex body in d-dimensional space have received a great deal of attention in the computational geometry community. In contrast, works involving multiple convex bodies are generally limited to dimensions $d \leq 3$ and/or do not consider approximation. In this paper, we consider approximations to two natural problems involving multiple convex bodies: detecting whether two polytopes intersect and computing their Minkowski sum. Given an approximation parameter $\epsilon > 0$, we show how to independently preprocess two polytopes A, B into data structures of size $O(1/\epsilon^{(d-1)/2})$ such that we can answer in polylogarithmic time whether A and B intersect approximately. More generally, we can answer this for the images of A and B under affine transformations. Next, we show how to ϵ-approximate the Minkowski sum of two given polytopes defined as the intersection of n halfspaces in $O(n \log(1/\epsilon) + 1/\epsilon^{(d-1)/2+\alpha})$ time, for any constant $\alpha > 0$. Finally, we present a surprising impact of these results to a well studied problem that considers a single convex body. We show how to ϵ-approximate the width of a set of n points in $O(n \log(1/\epsilon) + 1/\epsilon^{(d-1)/2+\alpha})$ time, for any constant $\alpha > 0$, a major improvement over the previous bound of roughly $O(n + 1/\epsilon^{d-1})$ time [22].

7.1.9. Approximating the Spectrum of a Graph

Participant: David Cohen-Steiner.

In collaboration with Weihao Kong (Stanford University), Christian Sohler (TU Dortmund) and Gregory Valiant (Stanford University).

The spectrum of a network or graph $G = (V, E)$ with adjacency matrix A , consists of the eigenvalues of the normalized Laplacian $L = I - D^{-1/2}AD^{-1/2}$. This set of eigenvalues encapsulates many aspects of the structure of the graph, including the extent to which the graph posses community structures at multiple scales. We study the problem of approximating the spectrum, $\lambda = (\lambda_1, \cdots, \lambda_{|V|})$, of G in the regime where the graph is too large to explicitly calculate the spectrum. We present a sublinear time algorithm that, given the ability to query a random node in the graph and select a random neighbor of a given node, computes a succinct representation of an approximation $\widetilde{\lambda} = (\widetilde{\lambda}_1, \cdots, \widetilde{\lambda}_{|V|})$, such that $\|\widetilde{\lambda} - \lambda\|_1 \leq \varepsilon|V|$. Our algorithm has query complexity and running time $\exp(O(1/\varepsilon))$, which is independent of the size of the graph, $|V|$. We demonstrate the practical viability of our algorithm on synthetically generated graphs, and on 15 different real-world graphs from the Stanford Large Network Dataset Collection, including social networks, academic collaboration graphs, and road networks. For the smallest of these graphs, we are able to validate the accuracy of our algorithm by explicitly calculating the true spectrum; for the larger graphs, such a calculation is computationally prohibitive. The spectra of these real-world networks reveal insights into the structural similarities and differences between them, illustrating the potential value of our algorithm for efficiently approximating the spectrum of large networks [29].

7.1.10. Spectral Properties of Radial Kernels and Clustering in High Dimensions

Participants: David Cohen-Steiner, Alba Chiara de Vitis.

In this paper [40], we study the spectrum and the eigenvectors of radial kernels for mixtures of distributions in $\mathbb{R}^n$. Our approach focuses on high dimensions and relies solely on the concentration properties of the components in the mixture. We give several results describing of the structure of kernel matrices for a sample drawn from such a mixture. Based on these results, we analyze the ability of kernel PCA to cluster high dimensional mixtures. In particular, we exhibit a specific kernel leading to a simple spectral algorithm for clustering mixtures with possibly common means but different covariance matrices. This algorithm will succeed if the angle between any two covariance matrices in the mixture (seen as vectors in $\mathbb{R}^{n^2}$) is larger than $\Omega(n^{-1/6}\log^{5/3} n)$. In particular, the required angular separation tends to 0 as the dimension tends to infinity. To the best of our knowledge, this is the first polynomial time algorithm for clustering such mixtures beyond the Gaussian case.

7.1.11. 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 [44] 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.

7.1.12. A Comparison Framework for Interleaved Persistence Modules

Participant: Miroslav Kramár.

In collaboration with Rachel Levanger (UPenn), Shaun Harker and Konstantin Mischaikow (Rutgers).

In [43], we present a generalization of the induced matching theorem of [1] and use it to prove a generalization of the algebraic stability theorem for R-indexed pointwise finite-dimensional persistence modules. Via numerous examples, we show how the generalized algebraic stability theorem enables the computation of rigorous error bounds in the space of persistence diagrams that go beyond the typical formulation in terms of bottleneck (or log bottleneck) distance.

7.1.13. 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 [45].

7.2. Statistical aspects of topological and geometric data analysis

7.2.1. Robust Bregman Clustering

Participants: Claire Brécheteau, Clément Levrard.

In collaboration with Aurélie Fischer (Université Paris-Diderot).

Using a trimming approach, in [38], we investigate a k-means type method based on Bregman divergences for clustering data possibly corrupted with clutter noise. The main interest of Bregman divergences is that the standard Lloyd algorithm adapts to these distortion measures, and they are well-suited for clustering data sampled according to mixture models from exponential families. We prove that there exists an optimal codebook, and that an empirically optimal codebook converges a.s. to an optimal codebook in the distortion sense. Moreover, we obtain the sub-Gaussian rate of convergence for k-means 1 $\sqrt{}$ n under mild tail assumptions. Also, we derive a Lloyd-type algorithm with a trimming parameter that can be selected from data according to some heuristic, and present some experimental results.

7.2.2. Statistical analysis and parameter selection for Mapper

Participants: Mathieu Carrière, Bertrand Michel, Steve Oudot.

In [15] we study the question of the statistical convergence of the 1-dimensional Mapper to its continuous analogue, the Reeb graph. We show that the Mapper is an optimal estimator of the Reeb graph, which gives, as a byproduct, a method to automatically tune its parameters and compute confidence regions on its topological features, such as its loops and flares. This allows to circumvent the issue of testing a large grid of parameters and keeping the most stable ones in the brute-force setting, which is widely used in visualization, clustering and feature selection with the Mapper.

7.2.3. A Fuzzy Clustering Algorithm for the Mode-Seeking Framework

Participants: Thomas Bonis, Steve Oudot.

In [13] we propose a new soft clustering algorithm based on the mode-seeking framework. Given a point cloud in $\mathbb{R}^d$, we define regions of high density that we call cluster cores, then we implement a random walk on a neighborhood graph built on top of the data points. This random walk is designed in such a way that it is attracted by high-density regions, the intensity of the attraction being controlled by a temperature parameter $\beta > 0$. The membership of a point to a given cluster is then the probability for the random walk starting at this point to hit the corresponding cluster core before any other. While many properties of random walks (such as hitting times, commute distances, etc) are known to eventually encode purely local information when the number of data points grows to infinity, the regularization introduced by the use of cluster cores allows the output of our algorithm to converge to quantities involving the global structure of the underlying density function. Empirically, we show how the choice of β influences the behavior of our algorithm: for small values of β the result is really close to hard mode-seeking, while for values of β close to 1 the result is similar to the output of the (soft) spectral clustering. We also demonstrate the scalability of our approach experimentally.

7.2.4. Large Scale computation of Means and Clusters for Persistence Diagrams using Optimal Transport

Participants: Théo Lacombe, Steve Oudot.

In collaboration with Marco Cuturi (ENSAE).

Persistence diagrams (PDs) are at the core of topological data analysis. They provide succinct descriptors encoding the underlying topology of sophisticated data. PDs are backed-up by strong theoretical results regarding their stability and have been used in various learning contexts. However, they do not live in a space naturally endowed with a Hilbert structure where natural metrics are not even differentiable, thus not suited to optimization process. Therefore, basic statistical notions such as the barycenter of a finite sample of PDs are not properly defined. In [30] we provide a theoretically good and computationally tractable framework to estimate the barycenter of a set of persistence diagrams. This construction is based on the theory of Optimal Transport (OT) and endows the space of PDs with a metric inspired from regularized Wasserstein distances.

7.2.5. The k-PDTM : a coreset for robust geometric inference

Participants: Claire Brécheteau, Clément Levrard.

Analyzing the sub-level sets of the distance to a compact sub-manifold of $\mathbb{R}^d$ is a common method in TDA to understand its topology. The distance to measure (DTM) was introduced by Chazal, Cohen-Steiner and Mérigot to face the non-robustness of the distance to a compact set to noise and outliers. This function makes possible the inference of the topology of a compact subset of $\mathbb{R}^d$ from a noisy cloud of n points lying nearby in the Wasserstein sense. In practice, these sub-level sets may be computed using approximations of the DTM such as the q-witnessed distance or other power distance. These approaches lead eventually to compute the homology of unions of n growing balls, that might become intractable whenever n is large. To simultaneously face the two problems of large number of points and noise, we introduce in [39] the k-power distance to measure (k-PDTM). This new approximation of the distance to measure may be thought of as a k-coreset based approximation of the DTM. Its sublevel sets consist in union of k-balls, $k << n$, and this distance is also proved robust to noise. We assess the quality of this approximation for k possibly dramatically smaller than n, for instance $k = n13$ is proved to be optimal for 2-dimensional shapes. We also provide an algorithm to compute this k-PDTM.

7.2.6. The density of expected persistence diagrams and its kernel based estimation

Participants: Frédéric Chazal, Vincent Divol.

Persistence diagrams play a fundamental role in Topological Data Analysis where they are used as topological descriptors of filtrations built on top of data. They consist in discrete multisets of points in the plane $\mathbb{R}^2$ that can equivalently be seen as discrete measures in $\mathbb{R}^2$. When the data come as a random point cloud, these discrete measures become random measures whose expectation is studied in this paper. In [28] we first show that for a wide class of filtrations, including the Čech and Rips-Vietoris filtrations, the expected persistence diagram, that is a deterministic measure on $\mathbb{R}^2$, has a density with respect to the Lebesgue measure. Second, building on the previous result we show that the persistence surface recently introduced by Adams et al can be seen as a kernel estimator of this density. We propose a cross-validation scheme for selecting an optimal bandwidth, which is proven to be a consistent procedure to estimate the density.

7.2.7. 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 [42], 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 X_n is an i.i.d. sample from a density on $[0,1]^d$. For the Cech 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 persistence of such diagrams. Both approaches 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 $\alpha \geq d$.

7.2.8. Estimating the Reach of a Manifold

Participants: Frédéric Chazal, Bertrand Michel.

In collaboration with E. Aamari (CNRS Paris 7), J.Kim, A. Rinaldo and L. Wasserman (Carnegie Mellon University).

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. [32] 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 a framework where tangent spaces are known, and bounds assessing its efficiency are derived. In the case of i.i.d. random point cloud $\mathbb{X}_n$, $\tau(\mathbb{X}_n)$ is showed to achieve uniform expected loss bounds over a $\mathcal{C}^3$-like model. Finally, we obtain upper and lower bounds on the minimax rate for estimating the reach.

7.2.9. Robust Topological Inference: Distance To a Measure and Kernel Distance

Participants: Frédéric Chazal, Bertrand Michel.

In collaboration with B. Fasy (Univ. Montana) and F. Lecci, A. Rinaldo and L. Wasserman (Carnegie Mellon University).

Let P be a distribution with support S. The salient features of S can be quantified with persistent homology, which summarizes topological features of the sublevel sets of the distance function (the distance of any point x to S). Given a sample from P we can infer the persistent homology using an empirical version of the distance function. However, the empirical distance function is highly non-robust to noise and outliers. Even one outlier is deadly. The distance-to-a-measure (DTM), introduced by Chazal et al. (2011), and the kernel distance, introduced by Phillips et al. (2014), are smooth functions that provide useful topological information but are robust to noise and outliers. Chazal et al. (2015) derived concentration bounds for DTM. Building on these results, in [16], we derive limiting distributions and confidence sets, and we propose a method for choosing tuning parameters.

7.3. Topological approach for multimodal data processing

7.3.1. Barcode Embeddings for Metric Graphs

Participants: Steve Oudot, Yitchzak Solomon.

Stable topological invariants are a cornerstone of persistence theory and applied topology, but their discriminative properties are often poorly-understood. In [46] we study a rich homology-based invariant first defined by Dey, Shi, and Wang, which we think of as embedding a metric graph in the barcode space. We prove that this invariant is locally injective on the space of metric graphs and globally injective on a GH-dense subset. Moreover, we define a new topology on MGraphs, which we call the fibered topology, for which the barcode transform is injective on a generic (open and dense) subset.

7.3.2. Inverse Problems in Topological Persistence: a Survey

Participants: Steve Oudot, Yitchzak Solomon.

In [47] 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 right inverses, and the second half focuses on injectivity, i.e. left inverses. Throughout, we highlight the tools and theorems that underlie these advances, and direct the reader's attention to open problems, both theoretical and applied.

7.4. Experimental research and software development

7.4.1. Activity recognition from stride detection: a machine learning approach based on geometric patterns and trajectory reconstruction.

Participants: Bertrand Beaufils, Frédéric Chazal, Bertrand Michel.

In collaboration with M. Grelet (Sysnav).

In [23] algorithm for activity recognition is proposed using inertial sensors worn on the ankle. This innovative approach based on geometric patterns uses a stride detector that can detect both normal walking strides and atypical strides such as small steps, side steps and backward walking that existing methods struggle to detect. It is also robust in critical situations, when for example the wearer is sitting and moving the ankle, while most algorithms in the literature would wrongly detect strides. A technique inspired by Zero Velocity Update is used on the stride detection to compute the trajectory of the device. It allows to compute relevant features for the activity recognition learning task. Compared to most algorithms in the literature, this method does not use fixed-size sliding window that could be too short to provide enough information or too long and leads to overlapping issue when the window covers two different activities.

7.4.2. Dynamics of silo deformation under granular discharge

Participant: Miroslav Kramár.

In collaboration with Claudia Colonnello.

In [17], we use Topological Data Analysis to study the post buckling behavior of laboratory scale cylindrical silos under gravity driven granular discharges. Thin walled silos buckle during the discharge if the initial height of the granular column is large enough. The deformation of the silo is reversible as long as the filling height does not exceed a critical value, Lc. Beyond this threshold the deformation becomes permanent and the silo often collapses. We study the dynamics of reversible and irreversible deformation processes, varying the initial filling height around Lc. We find that all reversible processes exhibit striking similarities and they alternate between regimes of slow and fast dynamics. The patterns that occur at the beginning of irreversible deformation processes are topologically very similar to those that arise during reversible processes. However, the dynamics of reversible and irreversible processes is significantly different. In particular, the evolution of irreversible processes is much faster. This allows us to make an early prediction of the collapse of the silo based solely on observations of the deformation patterns.

7.4.3. Characterizing Granular Networks Using Topological Metrics

Participant: Miroslav Kramár.

In collaboration with Joshua Dijksman (Duke Physics), Lenka Kovalcinova and Lou Kondic (NJIT), Jie Ren (Merck Research Lab), Robert Behringer (Duke), and Konstantin Mischaikow (Rutgers).

In [18], we carry out a direct comparison of experimental and numerical realizations of the exact same granular system as it undergoes shear jamming. We adjust the numerical methods used to optimally represent the experimental settings and outcomes up to microscopic contact force dynamics. Measures presented here range form microscopic, through mesoscopic to system-wide characteristics of the system. Topological properties of the mesoscopic force networks provide a key link between mi-cro and macro scales. We report two main findings: the number of particles in the packing that have at least two contacts is a good predictor for the mechanical state of the system, regardless of strain history and packing density. All measures explored in both experiments and numerics, including stress tensor derived measures and contact numbers depend in a universal manner on the fraction of non-rattler particles, fNR. The force network topology also tends to show this universality, yet the shape of the master curve depends much more on the details of the numerical simulations. In particular we show that adding force noise to the numerical data set can significantly alter the topological features in the data. We conclude that both fNR and topological metrics are useful measures to consider when quantifying the state of a granular system.

7.5. Miscellaneous

7.5.1. On Order Types of Random Point Sets

Participant: Marc Glisse.

In collaboration with Olivier Devillers and Xavier Goaoc (Inria team Gamble) and Philippe Duchon (LaBRI, Université de Bordeaux).

Let P be a set of n random points chosen uniformly in the unit square. In this paper [41], we examine the typical resolution of the order type of P. First, we show that with high probability, P can be rounded to the grid of step $\frac{1}{n^{3+\epsilon}}$ without changing its order type. Second, we study algorithms for determining the order type of a point set in terms of the number of coordinate bits they require to know. We give an algorithm that requires on average $4n\log_2 n + O(n)$ bits to determine the order type of P, and show that any algorithm requires at least $4n\log_2 n - O(n\log\log n)$ bits. Both results extend to more general models of random point sets.

DEDUCTEAM Project-Team

7. New Results

7.1. $\lambda\Pi$-calculus modulo theory

Gilles Dowek, Jean-Pierre Jouannaud and Jiaxiang Liu have started a program for developing new techniques for proving confluence of dependently typed theories, which do not rely on termination. These results have been presented at Types 2016, and will be submitted to a Journal early 2019. Target applications for these techniques are encodings of the Calculus of inductive constructions with polymorphic universes in the $\lambda\Pi$-calculus modulo theory.

Frédéric Blanqui has published in the Journal of Functional Programming a long article synthesizing his work on the use of size annotations for proving termination [12]. This paper provides a general and modular criterion for the termination of simply-typed λ-calculus extended with function symbols defined by user-defined rewrite rules. Following a work of Hughes, Pareto and Sabry, for functions defined with a fixpoint operator and pattern-matching, several criteria use typing rules for bounding the height of arguments in function calls. In this paper, we extend this approach to rewriting-based function definitions and more general user-defined notions of size.

Size-change termination is a technique introduced for first-order functional programs. In [16], Frédéric Blanqui and Guillaume Genestier show how it can be used to study the termination of higher-order rewriting in the $\lambda\Pi$-calculus modulo theory.

Dependency pairs are a key concept at the core of modern automated termination provers for first-order term rewrite systems. In [22], Frédéric Blanqui, Guillaume Genestier and Olivier Hermant introduced an extension of this technique for a large class of dependently-typed higher-order rewrite systems. This improves previous results by Wahlstedt on one hand and Frédéric Blanqui on the other hand to strong normalization and non-orthogonal rewrite systems. This new criterion has been implemented in the type-checker DEDUKTI.

7.2. Dedukti

Frédéric Blanqui and Guillaume Genestier have formally defined the operational semantics of DEDUKTI 2.5, showing some problems with non left-linear rewrite rules.

Rodolphe Lepigre, Frédéric Blanqui and Franck Slama developed a new version of DEDUKTI, available on https://github.com/Deducteam/lambdapi, with meta-variables and a small set of tactics in order to be able to build DEDUKTI proofs interactively.

Aristomenis-Dionysios Papadopoulos has added a rewrite tactic in the style of Ssreflect [27].

Emilio Gallego added an LSP server for communicating with editors.

Ismail Lachheb has developed a plugin for DEDUKTI based on the LSP protocol into the Atom editor [25].

Guillaume Burel added support for polarized Deduction modulo theory in DEDUKTI.

Quentin Ye has developed an algorithm to compare λ-terms. The main point was to take sharing into account, so as to relate the complexity with the space used to represent the term, rather than with the size of the term. He has implemented this algorithm in the DEDUKTI codebase. He has also run his algorithm on examples that show an exponential speed-up compared to the naive algorithm [21].

7.3. Theories

Gaspard Férey and François Thiré defined a new encoding for Cumulative type systems (CTS) in the $\lambda\Pi$-calculus modulo theory, extending the work of Ali Assaf's PhD [28]. This encoding relies on explicit subtyping which requires additional computational rules. It provides a way to encode a larger class of CTS, which sheds a new light on the computational content of explicit subtyping. This encoding should be extendable to express more advanced features such as universe polymorphism in the Calculus of Inductive Construction, a first step to have a faithful encoding of the COQ system. The encoding has been proven correct under the hypothesis that the computational rules are confluent.

François Thiré redesigned the tool UNIVERSO, so that it can be used for a larger class of CTS. The specification for UNIVERSO can be given by rewrite rules which makes UNIVERSO much easier to use. This tool is a first step to have an automatic chain of translations to translate proofs in the encoding of MATITA to $STT\forall_{\beta\delta}$.which would make these proofs interoperable with 5 different systems.

François Thiré changed the encoding provided by KRAJONO to integrate some ideas of the encoding discussed above. This encoding is compatible with the tool UNIVERSO.

Gaspard Férey updated the COQINE software to translate COQ's 8.8 version. In this version, the standard library relies on universe polymorphism so partial support for the translation of this feature was integrated. Since encodings of the many features of Coq (inductive constructions, floating universes, several kinds of universe polymorphisms, etc) are a current work in progress, the software was made parameterizable to allow experimentations of multiple encodings of these features.

Gaspard Férey showcased an encoding of the Calculus of Inductive Constructions (CiC) relying on associative-commutative (AC) rewriting on the arithmetic library translated from MATITA. This practical experiment shows the limitations of AC-rewriting (as implemented in DEDUKTI) in terms of performance and the need for special care when defining encodings relying on this feature.

Guillaume Burel began to write a tool translating SAT proof traces in LRAT format into DEDUKTI proofs. The main issue was that steps in LRAT traces are not logical consequences of previous clauses but only preserve provability.

Mohamed Yacine El Haddad developed a tool to extract TPTP problems from a TSTP trace (generated by automated theorem provers) and reconstruct the proof of the trace in DEDUKTI format.

Bruno Barras has started to develop a model of Homotopy Type Theory (HoTT) in DEDUKTI. This is basically a presheaf model, where the choice of the base category leads either to the simplicial sets model or to the cubical model of HoTT. This construction generalizes the setoid model construction [2] to an arbitrary dimension. Since this involves encoding notions of category theory, the rewriting feature of DEDUKTI is intensively used to represent, among others, the associativity of morphism composition, or the naturality conditions.

Guillaume Bury has proposed an automation-friendly set theory for the B method. This theory is expressed using first order logic extended to polymorphic types and rewriting. Rewriting is introduced along the lines of deduction modulo theory, where axioms are turned into rewrite rules over both propositions and terms. This work has been published in [30].

7.4. Interoperability

François Thiré has defined in DEDUKTI a constructive version of simple type theory with prenex polymorphism: $STT\forall_{\beta\delta}$. This work has been published at the LFMTP workshop in [15]. $STT\forall_{\beta\delta}$ has been used to encode an arithmetic library able to prove little Fermat's theorem. Then these proofs has been exported to different systems that are: COQ, MATITA, LEAN and OPENTHEORY. Gilles Dowek, César Muñoz, and François Thiré have developed a translation of $STT\forall_{\beta\delta}$ to PVS.

Then, Walid Moustaoui and François Thiré have built a website called LOGIPEDIA which allows the user to inspect this arithmetic library and the user can download the proof of this theorem to one of the systems mentioned above.

7.5. Drags

Shared and cyclic structures are very common in both programming and proving, which requires generalizing term rewriting techniques to graphs. Jean-Pierre Jouannaud and Nachum Dershowitz have introduced a very general class of multigraphs, called drags, equipped with a composition operator $\otimes$ which provides with a rich categorical structure. Rewriting a drag D can then be defined in a very simple way, by writing D as the composition of a left-hand side of rules L and a context C, and then replacing L by R, the right-hand side of the rule, which yields the rewritten drag $R \otimes C$. The fundamental aspects of the algebra of drags have been presented at TERMGRAPH'2018 and have also been submitted to a special issue of TCS. Termination of drag rewriting in investigated in [20].

7.6. SCTL

Gilles Dowek, Liu Jian, and Ying Jiang have reworked the presentation of CTL in sequent calculus proposed by Gilles Dowek and Ying Jiang in 2012 and provided an implementation of it. This work has been published in [13].

GRACE Project-Team

6. New Results

6.1. Fast transforms over fields of characteristic 2

Participant: Nicholas Coxon.

With the aim of reaching fast, linear time, algorithms for encoding multiplicity codes, which have good local properties, N. Coxon had to develop subalgorithms for dealing with the Hermite interpolation [13], which in turn relies on computer algebra for fast transforms over fields of characteritic two [14]. Locally decodable codes are used for private information retrieval, where a database can be privately queried by a user, in such a way that the user does not reveal his query. Using codes with locality for private information retrieval, the database is first encoded, then queried using the local property of the code. Since the databases in question can be large, only linear time algorithms can be used. Our results achieve linear-time complexity, and even with a non agressively optimized implementation, can encode as much as 10^9 bits in thirty seconds on a laptop.

6.2. Private information retrieval

Participants: Daniel Augot, Nicholas Coxon, Julien Lavauzelle, Françoise Levy-Dit-Vehel.

J. Lavauzelle continued his study on private information retrieval (PIR) protocols. First, he completed the construction of PIR protocols from transversal designs [8], initiated in 2017. Compared to existing protocols, the main benefit of the construction is to feature an optimal computation complexity for the servers. Sublinear communication complexity and negligeable storage overhead can also be achieved for some particular instances.

Second, in a joint work with R. Tajeddine, R. Freij-Hollanti and C. Hollanti from the University of Aalto (Finland), J. Lavauzelle considered the setting in which the database is encoded with an optimal regenerating code [16]. Quantitatively, their construction of PIR protocols improves upon a recent work of Dorkson and Ng, for every non-trivial set of parameters.

6.3. Locally correctable codes

Participant: Julien Lavauzelle.

In 2013, Guo, Kopparty and Sudan built a new family of locally correctable codes from lifting, achieving an arbitrarily high information rate for sublinear locality. J. Lavauzelle proposed an analogue of this construction in projective spaces [7]. The parameters of this construction are similar to the original work of Guo *et al.* Intertwined relations between the two families of codes were proven thanks to a careful analysis of their monomial bases. The practicality of the construction was also established through an implementation and a study of information sets and automorphisms of the code.

6.4. Cryptanalysis in code based cryptography

Participant: Alain Couvreur.

Following NIST call for post quantum cryptography, A. Couvreur and E. Barelli designed a key recovery attack against a McEliece–like encryption scheme called DAGS [9].

In addition, in collaboration with Matthieu Lequesne and Jean-Pierre Tillich (Inria Paris, SECRET team), A. Couvreur designed an attack against another proposal called RLCE (Random Linear Code Encryption) [12].

6.5. Commutative isogeny-based cryptography

Participants: Luca de Feo, Benjamin Smith.

Despite the many advances in post-quantum cryptography in recent years, efficient drop-in replacements for the classic Diffie–Hellman key exchange algorithm have proven elusive. L. De Feo, J. Kieffer, and B. Smith laid the algorithmic groundwork for *commutative isogeny-based key exchange* in [10]; this work became the basis of the exciting new CSIDH proposal [19].

6.6. Factoring oracles

Participants: François Morain, Benjamin Smith.

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 (ANSSI) 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, see [17].

MEXICO Project-Team

7. New Results

7.1. Contract Based Design of Symbolic Controllers for Interconnected Multiperiodic Sampled-Data Systems

This paper deals with the synthesis of symbolic controllers for interconnected sampled-data systems where each component has its own sampling period. A compositional approach based on continuous-time assume-guarantee contracts is used. We provide sufficient conditions guaranteeing for a sampled-data system, satisfaction of an assume-guarantee contract and completeness of trajectories. Then, compositional results can be used to reason about interconnection of mul-tiperiodic sampled-data systems. We then show how discrete abstractions and symbolic control techniques can be applied to enforce the satisfaction of contracts and ensure completeness of trajectories. Finally, theoretical results are applied to a vehicle platooning problem on a circular road, which show the effectiveness of our approach.

7.2. Boolean Networks: Beyond Generalized Asynchronicity

Boolean networks are commonly used in systems biology to model dynamics of biochemical networks by abstracting away many (and often unknown) parameters related to speed and species activity thresholds. It is then expected that Boolean networks produce an over-approximation of behaviours (reachable configurations), and that subsequent refinements would only prune some impossible transitions. However, we show that even generalized asynchronous updating of Boolean networks, which subsumes the usual updating modes including synchronous and fully asynchronous, does not capture all transitions doable in a multi-valued or timed refinement. We define a structural model transformation which takes a Boolean network as input and outputs a new Boolean network whose asynchronous updating simulates both synchronous and asynchronous updating of the original network, and exhibits even more behaviours than the generalized asynchronous updating. We argue that these new behaviours should not be ignored when analyzing Boolean networks, unless some knowledge about the characteristics of the system explicitly allows one to restrict its behaviour.

7.3. Most Permissive Semantics of Boolean Networks

The usual update modes of Boolean networks (BNs), including synchronous and (generalized) asynchronous, fail to capture behaviours introduced by multivalued refinements. Thus, update modes do not allow a correct abstract reasoning on dynamics of biological systems, as they may lead to reject valid BN models. We introduce a new semantics for interpreting BNs which meets with a correct abstraction of any multivalued refinements, with any update mode. This semantics subsumes all the usual updating modes, while enabling new behaviours achievable by more concrete models. Moreover, it appears that classical dynamical analyses of reachability and attractors have a simpler computational complexity: – reachability can be assessed in a polynomial number of iterations (instead of being PSPACE-complete with update modes); – attractors are hypercubes, and deciding the existence of attractors with a given upper-bounded dimension is in NP (instead of PSPACE-complete with update modes). The computation of iterations is in NP in the very general case, and is linear when local functions are monotonic, or with some usual representations of functions of BNs (binary decision diagrams, Petri nets, automata networks, etc.). In brief, the most permissive semantics of BNs enables a correct abstract reasoning on dynamics of BNs, with a greater tractability than previously introduced update modes. This technical report lists the main definitions and properties of the most permissive semantics of BNs, and draw some remaining open questions.

7.4. 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 components updates can have a dramatic impact on the predicted behaviours. In this paper, we explore the use of Contextual Petri Nets (CPNs) to study dynamics of BNs with a concurrency theory perspective. After showing bi-directional translations between CPNs and BNs and analogies between results on synchronism sensitivies, we illustrate that usual updating modes for BNs can miss plausible behaviours, i.e., incorrectly conclude on the absence/impossibility of reaching specific configurations. Taking advantage of CPN semantics enabling more behaviour than the generalized asynchronous updating mode, we propose an encoding of BNs ensuring a correct abstraction of any multivalued refinement, as one may expect to achieve when modelling biological systems with no assumption on its time features.

7.5. On the Composition of Discrete and Continuous-time Assume-Guarantee Contracts for Invariance

Many techniques for verifying invariance properties are limited to systems of moderate size. In this paper, we propose an approach based on assume-guarantee contracts and compositional reasoning for verifying invariance properties of a broad class of discrete-time and continuous-time systems consisting of interconnected components. The notion of assume-guarantee contracts makes it possible to divide responsibilities among the system components: a contract specifies an invariance property that a component must fulfill under some assumptions on the behavior of its environment (i.e. of the other components). We define weak and strong semantics of assume-guarantee contracts for both discrete-time and continuous-time systems. We then establish a certain number of results for compositional reasoning, which allow us to show that a global invariance property of the whole system is satisfied when all components satisfy their own contract. Interestingly, we show that the weak satisfaction of the contract is sufficient to deal with cascade compositions, while strong satisfaction is needed to reason about feedback composition. Specific results for systems described by differential inclusions are then developed. Throughout the paper, the main results are illustrated using simple examples.

7.6. Compositional synthesis of state-dependent switching control

We present a correct-by-design method of state-dependent control synthesis for sampled switching systems. Given a target region R of the state space, our method builds a capture set S and a control that steers any element of S into R. The method works by iterated backward reachability from R. The method is also used to synthesize a recurrence control that makes any state of R return to R infinitely often. We explain how the synthesis method can be performed in a compositional manner, and apply it to the synthesis of a compositional control of a concrete floor-heating system with 11 rooms and up to $2^1 1 = 2048$ toswitching modes.

7.7. An Improved Algorithm for the Co3ntrol Synthesis of Nonlinear Sampled Switched Systems

A novel algorithm for the control synthesis for nonlinear switched systems is presented in this paper. Based on an existing procedure of state-space bisection and made available for nonlinear systems with the help of guaranteed integration, the algorithm has been improved to be able to consider longer patterns of modes with a better pruning approach. Moreover, the use of guaranteed integration also permits to take bounded perturbations and varying parameters into account. It is particularly interesting for safety critical applications, such as in aeronautical, military or medical fields. The whole approach is entirely guaranteed and the induced controllers are correct-by-design. Some experimentations are performed to show the important gain of the new algorithm.

7.8. Control Synthesis for Stochastic Switched Systems using the Tamed Euler Method

In this paper, we explain how, under the one-sided Lipschitz (OSL) hypothesis, one can find an error bound for a variant of the Euler-Maruyama approximation method for stochastic switched systems. We then explain how this bound can be used to control stochastic switched switched system in order to stabilize them in a given region. The method is illustrated on several examples of the literature.

7.9. The Complexity of Diagnosability and Opacity Verification for Petri Nets

Diagnosability and opacity are two well-studied problems in discrete-event systems. We revisit these two problems with respect to expressiveness and complexity issues. We first relate different notions of diagnosability and opacity. We consider in particular fairness issues and extend the definition of Germanos et al. [ACM TECS, 2015] of weakly fair diagnosability for safe Petri nets to general Petri nets and to opacity questions. Second, we provide a global picture of complexity results for the verification of diagnosability and opacity. We show that diagnosability is NL-complete for finite state systems, PSPACE-complete for safe Petri nets (even with fairness), and EXPSPACE-complete for general Petri nets without fairness, while non diagnosability is inter-reducible with reachability when fault events are not weakly fair. Opacity is ESPACE-complete for safe Petri nets (even with fairness) and undecidable for general Petri nets already without fairness.

7.10. Integrating Simulink Models into the Model Checker Cosmos

We present an implementation for Simulink model executions in the statistical model-checker Cosmos. We take profit of this implementation for an hybrid modeling combining Petri nets and Simulink models.,Nous présentons une implémentation pour l'exécution de modèles Simulink dans le model-checker Cosmos. Cette implémentation est ensuite utilisée pour la simulation de modèles hybrides, combinant des réseaux de Petri et des modèles Simulink.

7.11. Bounds Computation for Symmetric Nets

Monotonicity in Markov chains is the starting point for quantitative abstraction of complex probabilistic systems leading to (upper or lower) bounds for probabilities and mean values relevant to their analysis. While numerous case studies exist in the literature, there is no generic model for which monotonicity is directly derived from its structure. Here we propose such a model and formalize it as a subclass of Stochastic Symmetric (Petri) Nets (SSNs) called Stochastic Monotonic SNs (SMSNs). On this subclass the monotonicity is proven by coupling arguments that can be applied on an abstract description of the state (symbolic marking). Our class includes both process synchronizations and resource sharings and can be extended to model open or cyclic closed systems. Automatic methods for transforming a non monotonic system into a monotonic one matching the MSN pattern, or for transforming a monotonic system with large state space into one with reduced state space are presented. We illustrate the interest of the proposed method by expressing standard monotonic models and modelling a flexible manufacturing system case study.

7.12. Distributed computation of vector clocks in Petri nets unfolding for test selection

Petri net unfoldings with time stamps allow to build distributed testers for distributed systems. However, the construction of the annotated unfolding of a distributed system currently remains a centralized task. In the aforemention paper, we extend a distributed unfolding technique in order to annotate the resulting unfolding with time stamps. This allows for distributed construction of distributed testers for distributed systems.

7.13. Hyper Partial Order Logic

We define HyPOL, a local hyper logic for partial order models, expressing properties of sets of runs. These properties depict shapes of causal dependencies in sets of partially ordered executions,with similarity relations defined as isomorphisms of past observations. Unsurprisingly, since comparison of projections are included, satisfiability of this logic is undecidable. We then addressmodel checking of HyPOL and show that, already for safe Petri nets, the problem is undecidable. Fortunately, sensible restrictions of observations and nets allow us to bring back model checking ofHyPOL to a decidable problem, namely model checking of MSO on graphs of bounded treewidth.

7.14. Integrating Simulink Models into the Model Checker Cosmos

We present an implementation for Simulink model executions in the statistical model-checker Cosmos. We take profit of this implementation for hybrid modeling and simulations combining Petri nets and Simulink models.

7.15. Site-Directed Deletion

We introduce a new bio-inspired operation called a site-directed deletion motivated from site-directed mutagenesis performed by enzymatic activity of DNA polymerase: Given two strings x and y, a site-directed deletion partially deletes a substring of x guided by the string y that specifies which part of a substring can be deleted. We study a few decision problems with respect to the new operation and examine the closure properties of the (iterated) site-directed deletion operations. We, then, define a site-directed deletion-closed (and-free) language L and investigate its decidability properties when L is regular or context-free.

7.16. Site-Directed Insertion: Decision Problems, Maximality and Minimality

Site-directed insertion is an overlapping insertion operation that can be viewed as analogous to the overlap assembly or chop operations that concatenate strings by overlapping a suffix and a prefix of the argument strings. We consider decision problems and language equations involving site-directed insertion. By relying on the tools provided by semantic shuffle on trajectories we show that one variable equations involving site-directed insertion and regular constants can be solved. We consider also maximal and minimal variants of the site-directed insertion operation.

7.17. A Faithful Binary Circuit Model with Adversarial Noise

Accurate delay models are important for static and dynamic timing analysis of digital circuits, and mandatory for formal verification. However, Függer et al. [IEEE TC 2016] proved that pure and inertial delays, which are employed for dynamic timing analysis in state-of-the-art tools like ModelSim, NC-Sim and VCS, do not yield faithful digital circuit models. Involution delays, which are based on delay functions that are mathematical involutions depending on the previous-output-to-input time offset, were introduced by Függer et al. [DATE'15] as a faithful alternative (that can easily be used with existing tools). Although involution delays were shown to predict real signal traces reasonably accurately, any model with a deterministic delay function is naturally limited in its modeling power. In this paper, we thus extend the involution model, by adding non-deterministic delay variations (random or even adversarial), and prove analytically that faithfulness is not impaired by this generalization. Albeit the amount of non-determinism must be considerably restricted to ensure this property, the result is surprising: the involution model differs from non-faithful models mainly in handling fast glitch trains, where small delay shifts have large effects. This originally suggested that adding even small variations should break the faithfulness of the model, which turned out not to be the case. Moreover, the results of our simulations also confirm that this generalized involution model has larger modeling power and, hence, applicability.

7.18. Tight Bounds for Asymptotic and Approximate Consensus

We study the performance of asymptotic and approximate consensus algorithms under harsh environmental conditions. The asymptotic consensus problem requires a set of agents to repeatedly set their outputs such that the outputs converge to a common value within the convex hull of initial values. This problem, and the related approximate consensus problem, are fundamental building blocks in distributed systems where exact consensus among agents is not required or possible, e.g., man-made distributed control systems , and have applications in the analysis of natural distributed systems, such as flocking and opinion dynamics. We prove tight lower bounds on the contraction rates of asymptotic consensus algorithms in dynamic networks, from which we deduce bounds on the time complexity of approximate consensus algorithms. In particular, the obtained bounds show optimality of asymptotic and approximate consensus algorithms presented in [Charron-Bost et al., ICALP'16] for certain dynamic networks, including the weakest dynamic network model in which asymptotic and approximate consensus are solvable. As a corollary we also obtain asymptotically tight bounds for asymptotic consensus in the classical asynchronous model with crashes. Central to our lower bound proofs is an extended notion of valency, the set of reachable limits of an asymptotic consensus algorithm starting from a given configuration. We further relate topological properties of valencies to the solvability of exact consensus , shedding some light on the relation of these three fundamental problems in dynamic networks.

7.19. Pomsets and Unfolding of Reset Petri Nets

Reset Petri nets are a particular class of Petri nets where transition firings can remove all tokens from a place without checking if this place actually holds tokens or not. In this paper we look at partial order semantics of such nets. In particular, we propose a pomset bisimulation for comparing their concurrent behaviours. Building on this pomset bisimulation we then propose a generalization of the standard finite complete prefixes of unfolding to the class of safe reset Petri nets.

7.20. Fast All-Digital Clock Frequency Adaptation Circuit for Voltage Droop Tolerance

Naive handling of supply voltage droops in synchronous circuits results in conservative bounds on clock speeds, resulting in poor performance even if droops are rare. Adaptive strategies detect such potentially hazardous events and either initiate a rollback to a previous state or proactively reduce clock speed in order to prevent timing violations. The performance of such solutions critically depends on a very fast response to droops. However, state-of-the-art solutions incur synchronization delay to avoid that the clock signal is affected by metastability. Addressing the challenges discussed by Keith Bowman in his ASYNC 2017 keynote talk, we present an all-digital circuit that can respond to droops within a fraction of a clock cycle. This is achieved by delaying clock signals based on measurement values while they undergo synchronization simultaneously. We verify our solution by formally proving correctness, complemented by VHDL and Spice simulations of a 65 nm ASIC design confirming the theoretically obtained results.

7.21. Fast Multidimensional Asymptotic and Approximate Consensus

We study the problems of asymptotic and approximate consensus in which agents have to get their values arbitrarily close to each others' inside the convex hull of initial values, either without or with an explicit decision by the agents. In particular, we are concerned with the case of multidimensional data, i.e., the agents' values are d-dimensional vectors. We introduce two new algorithms for dynamic networks, subsuming classical failure models like asynchronous message passing systems with Byzantine agents. The algorithms are the first to have a contraction rate and time complexity independent of the dimension d. In particular, we improve the time complexity from the previously fastest approximate consensus algorithm in asynchronous message passing systems with Byzantine faults by Mendes et al. [Distrib. Comput. 28].

7.22. 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. This article introduces 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.

7.23. Interval Iteration Algorithm for MDPs and IMDPs

Markov Decision Processes (MDP) are a widely used model including both non-deterministic and probabilistic choices. Minimal and maximal probabilities to reach a target set of states, with respect to a policy resolving non-determinism, may be computed by several methods including value iteration. This algorithm, easy to implement and efficient in terms of space complexity, iteratively computes the probabilities of paths of increasing length. However, it raises three issues: (1) defining a stopping criterion ensuring a bound on the approximation, (2) analysing the rate of convergence, and (3) specifying an additional procedure to obtain the exact values once a sufficient number of iterations has been performed. The first two issues are still open and, for the third one, an upper bound on the number of iterations has been proposed. Based on a graph analysis and transformation of MDPs, we address these problems. First we introduce an interval iteration algorithm, for which the stopping criterion is straightforward. Then we exhibit its convergence rate. Finally we significantly improve the upper bound on the number of iterations required to get the exact values. We extend our approach to also deal with Interval Markov Decision Processes (IMDP) that can be seen as symbolic representations of MDPs.

7.24. Diagnosability of Repairable Faults

The diagnosis problem for discrete event systems consists in deciding whether some fault event occurred or not in the system, given partial observations on the run of that system. Diagnosability checks whether a correct diagnosis can be issued in bounded time after a fault, for all faulty runs of that system. This problem appeared two decades ago and numerous facets of it have been explored, mostly for permanent faults. It is known for example that diagnosability of a system can be checked in polynomial time, while the construction of a diagnoser is exponential. The present paper examines the case of transient faults, that can appear and be repaired. Diagnosability in this setting means that the occurrence of a fault should always be detected in bounded time, but also before the fault is repaired. Checking this notion of diagnosability is proved to be PSPACE-complete. It is also shown that faults can be reliably counted provided the system is diagnosable for faults and for repairs.

7.25. Metastability-Containing Circuits

In digital circuits, metastability can cause deteriorated signals that neither are logical 0 nor logical 1, breaking the abstraction of Boolean logic. Synchronizers, the only traditional countermeasure, exponentially decrease the odds of maintained metastability over time. We propose a fundamentally different approach: It is possible to deterministically contain metastability by fine-grained logical masking so that it cannot infect the entire circuit. At the heart of our approach lies a time-and value-discrete model for metastability in synchronous clocked digital circuits, in which metastability is propagated in a worst-case fashion. The proposed model permits positive results and passes the test of reproducing Marino's impossibility results. We fully classify which functions can be computed by circuits with standard registers. Regarding masking registers, we show that more functions become computable with each clock cycle, and that masking registers permit exponentially smaller circuits for some tasks. Demonstrating the applicability of our approach, we present the first fault-tolerant distributed clock synchronization algorithm that deterministically guarantees correct behavior in the presence of metastability. As a consequence, clock domains can be synchronized without using synchronizers, enabling metastability-free communication between them.

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 [17]. 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.

The operational semantics of MLTS is given using natural semantics for evaluation. We shall view such natural semantics as a logical theory with a rich logic that includes both nominal abstraction and the ∇-quantifier: as a result, the natural semantic specification of MLTS can be given a succinct and elegant presentation.

We have developed a number of examples of how this new programming language can be used. Some of the most convincing of these examples are programs that manipuate untyped λ-terms. A web-based implementation of an MLTS interpreter is available to anyone with a modern web browser: simply visit https://trymlts.github.io/. Small MLTS programs can be composed and executed using that interpreter.

7.2. Proof theory for model checking

Participant: Dale Miller.

While model checking has often been considered as a practical alternative to building formal proofs, we have argued that the theory of sequent calculus proofs can be used to provide an appealing foundation for model checking [7]. Given that the emphasis of model checking is on establishing the truth of a property in a model, our framework concentrates on *additive* inference rules since these provide a natural description of truth values via inference rules. Unfortunately, using these rules alone can force the use of inference rules with an infinite number of premises. In order to accommodate more expressive and finitary inference rules, *multiplicative* rules must be used, but limited to the construction of *additive synthetic inference rules*: such synthetic rules are described using the proof-theoretic notions of polarization and focused proof systems. This framework provides a natural, proof-theoretic treatment of reachability and non-reachability problems, as well as tabled deduction, bisimulation, and winning strategies. (Q. Heath collaborated on several parts of this research effort.)

7.3. From syntactic proofs to combinatorial proofs

Participants: Matteo Acclavio, Lutz Straßburger.

We continued our research on combinatorial proofs as a notion of proof identity for classical logic. We managed to extend our results from last year: We show for various syntactic formalisms including sequent calculus, analytic tableaux, and resolution, how they can be translated into combinatorial proofs, and which notion of identity they enforce. This allows the comparison of proofs that are given in different formalisms.

These results have been presented at the MLA workshop ins Kanazawa and the IJCAR conference in Oxford, published in [25].

7.4. Proof nets for first-order additive linear logic

Participant: Lutz Straßburger.

In a joint work with Willem Heijltjes (University of Bath) and Dominic Hughes (UC Berkeley) we present canonical proof nets for first-order additive linear logic, the fragment of linear logic with sum, product, and first-order universal and existential quantification. We present two versions of our proof nets. One, witness nets, retains explicit witnessing information to existential quantification. For the other, unification nets, this information is absent but can be reconstructed through unification. Unification nets embody a central contribution of the paper: first-order witness information can be left implicit, and reconstructed as needed. Witness nets are canonical for first-order additive sequent calculus. Unification nets in addition factor out any inessential choice for existential witnesses. Both notions of proof net are defined through coalescence, an additive counterpart to multiplicative contractibility, and for witness nets an additional geometric correctness criterion is provided. Both capture sequent calculus cut-elimination as a one-step global composition operation.

These results are published in [26] and have been presented at the First workshop of the Proof Society in Ghent and at the 3rd FISP workshop in Vienna.

7.5. On the Decision Problem for MELL

Participant: Lutz Straßburger.

The decision problem for multiplicative exponential linear logic (MELL) is one of the most important open problems in the are of linear logic. in 2015 there has been an attempt by Bimbò to prove the decidability of MELL. However, we have found several mistakes in that work, and the main mistake is so serious that there is no obvious fix, and therefore the decidability of MELL remains to be open. As a side effect, our work contains a complete (syntactic) proof of the decidability of the relevant version of MELL, that is the logic obtained from MELL by replacing the linear logic contraction rule by a general unrestricted version of the contraction rule. These results are presented in [27].

7.6. OCaml metatheory

Participant: Gabriel Scherer.

We worked on the evolution of advanced features of the OCaml programming language, designing static analyses to ensure their safety through a scientific study their metatheory. Specifically, we worked on unboxed type declarations (during an internship by Simon Colin, M1 from École Polytechnique) and recursive value definitions (during an internship by Alban Reynaud, L3 from ENS Lyon). The two internships and followup work each resulted in both a change proposal to the OCaml implementation and a submission to an academic conference.

7.7. Merlin: understanding a language server

Participant: Gabriel Scherer.

Thomas Réfis (Jane Street) and Frédéric Bour maintain the Merlin language server of OCaml, a tool that provides language-aware features to text editors. We collaborated with them on dissecting the tool and explaining its design and evolution ([4]); the similarities and differences with usual compiler frontends may inform future language implementation work, and our language-agnostic presentation may be of use to tool designers for other languages and proof assistants.

7.8. Language interoperability: ML and a Linear language

Participant: Gabriel Scherer.

In a programming system where programs are created in one programming language, we consider the addition of another programming language that interoperates with the first – and the reimplementation of some library/system functions in this new language. This can increase expressivity, but it could also break some assumptions made by programmers. Typically, adding a bridge to C or assembly code can introduce memory-unsafe code in a previously-safe system. In [18], we formalize a notion of "graceful" interoperability between two languages in this setting, determined by full abstraction, that is, preservation of equational reasoning. We instantiate this general idea by extending ML with an advanced expert language with linear types and linear mutable cells.

7.9. First-class simultaneous substitutions in the two-level logic approach

Participant: Kaustuv Chaudhuri.

The *two-level logic approach* that underlies the Abella prover is excellent at reasoning about the inductive structure of terms with binding constructs, such as λ-terms from the λ-calculus. However, there is no built in support in Abella for reasoning about the inductive structure of (simultaneous) substitutions. This lack of this kind of support is often criticized in the λ-tree syntax representational style that is used in Abella; indeed, in a number of other systems based on this style, support for reasoning about substitutions is explicitly added into the trusted kernel. In [14] we show how to formalize substitutions in Abella in a fluent and high level manner, where all the meta-theory can be proven in a straightforward manner. We illustrate its use in giving a clean formulation of fact that the Howe extension of applicative similarity is a pre-congruence, a standard result from the meta-theory of the λ-calculus that requires sophistication in treating simultaneous substitutions.

7.10. Hybrid Linear Logic, revisited

Participant: Kaustuv Chaudhuri.

Hybrid Linear Logic (HyLL) was proposed by Chaudhuri and Despeyroux in 2010 as a meta-logic for reasoning about constrained transition systems, with applications to a number of domains including formal molecular biology [36]. This logic is an extension of (intuitionistic) linear logic with hybrid connectives that can reason about monoidal constraint domains such as instants of time or rate functions. *Linear logic with subexponential* is a different extension of linear logic that has been proposed as a mechanism for capturing certain well known constrained settings such as bigraphs [39] or concurrent constraint programming [65]. In a paper accepted to MSCS [5] we show how to relate these two extensions of linear logic by giving an embedding of HyLL into linear logic with subexponentials. Furthermore, we show that subexponentials are able to give an adequate encoding of CTL$*$, which is beyond the expressive power of HyLL. Thus, subexponentials appear to be the better choice as a foundation for constraints in linear logic.

7.11. Proof Nets and the Linear Substitution Calculus

Participant: Beniamino Accattoli.

This work [21] belongs to line of work *Cost Models and Abstract Machines for Functional Programs*, supported by the ANR project COCA HOLA, and it has been published in the proceedings of the international conference ICTAC 2018.

The *Linear Substitution Calculus* (LSC) is a refinement of the λ-calculus that is crucial for the study of cost models for functional programs, as it enables a sharp and yet simple decomposition of the evaluation of λ-terms, and it is employed in the proof of various results about cost models in the literature.

In this work we show that the LSC is isomorphic to the linear logic representation of the λ-calculus. More precisely, it is isomorphic to the *proof nets* presentation of such a fragment of linear logic. Proof nets are a graphical formalism, which—as most graphical formalisms—is handy for intuitions but not prone to formal reasoning. The result is relevant because it allows to manipulate formally a graphical formalism (proof nets) by means of an ordinary term syntax (the LSC).

7.12. Tight Typings and Split Bounds

Participants: Beniamino Accattoli, Stéphane Graham-Lengrand.

This joint work with Delia Kesner (Paris Diderot University) [12] belongs to line of work *Cost Models and Abstract Machines for Functional Programs*, supported by the ANR project COCA HOLA, and it has been published in the proceedings of the international conference ICFP 2018.

Intersection types are a classic tool in the study of the λ-calculus. They are known to characterise various termination properties.

It is also well-known that *multi types*, a variant of intersection types strongly related to linear logic, also characterise termination properties. Typing derivation of multi types, moreover, provide quantitative information such as the number of evaluation step and the size of the results, as first shown by de Carvalho.

In this work we provide some new results on this line of work, notably we provide the first quantitative study via multi types of the leftmost and linear head evaluation strategies. Moreover, we show that our approach covers also the other cases in the literature.

7.13. Types of Fireballs

Participant: Beniamino Accattoli.

This joint work with Giulio Guerrieri (Bologna University) [22] belongs to line of work *Cost Models and Abstract Machines for Functional Programs*, supported by the ANR project COCA HOLA, and it has been published in the proceedings of the international conference APLAS 2018.

The theory of the call-by-value λ-calculus has mostly been developed for *closed* programs, that is, programs without free variables. In the last few years, the authors dedicated considerable efforts to extend it to open terms, that is the case relevant for the implementation of proof assistants. The simplest presentation of the call-by-value λ-calculus for open terms is the *fireball calculus*.

In this work we extend the quantitative study via multi types mentioned in *Tight Typings and Split Bounds* to the fireball calculus.

7.14. Decision procedures for intuitionistic propositional logic

Participant: Stéphane Graham-Lengrand.

Provability in intuitionistic propositional logic is decidable and, as revealed by the works of, e.g., Vorobev [72], Hudelmaier [51] and Dyckhoff [42], proof theory can provide natural decision procedures, which have been implemented in various software. More precisely, a decision procedure is obtained by performing direct root-first proof-search in (different variants of) a sequent calculus system called LJT (aka G4ip); termination is ensured by a property of the sequent calculus called depth-boundedness.

Independently from this, Claessen and Rosen [40] recently proposed a decision procedure for the same logic, based on a methodology used in the field of Satisfiability-Modulo-Theories (SMT). Their implementation clearly outperforms the sequent-calculus-based implementations.

In 2018 we managed to establish of formal connection between the G4ip sequent calculus and the algorithm from [40], revealing the features that they share and the features that distinguish them. This connection is interesting because it gives a proof-theoretical light on SMT-solving techniques, and it opens the door to the design of an intuitionistic version of the CDCL algorithm used in SAT-solvers, which decides provability in classical logic.

7.15. Admissible Tools in the Kitchen of Intuitionistic Logic

Participants: Matteo Manighetti, Andrea Condoluci.

In this work we study the computational meaning of the inference rules that are admissible, but not derivable, in intuitionistic logic [16].

An inference rule is admissible for a logic if whenever its antecedent is derivable, its conclusion was already derivable without the rule. In classical logic, whenever this is the case, then also the implication between antecedent and conclusion is derivable. The notion of an admissible rule is therefore internalized in the logic.

This is not the case for intuitionistic logic, and some rules that are admissible are not derivable: therefore they need reasoning outside the usual intuitionistic logic in order to be reduced to purely intuitionistic derivation.

In this work we propose a proof system with term annotations and reduction rules to give a computational meaning to these reductions.

SPECFUN Project-Team

7. New Results

7.1. Computing solutions of linear Mahler equations

Mahler equations relate evaluations of the same function f at iterated bth powers of the variable. They arise in particular in the study of automatic sequences and in the complexity analysis of divide-and-conquer algorithms. Recently, the problem of solving Mahler equations in closed form has occurred in connection with number-theoretic questions. A difficulty in the manipulation of Mahler equations is the exponential blow-up of degrees when applying a Mahler operator to a polynomial. In [3], Frédéric Chyzak and Philippe Dumas, together with Thomas Dreyfus (IRMA, Université de Strasbourg) and Marc Mezzarobba (external collaborator from Sorbonne Université), have presented algorithms for solving linear Mahler equations for series, polynomials, and rational functions, and have obtained polynomial-time complexity under a mild assumption. The article was formally accepted and published this year.

7.2. 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 where the initial coefficient satisfies $a_0(z) = 1$. In [1], 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 formally accepted this year.

7.3. Generalized Hermite reduction, creative telescoping and definite integration of D-finite functions

Hermite reduction is a classical algorithmic tool in symbolic integration. It is used to decompose a given rational function as a sum of a function with simple poles and the derivative of another rational function. Alin Bostan, Frédéric Chyzak, and Pierre Lairez, together with Bruno Salvy (project-team AriC) have extended Hermite reduction to arbitrary linear differential operators instead of the pure derivative. They have also developped efficient algorithms for this reduction, and then applied the generalized Hermite reduction to the computation of linear operators satisfied by single definite integrals of D-finite functions of several continuous or discrete parameters. The resulting algorithm is a generalization of reduction-based methods for creative telescoping. Their article [6] was published at the ISSAC conference.

7.4. Bijections between Łukasiewicz walks and generalized tandem walks

In [9], Frédéric Chyzak, together with Karen Yeats (University of Waterloo, Canada), have studied the enumeration by length of several walk models on the square lattice. They have obtained bijections between walks in the upper half-plane returning to the x-axis and walks in the quarter plane. An ongoing work by Bostan, Chyzak, and Mahboubi has given a bijection for models using small north, west, and south-east steps. The work in [9] has adapted and generalized it to a bijection between half-plane walks using those three steps in two colours and a quarter-plane model over the symmetrized step set consisting of north, north-west, west, south, south-east, and east. They have then generalized their bijections to certain models with large steps: for given $p \geq 1$, a bijection has been given between the half-plane and quarter-plane models obtained by keeping the small south-east step and replacing the two steps north and west of length 1 by the $p + 1$ steps of length p in directions between north and west. An article was submitted this year.

7.5. Putting Fürer's algorithm into practice with the BPAS library

Fast algorithms for integer and polynomial multiplication play an important role in scientific computing as well as in other disciplines. In 1971, Schönhage and Strassen designed an algorithm that improved the multiplication time for two integers of at most n bits to $O(\log n \log \log n)$. Martin Fürer presented a new algorithm that runs in $O(n \log n \cdot 2^{O(\log^* n)})$, where $\log^* n$ is the iterated logarithm of n. In a submitted article, Svyatoslav Covanov, together with Davood Mohajerani, Marc Moreno Maza and Lin-Xiao Wang, have explained how one can put Fürer's ideas into practice for multiplying polynomials over a prime field $\mathbb{Z}/p\mathbb{Z}$, for which p is a Generalized Fermat prime of the form $p = r^k + 1$ where k is a power of 2 and r is of machine word size. When k is at least 8, they have shown that multiplication inside such a prime field can be efficiently implemented via Fast Fourier Transform (FFT). Taking advantage of Cooley-Tukey tensor formula and the fact that r is a $2k$-th primitive root of unity in $\mathbb{Z}/p\mathbb{Z}$, they have obtained an efficient implementation of FFT over $\mathbb{Z}/p\mathbb{Z}$. This implementation outperforms comparable implementations either using other encodings of $\mathbb{Z}/p\mathbb{Z}$ or other ways to perform multiplication in $\mathbb{Z}/p\mathbb{Z}$.

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

In [5], 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 $\sqrt{p}$.

7.7. Counting walks with large steps in an orthant

In the past fifteen years, the enumeration of lattice walks with steps taken in a prescribed set and confined to a given cone, especially the first quadrant of the plane, has been intensely studied. As a result, the generating functions of quadrant walks are now well-understood, provided the allowed steps are *small*. In particular, having small steps is crucial for the definition of a certain group of bi-rational transformations of the plane. It has been proved that this group is finite if and only if the corresponding generating function is D-finite. This group is also the key to the uniform solution of 19 of the 23 small step models possessing a finite group. In contrast, almost nothing was known for walks with arbitrary steps. In [7], Alin Bostan together with Mireille Bousquet-Mélou (CNRS, Bordeaux) and Stephen Melczer (U. Pennsylvania, Philadelphia, USA), extended the definition of the group, or rather of the associated orbit, to this general case, and generalized the above uniform solution of small step models. When this approach works, it invariably yields a D-finite generating function. They applied it to many quadrant problems, including some infinite families. After developing the general theory, the authors of [7] considered the 13 110 two-dimensional models with steps in $\{-2, -1, 0, 1\}^2$ having at least one -2 coordinate. They proved that only 240 of them have a finite orbit, and solve 231 of them with our method. The 9 remaining models are the counterparts of the 4 models of the small step case that resist the uniform solution method (and which are known to have an algebraic generating function). They conjecture D-finiteness for their generating functions (but only two of them are likely to be algebraic!), and proved non-D-finiteness for the 12 870 models with an infinite orbit, except for 16 of them.

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

A previous article in 2017 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 [8], 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.

7.9. A numerical transcendental method in algebraic geometry

In "A transcendental method in algebraic geometry", Griffiths emphasized the role of certain multivariate integrals, known as *periods*, "to construct a continuous invariant of arbitrary smooth projective varieties". Periods often determine the projective variety completely and therefore its algebraic invariants. Translating periods into discrete algebraic invariants is a difficult problem, exemplified by the long standing Hodge conjecture which describes how periods determine the algebraic cycles within a projective variety.

Recent progress in computer algebra makes it possible to compute periods with high precision and put transcendental methods into practice. In [10], Pierre Lairez and Emre Sertöz focus on algebraic surfaces and give a numerical method to compute Picard groups. As an application, they count smooth rational curves on quartic surfaces using the Picard group. It is the first time that this kind of computation is performed.

TOCCATA Project-Team

7. New Results

7.1. Deductive Verification

Synthetic topology in HoTT for probabilistic programming. F. Faissole and B. Spitters have developed a mathematical formalism based on synthetic topology and homotopy type theory to interpret probabilistic algorithms. They suggest to use proof assistants to prove such programs [91] [92]. They also have formalized synthetic topology in the Coq proof assistant using the HoTT library. It consists of a theory of lower reals, valuations and lower integrals. All the results are constructive. They apply their results to interpret probabilistic programs using a monadic approach [23].

A Toolchain to Produce Correct-by-Construction OCaml Programs In the context of the research project Vocal, J.-C. Filliâtre, A. Paskevich, and M. Pereira, together with L. Gondelman (postdoc in January 2017) and S. Melo de Sousa (visiting Associate Professor from UBI, Portugal, in Sep/Oct 2017), designed and implemented a toolchain for the verification of OCaml code using Why3 [33]. In this framework, the user provides a formal specification within comments embedded in the OCaml interface file together with an implementation in Why3. Two tools automatically translate the former to a Why3 specification and the latter to an OCaml code. One the refinement proof is completed on the Why3 side, the overall diagram commutes, ensuring the soundness of the OCaml code.

Ghost monitors M. Clochard, C. Marché, and A. Paskevich designed 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. The 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. 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 [32] [29].

This approach is based on an earlier variant proposed in M. Clochard's PhD thesis [11]. 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. M. Clochard introduced one such framework, with an original extension that allows one to specify and prove fine-grained properties about infinite behaviors of target programs. The proof of correctness of this approach relies on a particular flavor of transfinite games. This proof is formalized and verified using the Why3 tool (http://toccata.lri.fr/gallery/hoare_logic_and_games.en.html).

Extracting Why3 programs to C programs. R. Rieu-Helft, C. Marché, and G. Melquiond devised a simple memory model for representing C-like pointers in the Why3 system. This makes it possible to translate a small fragment of Why3 verified programs into idiomatic C code [26]. This extraction mechanism was used to turn a verified Why3 library of arbitrary-precision integer arithmetic into a C library that can be substituted to part of the GNU Multi-Precision (GMP) library [128].

Verification of highly imperative OCaml programs with Why3 J.-C. Filliâtre, M. Pereira, and S. Melo de Sousa proposed a new methodology for proving highly imperative OCaml programs with Why3. For a given OCaml program, a specific memory model is built and one checks a Why3 program that operates on it. Once the proof is complete, they use Why3's extraction mechanism to translate its programs to OCaml, while replacing the operations on the memory model with the corresponding operations on mutable types of OCaml. This method is evaluated on several examples that manipulate linked lists and mutable graphs [24].

Verification of Parameterized Concurrent Programs on Weak Memory Models Modern multiprocessors and microprocesseurs implement weak or relaxed memory models, in which the apparent order of memory operation does not follow the sequential consistency (SC) proposed by Leslie Lamport. Any concurrent program running on such architecture and designed with an SC model in mind may exhibit new behaviors during its execution, some of which may potentially be incorrect. For instance, a mutual exclusion algorithm, correct under an interleaving semantics, may no longer guarantee mutual exclusion when implemented on a weaker architecture. Reasoning about the semantics of such programs is a difficult task. Moreover, most concurrent algorithms are designed for an arbitrary number of processes. D. Declerck [12] proposed an approach to ensure the correctness of such concurrent algorithms, regardless of the number of processes involved. It relies on the Model Checking Modulo Theories (MCMT) framework, developed by Ghilardi and Ranise, which allows for the verification of safety properties of parameterized concurrent programs, that is to say, programs involving an arbitrary number of processes. This technology is extended with a theory for reasoning about weak memory models. The result is an extension of the Cubicle model checker called Cubicle-W, which allows the verification of safety properties of parameterized transition systems running under a weak memory model similar to TSO.

Counterexample Generation S. Dailler and C. Marché worked on extensions and improvements of the counterexample generation feature of Why3, used in particular by the SPARK front-end for Ada [102] [101]. When the logic goal generated for a given verification condition is not shown unsatisfiable by an SMT solvers, some solver can propose a model. By carefully reverting the transformation chain (from an input program through the VC generator and the various translation steps to solvers), this model is turned into a potential counterexample that the user can exploit to analyze why its original code is not proved. The extension consists in a deep analysis of the complete model generated by the solver, so as to extract more information and produce better counterexamples. A journal paper giving the details of the whole process was published [14]

Alias Control for SPARK Program Verification G.-A. Jaloyan and A. Paskevich, together with C. Dross, M. Maalej, and Y. Moy made a proposal for introduction of pointers to the SPARK language, based on permission-driven static alias analysis method inspired by Rust's borrow-checker and affine types [35]. By ensuring that at any point of execution any writable value can only be accessed through a single name, it is possible to apply the standard rules of Hoare logic (or weakest precondition calculus) to verify programs with pointers. The proposed framework was implemented in the GNAT Ada compiler and the SPARK toolset.

7.2. Automated Reasoning

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-Helf 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 [20], [27].

Expressive and extensible automated reasoning tactics for Coq Proof assistants based on Type Theory, such as Coq, allow implementing effective automatic tactics based on computational reasoning (e.g. `lia` for linear integer arithmetic, or `ring` for ring theory). Unfortunately, these are usually limited to one particular domain. In contrast, SMTCoq is a modular and extensible tool, using external provers, which generalizes these computational approaches to combine multiple theories. It relies on a high-level interface, which offers a greater expressiveness, at the cost of more complex automation. Q. Garchery, in collaboration with C. Keller and V .Blot, designed two improvements to increase expressiveness of SMTCoq without impeding its modularity and its efficiency: the first adds some support for universally quantified hypotheses, while the second generalizes the support for integer arithmetic to the different representations of natural numbers and integers in Coq. This work will be presented in the next JFLA [30]

Non-linear Arithmetic Reasoning for Control-Command Software State-of-the-art (semi-)decision procedures for non-linear real arithmetic address polynomial inequalities by mean of symbolic methods, such as quantifier elimination, or numerical approaches such as interval arithmetic. Although (some of) these methods offer nice completeness properties, their high complexity remains a limit, despite the impressive efficiency of modern implementations. This appears to be an obstacle to the use of SMT solvers when verifying, for instance, functional properties of control-command programs. Using off-the-shelf convex optimization solvers is known to constitute an appealing alternative. However, these solvers only deliver approximate solutions, which means they do not readily provide the soundness expected for applications such as software verification. S. Conchon, together with P. Roux and M. Iguernelala [21], investigated a-posteriori validation methods and their integration in the SMT framework. Although their early prototype, implemented in the Alt-Ergo SMT solver, often does not prove competitive with state of the art solvers, it already gives some interesting results, particularly on control-command programs.

Lightweight Interactive Proving for Automated Program Verification Deductive verification approach allows establishing the strongest possible formal guarantees on critical software. The downside is the cost in terms of human effort required to design adequate formal specifications and to successfully discharge the required proof obligations. To popularize deductive verification in an industrial software development environment, it is essential to provide means to progressively transition from simple and automated approaches to deductive verification. The SPARK environment, for development of critical software written in Ada, goes towards this goal by providing automated tools for formally proving that some code fulfills the requirements expressed in Ada contracts.

In a program verifier that makes use of automatic provers to discharge the proof obligations, a need for some additional user interaction with proof tasks shows up: either to help analyzing the reason of a proof failure or, ultimately, to discharge the verification conditions that are out-of-reach of state-of-the-art automatic provers. Adding interactive proof features in SPARK appears to be complicated by the fact that the proof toolchain makes use of the independent, intermediate verification tool Why3, which is generic enough to accept multiple front-ends for different input languages. S. Dailler, C. Marché and Y. Moy proposed an approach to extend Why3 with interactive proof features and also with a generic client-server infrastructure allowing integration of proof interaction into an external, front-end graphical user interface such as the one of SPARK. This was presented at the F-IDE symposium [18].

7.3. Certification of Algorithms, Languages, Tools and Systems

Formalization and closedness of finite dimensional subspaces. F. Faissole formalized a theory of finite dimensional subspaces of Hilbert spaces in order to apply the Lax-Milgram Theorem on such subspaces. He had to prove, in the Coq proof assistant, that finite dimensional subspaces of Hilbert spaces are closed in the context of general topology using filters [90]. He also formalized both finite dimensional modules and finite dimensional subspaces of modules. He compared the two formalizations and showed a complementarity between them. He proved that the product of two finite dimensional modules is a finite dimensional module [22].

Analysis of explicit Runge-Kutta methods Numerical integration schemes are mandatory to understand complex behaviors of dynamical systems described by ordinary differential equations. Implementation of these numerical methods involve floating-point computations and propagation of round-off errors. In the spirit of [58], S. Boldo, F. Faissole and A. Chapoutot developed a fine-grained analysis of round-off errors in explicit Runge-Kutta integration methods, taking into account exceptional behaviors, such as underflow and overflow [31].

Verified numerical approximations of improper 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 [113]. 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 [15]. This makes CoqInterval one of the very few tools able to produce reliable results for improper integrals, be they formally verified or not.

Case study: algorithms for matrix multiplication. M. Clochard, L. Gondelman and M. Pereira worked on a case study about matrix multiplication. Two variants for the multiplication of matrices are proved: a naive version using three nested loops and Strassen's algorithm. To formally specify the two multiplication algorithms, they developed a new Why3 theory of matrices, and they applied a reflection methodology to conduct some of the proofs. A first version of this work was presented at the VSTTE Conference in 2016 [74]. An extended version that considers arbitrary rectangular matrices instead of square ones is published in the Journal of Automated Reasoning [13]. The development is available in Toccata's gallery http://toccata.lri.fr/gallery/verifythis_2016_matrix_multiplication.en.html.

Digital Filters Digital filters are small iterative algorithms, used as basic bricks in signal processing (filters) and control theory (controllers). D. Gallois-Wong, S. Boldo and T. Hilaire formally proved in Coq some error analysis theorems about digital filters, namely the Worst-Case Peak Gain theorem and the existence of a filter characterizing the difference between the exact filter and the implemented one. Moreover, as the digital signal processing literature provides many equivalent algorithms, called realizations, they formally defined and proved the equivalence of several realizations (Direct Forms and State-Space) [19]. Another Coq development dedicated the a realization called SIF (Specialized Implicit Form) has been done, in order to encompass all the other realizations up to the order of computation, which is very important in finite precision [25].

7.4. Floating-Point and Numerical Programs

Correct Average of Decimal Floating-Point Numbers Some modern processors include decimal floating-point units, with a conforming implementation of the IEEE-754 2008 standard. Unfortunately, many algorithms from the computer arithmetic literature are not correct anymore when computations are done in radix 10. This is in particular the case for the computation of the average of two floating-point numbers. S. Boldo, F. Faissole and V. Tourneur developed a new radix-10 algorithm that computes the correctly-rounded average, with a Coq formal proof of its correctness, that takes gradual underflow into account [17].

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. It also appears in abstract interpretation for the analysis of programs containing IEEE 754 operations. D. Gallois-Wong, S. Boldo and P. Cuoq proposed floating-point theorems that provide optimal bounds for all the intervals. Fast loop-free algorithms compute these optimal bounds using only floating-point computations at the target precision [34].

Handbook of Floating-point Arithmetic Initially published in 2010, the *Handbook of Floating-Point Arithmetic* has been heavily updated. G. Melquiond contributed to the second edition [28].

Error analysis of finite precision digital filters and controllers The effort to provide accurate and reliable error analysis of fixed-point implementations of Signal Processing and Control algorithms was continued (see also the formalization effort above). A. Volkova, M. Istoan, F. de Dinechin and T. Hilaire (Citi Lyon, INSA Lyon) created an automatic code generator for FPGAs and dedicated roundoff analysis in order to minimize the bit-widths used for the intern computations while guaranteeing a bound on the output error [16]. The global workflow for the rigorous design of reliable Fixed-Point filters has been studied by A. Volkova, T. Hilaire and C. Lauter and submitted to a journal [36] : it concerns the rigorous determination of the Most Significant Bit of each variable, to guaranty that no overflow will ever occur, also taking into account the roundoff error propagation.

COMMANDS Project-Team

7. New Results

7.1. Optimal control of ODEs

7.1.1. Optimal healh insurance design

In [7] we analyze the design of optimal medical insurance under ex post moral hazard, i.e., when illness severity cannot be observed by insurers and policyholders decide for themselves on their health expenditures. The trade-off between ex anterisk sharing and ex post incentive compatibility is analyzed in an optimal revelation mechanism under hidden information and risk aversion. The optimal contract provides partial insurance at the margin, with a deductible when insurers' rates are affected by a positive loading, and it may also include an upper limit on coverage. The potential to audit the health state leads to an upper limit on out-of-pocket expenses.

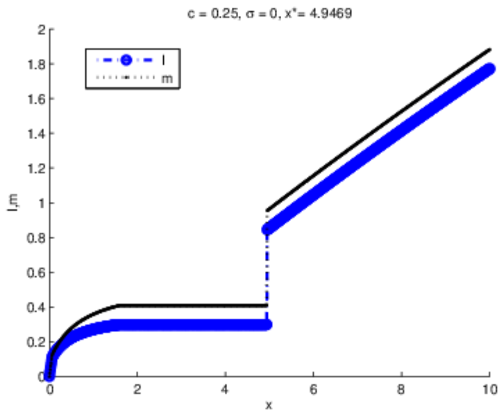

Figure 1.

Health insurance with audit. The 'out-of-pocket' expense $(m - I)$ remains bounded.

7.1.2. Optimal Battery Aging: an Adaptive Weights Dynamic Programming Algorithm

In [5] we present an algorithm to handle the optimization over a long horizon of an electric microgrid including a battery energy storage system. While the battery is an important and costly component of the microgrid, its aging process is often not taken into account by the Energy Management System, mostly because of modeling and computing challenges. We address the computing aspect by a new approach combining dynamic programming, decomposition and relaxation techniques. We illustrate this 'adaptive weight' method with numerical simulations for a toy microgrid model. Compared to a straightforward resolution by dynamic programming, our algorithm decreases the computing time by more than one order of magnitude, can be parallelized, and allows for online implementations. We believe that this approach can be used for other applications presenting fast and slow variables.

Optimal battery aging. Comparison of brute-force and adaptive weights algorithm.

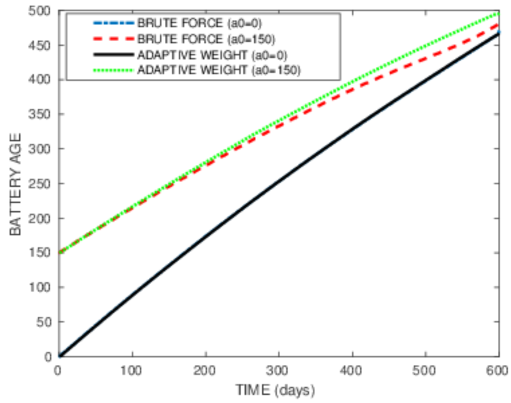

Figure 2.

7.1.3. Aircraft model identification and trajectory optimization

During the PhD of C. Rommel co-supervised with startup Safety Line, we investigated several formulations and methods for identifying an aircraft dynamics from recorded flight data. In particular, in [14] we introduce a block-sparse Bolasso approach for variable selection. In [12] we study how to quantify the closedness of a trajectory to a set of reference ones, based on the meean marginal likelihood. These works are combined with a gaussian mixture model in [15], allowing for a trade-off between optimality and acceptability of the aircraft trajectories.

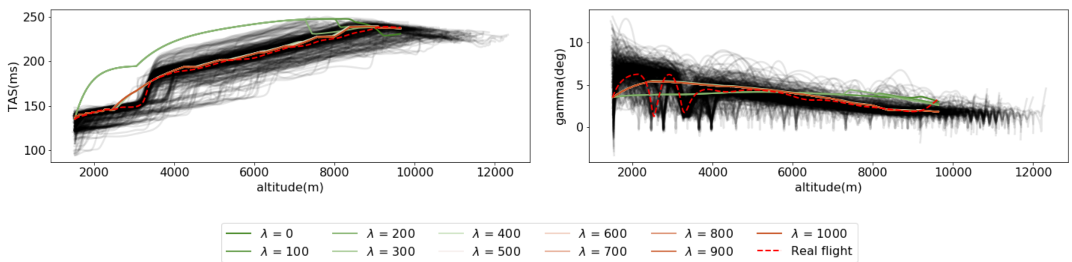

Figure 3.

Aircraft trajectory optimization. Illustration of the trade-off between performance (consumption) and acceptability (weighted by λ).

7.1.4. Microalgae cultivation in a turbid medium

In the context of IPL Algae in Silico, we study in [11] the cultivation of microalgae in a turbid medium. Microalgae cultivation with wastewater is a promising way of reducing the energetic needs for wastewater treatment and the costs of biofuel production. However, the very turbid medium is not favorable for the development of microalgae. Indeed, light, the key element for photosynthesis, rapidly vanishes along depth due to absorption and scattering. Therefore it is crucial to understand the effects of the depth on turbid cultures. In this work, we study theoretically the long-term behavior of a continuous culture of microalgae exposed to a periodic source of light. By allowing periodic variations of the depth and the hydraulic retention time, we show that the microalgae population is forced to a periodic regime. Finally, we address numerically the problem of determining the optimal variations of the depth and the hydraulic retention time for maximizing the productivity of the culture in the periodic regime.

7.1.5. Optimizing running a race on a curved track

Following on a previous study of optimal running strategies [16], we investigate in [9] the case of a curved track. In order to determine the optimal strategy to run a race on a curved track according to the lane number, we introduce a model based on differential equations for the velocity, the propulsive force and the anaerobic energy which takes into account the centrifugal force. This allows us to analyze numerically the different strategies according to the different types of track since the straight line is not always of the same length. In particular, we find that the tracks with shorter straight lines lead to better performances, while the double bend track with the longest straight line leads to the worst performances and the biggest difference between lanes. Then for a race with two runners, we introduce a psychological attraction to follow someone just ahead and the delay to benefit again from this interaction after being overtaken. We provide numerical simulations in different cases. Results are overall consistent with the IAAF rules for lanes drawing, indicating that middle lanes are the best, followed by the exterior lanes, interior lanes being the worst.

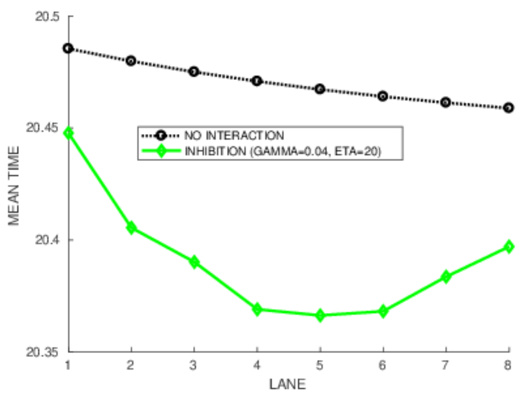

Figure 4.

Running on a curved track. Mean race times per lane, taking into account centrifugal force and psychological interaction.

7.2. Optimal control of PDEs and stochastic control

7.2.1. Sufficient optimality conditions for bilinear optimal control of the linear damped wave equation

In [8] we discuss sufficient optimality conditions for an optimal control problem for the linear damped wave equation with the damping parameter as the control. We address the case that the control enters quadratic in the cost function as well as the singular case that the control enters affine. For the non-singular case we consider strong and weak local minima , in the singular case we derive sufficient optimality conditions for weak local minima. Thereby, we take advantage of the Goh transformation applying techniques recently established in

Aronna, Bonnans, and Kröner [Math. Program. 168(1):717–757, 2018]. Moreover, a numerical example for the singular case is presented.

7.2.2. Variational analysis for options with stochastic volatility and multiple factors

In [3] we perform a variational analysis for a class of European or American options with stochastic volatility models, including those of Heston and Achdou-Tchou. Taking into account partial correlations and the presence of multiple factors, we obtain the well-posedness of the related partial differential equations, in some weigthed Sobolev spaces. This involves a generalization of the commutator analysis introduced by Achdou and Tchou.

7.2.3. Infinite Horizon Stochastic Optimal Control Problems with Running Maximum Cost

In [6] we analyze an infinite horizon stochastic optimal control problem with running maximum cost. The value function is characterized as the viscosity solution of a second-order Hamilton-Jacobi-Bellman (HJB) equation with mixed boundary condition. A general numerical scheme is proposed and convergence is established under the assumptions of consistency, monotonicity and stability of the scheme. These properties are verified for a specific semi-Lagrangian scheme.

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

In the framework of the PhD of A. Le Rhun, we present in [10] a new approach to estimate traffic energy consumption via traffic data aggregation in (speed,acceleration) probability distributions. 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.

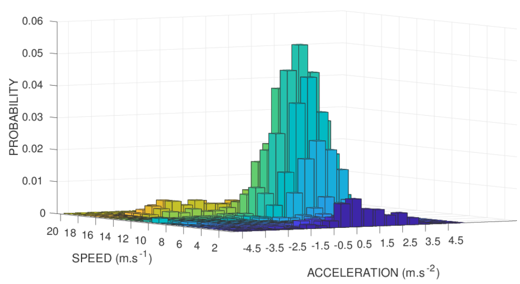

Figure 5.

Traffic modeling. Example of (speed,acceleration) distribution and illustration of clustering results with respect to day time. Slow traffic for yellow and purple clusters clearly corresponds to peak hours.

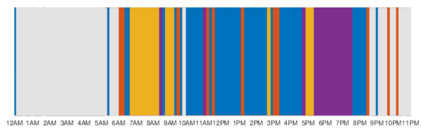
12AM 1AM 2AM 3AM 4AM 5AM 6AM 7AM 8AM 9AM 10AM 11AM 12PM 1PM 2PM 3PM 4PM 5PM 6PM 7PM 8PM 9PM 10PM 11PM

Figure 6.

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7. New Results

7.1. Qualitative and quantitative methods for inverse problems

7.1.1. On the Factorization Method for a Far Field Inverse Scattering Problem in the Time Domain

F. Cakoni, H. Haddar and A. Lechleiter

We develop a factorization method to obtain explicit characterization of a (possibly non-convex) Dirichlet 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 Dirichlet 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.

7.1.2. New interior transmission problem applied to a single Floquet–Bloch mode imaging of local perturbations in periodic media

F. Cakoni, H. Haddar and T.P Nguyen

We consider the imaging of local perturbations of an infinite penetrable periodic layer. A cell of this periodic layer consists of several bounded inhomogeneities situated in a known homogeneous media. We use a differential linear sampling method to reconstruct the support of perturbations without using the Green's function of the periodic layer nor reconstruct the periodic background inhomogeneities. The justification of this imaging method relies on the well-posedeness of a nonstandard interior transmission problem, which until now was an open problem except for the special case when the local perturbation did not intersect the background inhomogeneities. The analysis of this new interior transmission problem is the main focus of this paper. We then complete the justification of our inversion method and present some numerical examples that confirm the theoretical behavior of the differential indicator function determining the reconstructable regions in the periodic layer.

7.1.3. 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.

7.1.4. Detecting Sound Hard Cracks in Isotropic Inhomogeneities

L. Audibert, L. Chesnel, H. Haddar and Kevish Napal

We consider the problem of detecting the presence of sound-hard cracks in a non homogeneous reference medium from the measurement of multi-static far field data. First, we provide a factorization of the far field operator in order to implement the Generalized Linear Sampling Method (GLSM). The justification of the analysis is also based on the study of a special interior transmission problem. This technique allows us to recover the support of the inhomogeneity of the medium but fails to locate cracks. In a second step, we consider a medium with a multiply connected inhomogeneity assuming that we know the far field data at one given frequency both before and after the appearance of cracks. Using the Differential Linear Sampling Method (DLSM), we explain how to identify the component(s) of the inhomogeneity where cracks have emerged. The theoretical justification of the procedure relies on the comparison of the solutions of the corresponding interior transmission problems without and with cracks. Finally we illustrate the GLSM and the DLSM providing numerical results in 2D. In particular, we show that our method is reliable for different scenarios simulating the appearance of cracks between two measurements campaigns

7.1.5. Uncertainty Analysis and Calibration of the Catalytic Properties of Thermal Protection Materials: Formulation of the Bayesian Inference Problem

P.M. Congedo, F. Sanson, T. Magin, F. Panerai

Quantifying the catalytic properties of reusable thermal protection system materials is essential for the design of atmospheric entry vehicles. Their properties quantify the recombination of oxygen and nitrogen atoms into molecules, and allow for accurate computation of the heat flux to the spacecraft. Their rebuilding from ground test data, however, is not straightforward and subject to uncertainties. We propose a fully Bayesian approach to reconstruct the catalytic properties of ceramic matrix composites from sparse high-enthalpy facility experimental data with uncertainty estimates. The results are compared to those obtained by means of an alternative reconstruction procedure, where the experimental measurements are also treated as random variables but propagated through a deterministic solver. For the testing conditions presented in this work, the contribution to the measured heat flux of the molecular recombination is negligible. Therefore, the material catalytic property cannot be estimated precisely. Moreover, epistemic uncertainties are rigorously included, such as the unknown reference calorimeter catalytic property.

7.1.6. A Bayesian framework for the investigation of complex fluid vapor flows

P.M. Congedo, G. Gori, O. Le Maitre, A. Guardone

The present work develops a Bayesian framework for the inference of complex fluid thermodynamic model parameters. The objective is to numerically assess the potential of using experimental measurements to reduce the aleatoric and epistemic uncertainties inherent the Peng-Robinson thermodynamic fluid model for flows of fluids in the non-ideal regimes. Our Bayesian framework is tailored to the design of the TROVA (Test-Rig for Organic VApors) experimental facility, at Politecnico di Milano. Computational Fluid Dynamics (CFD) simulations are used to predict the flow field within the designed test section whereas surrogate models (Polynomial-Chaos expansion) are constructed to account for the predictions dependence on the thermodynamic model parameters. First, synthetic data are generated in the attempt of reproducing a real test case, which is considered as the reference experiment, actually achieved in the TROVA facility. We investigate the resulting posterior uncertainties and assess the knowledge brought by using diverse type of measurements obtained for a flow in the non-ideal regime. Results reveal that the exploitation of pressure measurements only do not allow to infer the thermodynamic coefficients. Indeed, the material-dependent parameters remain highly uncertain.

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

H. Girardon, H. Haddar and L. Audibert

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 experimentations with synthetic data demonstrated the viability of our approach.

7.2. Invisiblity and transmission eigenvalues

7.2.1. Trapped modes and reflectionless modes as eigenfunctions of the same spectral problem

A.-S. Bonnet-Ben Dhia, L. Chesnel and V. Pagneux

We consider the reflection-transmission problem in a waveguide with obstacle. At certain frequencies, for some incident waves, intensity is perfectly transmitted and the reflected field decays exponentially at infinity. We show that such reflectionless modes can be characterized as eigenfunctions of an original non-selfadjoint spectral problem. In order to select ingoing waves on one side of the obstacle and outgoing waves on the other side, we use complex scalings (or Perfectly Matched Layers) with imaginary parts of different signs. We prove that the real eigenvalues of the obtained spectrum correspond either to trapped modes (or bound states in the continuum) or to reflectionless modes. Interestingly, complex eigenvalues also contain useful information on weak reflection cases. When the geometry has certain symmetries, the new spectral problem enters the class of $\mathcal{PT}$-symmetric problems.

7.2.2. Transmission eigenvalues with artificial background for explicit material index identification

L. Audibert, L. Chesnel and H. Haddar

We are interested in the problem of retrieving information on the refractive index n of a penetrable inclusion embedded in a reference medium from farfield data associated with incident plane waves. Our approach relies on the use of transmission eigenvalues (TEs) that carry information on n and that can be determined from the knowledge of the farfield operator F. We explain how to modify F into a farfield operator $F^{\mathrm{a}} = F - \widetilde{F}$, where $\widetilde{F}$ is computed numerically, corresponding to well chosen artificial background and for which the associated TEs provide more accessible information on n.

7.2.3. Simple examples of perfectly invisible and trapped modes in waveguides

L. Chesnel and V. Pagneux

We consider the propagation of waves in a waveguide with Neumann boundary conditions. We work at low wavenumber focusing our attention on the monomode regime. We assume that the waveguide is symmetric with respect to an axis orthogonal to the longitudinal direction and is endowed with a branch of height L whose width coincides with the wavelength of the propagating modes. In this setting, tuning the parameter L, we prove the existence of simple geometries where the transmission coefficient is equal to one (perfect invisibility). We also show that these geometries, for possibly different values of L, support so called trapped modes (non zero solutions of finite energy of the homogeneous problem) associated with eigenvalues embedded in the continuous spectrum.

7.2.4. New sets of eigenvalues in inverse scattering for inhomogeneous media and their determination from scattering data

F. Cakoni, H. Haddar and L. Audibert

We developed a general mathematical framework to determine interior eigenvalues from a knowledge of the modified far field operator associated with an unknown (anisotropic) inhomogeneity. The modified far field operator is obtained by subtracting from the measured far field operator the computed far field operator corresponding to a well-posed scattering problem depending on one (possibly complex) parameter. Injectivity of this modified far field operator is related to an appropriate eigenvalue problem whose eigenvalues can be determined from the scattering data, and thus can be used to obtain information about material properties of the unknown inhomogeneity. We discuss here two examples of such modification leading to a Steklov eigenvalue problem, and a new type of the transmission eigenvalue problem. We present some numerical examples demonstrating the viability of our method for determining the interior eigenvalues form far field data.

7.2.5. The Asymptotic of Transmission Eigenvalues for a Domain with a Thin Coating

H. Boujlida, H Haddar and M. Khenissi

We consider the transmission eigenvalue problem for a medium surrounded by a thin layer of inhomogeneous material with different refractive index. We derive explicit asymptotic expansion for the transmission eigenvalues with respect to the thickness of the thin layer. We prove error estimate for the asymptotic expansion up to order 1 for simple eigenvalues. This expansion can be used to obtain explicit expressions for constant index of refraction.

7.2.6. The spectral analysis of the interior transmission eigenvalue problem for Maxwell's equations

H. Haddar and S. Meng

we consider the transmission eigenvalue problem for Maxwell's equations corresponding to non-magnetic inhomogeneities with contrast in electric permittivity that has fixed sign (only) in a neighborhood of the boundary. Following the analysis made by Robbiano in the scalar case we study this problem in the framework of semiclassical analysis and relate the transmission eigenvalues to the spectrum of a Hilbert-Schmidt operator. Under the additional assumption that the contrast is constant in a neighborhood of the boundary, we prove that the set of transmission eigenvalues is discrete, infinite and without finite accumulation points. A notion of generalized eigenfunctions is introduced and a denseness result is obtained in an appropriate solution space.

7.2.7. Non reflection and perfect reflection via Fano resonance in waveguides

L. Chesnel, S.A. Nazarov

We investigate a time-harmonic wave problem in a waveguide. By means of asymptotic analysis techniques, we justify the so-called Fano resonance phenomenon. More precisely, we show that the scattering matrix considered as a function of a geometrical parameter ε and of the frequency λ is in general not continuous at a point $(\varepsilon, \lambda) = (0, \lambda^0)$ where trapped modes exist. In particular, we prove that for a given $\varepsilon \neq 0$ small, the scattering matrix exhibits a rapid change for frequencies varying in a neighbourhood of λ^0. We use this property to construct examples of waveguides such that the energy of an incident wave propagating through the structure is perfectly transmitted (non reflection) or perfectly reflected in monomode regime. We provide numerical results to illustrate our theorems.

7.2.8. From zero transmission to trapped modes in waveguides

L. Chesnel, V. Pagneux

We consider a time-harmonic scattering wave problem in a 2D waveguide at wavenumber k such that one mode is propagating in the far field. For a given k, playing with one scattering branch of finite length, we demonstrate how to construct geometries with zero transmission. The main novelty in this result is that the symmetry of the geometry is not needed: the proof relies on the unitary structure of the scattering matrix. Then, from a waveguide with zero transmission, we show how to build geometries supporting trapped modes associated with eigenvalues embedded in the continuous spectrum. For this second construction, using the augmented scattering matrix and its unitarity, we play both with the geometry and the wavenumber. The mathematical analysis is supplemented by numerical illustrations of the results.

7.3. Shape and topology optimization

7.3.1. Taking into account thermal residual stresses in topology optimization of structures built by additive manufacturing

G. Allaire and L. Jakabcin.

We introduce a model and several constraints for shape and topology optimization of structures, built by additive manufacturing techniques. The goal of these constraints is to take into account the thermal residual stresses or the thermal deformations, generated by processes like Selective Laser Melting, right from the beginning of the structural design optimization. In other words, the structure is optimized concurrently for its final use and for its behavior during the layer by layer production process. It is well known that metallic additive manufacturing generates very high temperatures and heat fluxes, which in turn yield thermal deformations that may prevent the coating of a new powder layer, or thermal residual stresses that may hinder the mechanical properties of the final design. Our proposed constraints are targeted to avoid these undesired effects. Shape derivatives are computed by an adjoint method and are incorporated into a level set numerical optimization algorithm. Several 2-d and 3-d numerical examples demonstrate the interest and effectiveness of our approach.

7.3.2. Topology optimization of modulated and oriented periodic microstructures by the homogenization method

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

This work is concerned with the topology optimization of structures made of periodically perforated material, where the microscopic periodic cell can be macroscopically modulated and oriented. The main idea is to optimize the homogenized formulation of this problem, which is an easy task of parametric optimization, then to project the optimal microstructure at a desired lengthscale, which is a delicate issue, albeit computationally cheap. The main novelty of our work is, in a plane setting, the conformal treatment of the optimal orientation of the microstructure. In other words, although the periodicity cell has varying parameters and orientation throughout the computational domain, the angles between its members or bars are conserved. The main application of our work is the optimization of so-called lattice materials which are becoming increasingly popular in the context of additive manufacturing. Several numerical examples are presented for single and multiple loads problems, as well as for compliance or more general objective functions.

7.3.3. Shape optimization of a coupled thermal fluid-structure problem in a level set mesh evolution framework

G. Allaire, F. Feppon, F. Bordeu, J. Cortial and C. Dapogny

Hadamard's method of shape differentiation is applied to topology optimization of a weakly coupled three physics problem. The coupling is weak because the equations involved are solved consecutively, namely the steady state Navier-Stokes equations for the fluid domain, first, the convection diffusion equation for the whole domain, second, and the linear thermo-elasticity system in the solid domain, third. Shape sensitivities are derived in a fully Lagrangian setting which allows us to obtain shape derivatives of general objective functions. An emphasis is given on the derivation of the adjoint interface condition dual to the one of equality of the normal stresses at the fluid solid interface. The arguments allowing to obtain this surprising condition are specifically detailed on a simplified scalar problem. Numerical test cases are presented using a level set mesh evolution method. It is demonstrated how the implementation enables to treat a variety of shape optimization problems.

7.3.4. Optimizing supports for additive manufacturing

G. Allaire and B. Bogosel

In additive manufacturing process support structures are often required to ensure the quality of the final built part. In this article we present mathematical models and their numerical implementations in an optimization loop, which allow us to design optimal support structures. Our models are derived with the requirement that they should be as simple as possible, computationally cheap and yet based on a realistic physical modeling. Supports are optimized with respect to two different physical properties. First, they must support overhanging regions of the structure for improving the stiffness of the supported structure during the building process. Second, supports can help in channeling the heat flux produced by the source term (typically a laser beam) and thus improving the cooling down of the structure during the fabrication process. Of course, more involved constraints or manufacturability conditions could be taken into account, most notably removal of supports. Our work is just a first step, proposing a general framework for support optimization. Our optimization algorithm is based on the level set method and on the computation of shape derivatives by the Hadamard method. In a first approach, only the shape and topology of the supports are optimized, for a given and fixed structure. In second and more elaborated strategy, both the supports and the structure are optimized, which amounts to a specific multiphase optimization problem. Numerical examples are given in 2-d and 3-d.

7.3.5. Structural optimization under internal porosity constraints using topological derivatives

G. Allaire, J.Martinez-Frutos, C. Dapogny, F. Periago

Porosity is a well-known phenomenon occurring during various manufacturing processes (casting, welding, additive manufacturing) of solid structures, which undermines their reliability and mechanical performance. The main purpose of this article is to introduce a new constraint functional of the domain which controls the negative impact of porosity on elastic structures in the framework of shape and topology optimization. The main ingredient of our modelling is the notion of topological derivative, which is used in a slightly unusual way: instead of being an indicator of where to nucleate holes in the course of the optimization process, it is a component of a new constraint functional which assesses the influence of pores on the mechanical performance of structures. The shape derivative of this constraint is calculated and incorporated into a level set based shape optimization algorithm. Our approach is illustrated by several two- and three-dimensional numerical experiments of topology optimization problems constrained by a control on the porosity effect.

7.4. Analysis of some wave problems

7.4.1. 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 pre- scribe 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.

7.4.2. Crime Pays: Homogenized Wave Equations for Long Times

G. Allaire, A. Lamacz and J. Rauch

This work examines the accuracy for large times of asymptotic expansions from periodic homogenization of wave equations. As usual, ϵ denotes the small period of the coefficients in the wave equation. We first prove that the standard two scale asymptotic expansion provides an accurate approximation of the exact solution for times t of order $\epsilon^{-2+\delta}$ for any $\delta > 0$. Second, for longer times, we show that a different algorithm, that is called criminal because it mixes different powers of ϵ, yields an approximation of the exact solution with error $O(\epsilon^N)$ for times ϵ^{-N} with N as large as one likes. The criminal algorithm involves high order homogenized equations that, in the context of the wave equation, were first proposed by Santosa and Symes and analyzed by Lamacz. The high order homogenized equations yield dispersive corrections for moderate wave numbers. We give a systematic analysis for all time scales and all high order corrective terms.

7.5. Diffusion MRI

7.5.1. A partition of unity finite element method for computational diffusion MRI

D. V. Nguyen, J. Jansson, J. Hoffman and J.-R. Li.

The Bloch-Torrey equation describes the evolution of the spin (usually water proton) magnetization under the influence of applied magnetic field gradients and is commonly used in numerical simulations for diffusion MRI and NMR. Microscopic heterogeneity inside the imaging voxel is modeled by interfaces inside the simulation domain, where a discontinuity in the magnetization across the interfaces is produced via a permeability coefficient on the interfaces. To avoid having to simulate on a computational domain that is the size of an entire imaging voxel, which is often much larger than the scale of the microscopic heterogeneity as well as the mean spin diffusion displacement, smaller representative volumes of the imaging medium can be used as the simulation domain. In this case, the exterior boundaries of a representative volume either must be far away from the initial positions of the spins or suitable boundary conditions must be found to allow the movement of spins across these exterior boundaries.

Many approaches have been taken to solve the Bloch-Torrey equation but an efficient high performance computing framework is still missing. In this paper, we present formulations of the interface as well as the exterior boundary conditions that are computationally efficient and suitable for arbitrary order finite elements and parallelization. In particular, the formulations are based on the partition of unity concept which allows for a discontinuous solution across interfaces conforming with the mesh with weak enforcement of real (in the case of interior interfaces) and artificial (in the case of exterior boundaries) permeability conditions as well as an operator splitting for the exterior boundary conditions. The method is straightforward to implement and it is available in FEniCS for moderate-scale simulations and in FEniCS-HPC for large-scale simulations. The order of accuracy of the resulting method is validated in numerical tests and a good scalability is shown for the parallel implementation. We show that the simulated dMRI signals offer good approximations to reference signals in cases where the latter are available and we performed simulations for a realistic model of a neuron to show that the method can be used for complex geometries.

7.5.2. Diffusion MRI simulation in thin-layer and thin-tube media using a discretization on manifolds

D. V. Nguyen, J. Jansson, H. T. A. Tran, J. Hoffman and J.-R. Li.

The Bloch-Torrey partial differential equation describes 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 paper proposes a finite element discretization on manifolds in order to simulate the diffusion MRI signal in domains that have a thin layer or a thin tube geometrical structure. Suppose that the three-dimensional domain has a thin layer structure: points in the domain can be obtained by starting on the two-dimensional manifold and moving along a depth (thickness) function. For this type of domains, we propose a finite element discretization formulated on a surface triangulation of the manifold. The variable thickness of the domain is included in the weak formulation on the surface triangular elements. A simple modification extends the approach to 'thin tube' domains where a manifold in one dimension and a two-dimensional variable cross-section describe the points in the domain. 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 agreement between the simulated signals using our proposed method and the reference signals. 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.

7.5.3. The time-dependent diffusivity in the abdominal ganglion of Aplysia californica, experiments and simulations

K. V. Nguyen, D. Le Bihana, L. Ciobanua and J.-R. Li

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 three types of cells in the abdominal ganglia: the large cell neurons, the bag cells, and the nerve cells. For the bag cells and nerves cells, we created spherical and cylindrical geometrical configurations that are consistent with known information about the cellular structures from the literature. We used the simulation results to obtain information about the intrinsic diffusion coefficient in these cells.

For the large cell neurons, we created geometrical configurations by segmenting high resolution T_2-weighted (T_2w) images to obtain the cell outline and then incorporated a manually generated nucleus. We used numerical simulations to validate the claim that water diffusion in the large cell neurons is in the short diffusion time regime for 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 in the large cell neurons, 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.

7.5.4. The derivation of homogenized diffusion kurtosis models for diffusion MRI

H. Haddar, M. Kchaou and M. Moakher

We use homogenization theory to establish a new macroscopic model for the complex transverse water proton magnetization in a voxel due to diffusion-encoding magnetic field gradient pulses in the case of biological tissue with impermeable membranes. In this model, new higher-order diffusion tensors emerge and offer more information about the structure of the biological tissues. We explicitly solve the macroscopic model to obtain an ordinary differential equation for the diffusion MRI signal that has similar structure as diffusional kurtosis imaging models. We finally present some validating numerical results on synthetic examples showing the accuracy of the model with respect to signals obtained by solving the Bloch-Torrey equation.

7.5.5. On-going collaborative projects on DMRI

J.R. Li, H. Haddar and I. Mekkaoui

- 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.
- We continue 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.

7.6. Mathematical tools for Psychology

J. R. Li and J. Hao

This is the start of a collaborative effort between the Defi team and Dr. Hassan Rahioui at the centre hospitalier Sainte Anne and l'Université Paris Diderot.

- We started a new research direction in algorithm and software development for analysis and classification of EEG measurements during the administration of neuropsychological tests for AD/HD with the PhD project of Jingjing Hao, co-supervised with Dr. Hassan Rahioui, Chef du pôle psychiatrique du 7e arrondissement de Paris rattaché au centre hospitalier Sainte-Anne.

  Result: unfortunately Jingjing Hao will not be able to continue with this PhD project as of Jan 2019. We will modify the project in consultation with Dr. Rahioui and continue it in another format.

7.7. Shape optimization under uncertainties

7.7.1. Surrogate-Assisted Bounding-Box Approach Applied to Constrained Multi-Objective Optimisation Under Uncertainty

P.M. Congedo, M. Rivier

This work is devoted to tackling constrained multi-objective optimisation under uncertainty problems. In particular, the SABBa (Surrogate-Assisted Bounding-Box approach) framework is applied and extended to handle both robust and reliability-based constrained optimisation problems. This approach aims at efficiently dealing with uncertainty-based optimisation problems, with approximated robustness and reliability measures. A Bounding-Box (or conservative box) is defined as a multi-dimensional product of intervals centred on approximated objectives and constraints and containing the underlying true values. In SABBa, this approach is supplemented with a Surrogate-Assisting strategy, which is very effective to reduce the overall computational cost, notably during the last iterations of the optimisation. The efficiency of the method is further increased using the concept of Pareto Optimal Probability (POP) computed for each box, and proposing some estimations for conservative error computation and box refinement using a Gaussian Process (GP).

7.7.2. A quantile-based optimization under uncertainty of an ORC turbine cascade

P.M. Congedo, N. Razaaly

This study presents an original and fast robust shape optimization approach to overcome the limitation of a deterministic optimization that neglects operating conditions variability, applied on a typical 2D ORC turbine cascade (Biere). Flow around the blade is solved by means of inviscid simulation using the open-source SU2 code, considering Non-Ideal gas effects modeled through the use of the Peng-Robinson-Stryjek-Vera equation of state, from which a Quantity of Interest (QoI) is recovered. We propose here a mono-objective formulation consisting in minimizing the α-quantile of the QoI under a constraint, at a low computational cost. This is performed by using an efficient robust optimization approach, coupling a state-of- the-art quantile estimation and a classical bayesian optimization method. First, the advantages of a quantile-based formulations are illustrated with respect to a classical mean-based robust optimization. Secondly, we demonstrate the effectiveness of applying this robust optimization framework with a low-fidelity inviscid solver by comparing the resulting optimal design with the ones obtained with a deterministic optimization using a high-fidelity turbulent solver.

7.8. Uncertainty Quantification methods for uncertainty propagation

7.8.1. Kriging-sparse Polynomial Dimensional Decomposition surrogate model with adaptive refinement

P.M. Congedo, A. Cortesi, G. El Jannoun

In this work, an algorithm for the construction of a low-cost and accurate metamodel is proposed, having in mind redcomputationally expensive applications. It has two main features. First, Universal Kriging is coupled with sparse Polynomial Dimensional Decomposition (PDD) to build a metamodel with improved accuracy. The polynomials selected by the adaptive PDD representation are used as a sparse basis to build a Universal Kriging surrogate model. Secondly, a numerical method, derived from anisotropic mesh adaptation, is formulated in order to adaptively insert a fixed number of new training points to an existing Design of Experiments. The convergence of the proposed algorithm is analyzed and assessed on different test functions with an increasing size of the input space. Finally, the algorithm is used to propagate uncertainties in two high-dimensional real problems related to the atmospheric reentry.

7.8.2. Novel algorithm using Active Metamodel Learning and Importance Sampling: Application to multiple failure regions of low probability

P.M. Congedo, N. Razaaly

Calculation of tail probabilities is of fundamental importance in several domains, such as in risk assessment. One major challenge consists in the computation of low-failure probability in cases characterized by multiple-failure regions, especially when an unbiased estimation of the error is required. Methods developed in literature rely mostly on the construction of an adaptive surrogate, tackling some problems such as the metamodel building criterion and the global computational cost, at the price of a generally biased estimation of the failure probability. In this work, we propose a novel algorithm suitable for low-failure probability and multiple-failure regions, permitting to both building an accurate metamodel and to provide a statistically consistent error. Indeed, an importance sampling technique is used, which is quasi-optimal since permits, by exploiting the knowledge of the metamodel, to provide two unbiased estimators of the failure probability. Additionally, a gaussian mixture-based importance sampling technique is proposed, permitting to drastically reduce the computational cost when estimating some reference values, or the failure probability directly from the metamodel. Several numerical examples are carried out, showing the very good performances of the proposed method with respect to the state-of-the-art in terms of accuracy and computational cost. A physical test-case, focused on the numerical simulation of non-ideal gas turbine cascades, is also investigated to illustrate the capabilities of the method on an industrial case.

7.8.3. Uncertainty propagation framework for systems of codes

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

The simulation of complex multi-physics phenomena often requires the use of coupled solvers, modelling different physics (fluids, structures, chemistry, etc) with largely differing computational complexities. We call Systems of Solvers (SoS) a set of interdependent solvers where the output of an upstream solver can be the input of a downstream solvers. In this work we restrict ourselves to weakly coupled problems. A system of solvers typically encapsulate a large number of uncertain input parameters, challenging classical Uncertainty Quantification (UQ) methods such as spectral expansions and Gaussian process models which are affected by the curse of dimensionality. In this work, we develop an original mathematical framework, based on Gaussian Processes (GP) to construct a global metamodel of the uncertain SoS that can be used to solve forward and backward UQ problems. The key idea of the proposed approach is to determine a local GP model for each solver of the SoS. These local GP models are built adaptively to satisfy criteria based on the global output error estimation, which can be decomposed (following an ANOVA-like decomposition) into contributions from individual GP models. This decomposition enables one to select the local GP models that need be refined to efficiently reduce the global error using computer experiment design methods or Bayesian optimization. This framework is then applied to a space object reentry problem.

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

7.9.1. Validation of the Non-Ideal Compressible-Fluid Dynamics solver from the open-source SU2 suite

P.M. Congedo, G. Gori, A. Guardone, M. Zocca

The first-ever experimental validation of a flow simulation software for Non-Ideal Compressible-Fluid Dynamics (NICFD) flows is presented. Numerical results from the open-source suite SU2 are compared against pressure and Mach number measurements of supersonic flows of siloxane fluid MDM (Octamethyltrisiloxane, $C_8H_{24}O_2Si_3$) at conditions in the close proximity of the liquid-vapour saturation curve. The test set is representative of typical operating conditions of Organic Rankine Cycle systems and it includes expanding flows through a converging-diverging nozzle in mildly-to-highly non-ideal conditions. The validation process takes advantage of an Uncertainty Quantification analysis, to estimate the variability of the numerical solution with respect to the physical uncertainties and to provide a robust assessment of the SU2 capabilities. All considered flows are well represented by the numerical solutions and therefore the reliability of the numerical implementation and the predictiveness of the NICFD solver are confirmed.

7.9.2. Impact of geometric, operational, and model uncertainties on the non-ideal flow through a supersonic ORC turbine cascade

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

Typical energy sources for Organic Rankine Cycle (ORC) power systems feature variable heat load and turbine inlet/outlet thermodynamic conditions. The use of organic compounds with heavy molecular weight introduces uncertainties in the fluid thermodynamic modeling. In addition, the peculiarities of organic fluids typically lead to supersonic turbine configurations featuring supersonic flows and shocks, which grow in relevance in the aforementioned off-design conditions; these features also depend strongly on the local blade shape, which can be influenced by the geometric tolerances of the blade manufacturing. This study presents an Uncertainty Quantification (UQ) analysis on a typical supersonic nozzle cascade for ORC applications, by considering a two-dimensional high-fidelity turbulent Computational Fluid Dynamic (CFD) model. Kriging-based techniques are used in order to take into account at a low computational cost, the combined effect of uncertainties associated to operating conditions, fluid parameters, and geometric tolerances. The geometric variability is described by a finite Karhunen-Loeve expansion representing a non-stationary Gaussian random field, entirely defined by a null mean and its autocorrelation function. Several results are illustrated about the ANOVA decomposition of several quantities of interest for different operating conditions, showing the importance of geometric uncertainties on the turbine performances.

7.9.3. Efficient surrogate based human risk estimation of a space object reentry

P.M. Congedo, F. Sanson, O. Le Maitre, J.-M. Bouilly, C. Bertorello

The prediction of risk associated with the reentry of a man made space object is critical but subject to input parameter uncertainties. To compute the risk one needs to determine whether the object survives to reentry and if it does where it falls on Earth. Expensive numerical models can be used to answer both questions but they can only be evaluated a limited number of times to propagate the uncertainties. In this work, we present an original approach to construct an accurate surrogate model of the numerical models using a limited number of solver evaluations. Using Gaussian Processes, the constructed surrogate model is able two answer both questions (survivability and impact location) in order to provide an accurate description of the risk. The surrogate model can achieve high level of accuracy in terms of risk estimation using dedicated active learning strategies. The efficiency of the method is illustrated on analytical test cases and an actual space object reentry case.

DISCO Project-Team

6. New Results

6.1. Spectral abscissa characterization for Time-delay systems

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [Université Paris Sud], Thomas Vyhlidal [Czech technical university in Prague], Karim Trabelsi [IPSA].

It is well known that the spectral abscissa of a given dynamical is nothing but the corresponding solutions' exponential decay. The analytical characterization of the spectral abscissa for infinite dimensional dynamical systems is an old problem which is still nowadays a question of ongoing interest due to its links with stability problems. We produced several works in this topic dealing with reduced order retarded Time-delay systems and emphasized a property that we call *multiplicity induced-dominancy*. In the paper [13], the interest of using time-delay in the controller design as a control parameter is underlined and the way to assign a dominant spectral value is demonstrated. As a matter of fact, it is shown that the multiplicity of given spectral value may reach the degree of the corresponding quasipolynomial. Furthermore, when this holds, then using a particular factorization of the quasipolynomial, such a multiple spectral value is shown to be the corresponding spectral abscissa. A generalization of such a result to generic second order retarded equation with a single delay is established in [12]. More precisely, a parametric characterization of the spectral abscissa is established using the principle argument theorem. Furthermore, in the work [45], the potential applicability of such a parametric characterization in controller design in concrete application is demonstrated. As a matter of fact, a third order retarded system modeling the dynamics of Mach number in a wind tunnel is considered and a delayed controller design based on the spectral abscissa assignment is proposed.

6.2. Poles placement for reduced order Time-delay systems

Participants: Souad Amrane [University Mouloud Mammeri], Islam Boussaada, Fazia Bedouhen [University Mouloud Mammeri], Silviu-Iulian Niculescu, Matej Kure [Czech technical university in Prague], Wim Michiels [KU Leuven], Thomas Vyhlidal [Czech technical university in Prague].

It is well known in dynamical system theory that real spectral values correspond to non oscillating solutions. In the paper [11]we made a connexion between the degree of a given quasipolynomial and the admissible number of non oscillating modes for the corresponding Time-delay system. More precisely, we have shown that the assignment of at most n real spectral values is possible for generic quasipolynomial function of degree n. Namely, explicit formulas on the quasipolynomial's coefficients guaranteeing the coexistence of n negative spectral values are obtained. Furthermore, a new quasipolynomial factorization technique, analogous to the one we developed for multiple spectral values for the proof of the dominancy of n distinct negative spectral values is obtained.

In the paper [23] a robust alternative of the delayed resonator is proposed by spectral approach where a double root assignment at the excitation frequency is proposed. Such an excitation frequency is projected to widening the stop-band in the active absorber frequency response. It is shown that the performance sensitivity to the mismatch between the design and true excitation frequency is considerably decreased. Additionally, the overall scheme is supplemented by a control loop which improves the stability margin.

6.3. Asymptotic behavior of critical imaginary roots for retarded differential equations

Participants: Islam Boussaada, Jie Chen [City University of Hong Kong], Liana Felix [Universidad Autonoma de San Luis Potosi], Keqin Gu [Southern Illinois University], Fernando Mendez-Barrios [Universidad Autonoma de San Luis Potosi], Dina Irofti, Silviu-Iulian Niculescu, Alejandro Martinez.

The behavior of characteristic roots of time-delay systems, when the delay is subject to small variations is investigated in [26]. We performed an analysis by means of the Weierstrass polynomial which are employed to study the stability behavior of the characteristic roots with respect to small variations on parameters. Analytic description and splitting properties of the Puiseux series expansions of critical roots are characterized by allowing a full description covering all the cases that can be encountered.

In the paper [21] the migration of double imaginary roots of the systems characteristic equation when two parameters are subjected to small deviations is geometrically investigated. Under the least degeneracy assumptions, the local stability crossing curve is shown to have a cusp at the point that corresponds to the double root, which divides the neighborhood of this point into two sectors (called S-sector and a G-sector). We have shown that when the parameters move into the G-sector, one of the roots moves to the right half-plane, and the other moves to the left half-plane. However, when the parameters move into the S-sector, both roots move either to the left half-plane or the right half-plane depending on the sign of a quantity that depends on the characteristic function and its derivatives up to the third order.

6.4. Stability analysis of retarded differential equations with delay-dependent coefficients

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Chi Jin [IPSA], Keqin Gu [Southern Illinois University].

Retarded dynamical systems with delay dependent coefficients is a class of systems which is frequently encountered in various scientific and engineering applications. The paper [36] provides an overview of the stability analysis of such systems which generalizes those on systems with delay-independent coefficients. Methods of analysis for systems with a single delay and commensurate delays are presented, their application to output feedback control and a geometric perspective that establishes a link between systems with and without delay-dependent coefficients.

The paper [22] presents a systematic method to analyse the stability of systems with single delay in which the coefficient polynomials of the characteristic equation depend on the delay. With respect to the literature on the topic, a less restrictive method to analyse stability is presented. It is found that a much richer behavior is possible when the restrictive assumptions are removed. The interval of interest for the delay is partitioned into subintervals so that the magnitude condition generates a fixed number of frequencies as functions of the delay within each subinterval. The crossing conditions are expressed in a general form, and a simplified derivation for the first-order derivative criterion is obtained.

6.5. Stability and Stabilisability Through Envelopes for Retarded and Neutral Time-Delay Systems

Participants: Catherine Bonnet, Caetano Cardeliquio, Silviu Niculescu, André Fioravanti [FEM-UNICAMP, Brazil].

Through an LMI approach it was possible to determine envelopes and use them not only to study stability but to design robust controllers for retarded and neutral time-delay systems. The controller designed is robust to parametric uncertainties and can guarantee delay independant stability or delay-dependant $\alpha - stability$ [46].

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

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

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 [66] and analyzed carefully the position of the poles of such systems in the right half-plane.

6.7. Local Analysis of Lurie Systems

Participants: Elena Panteley [L2S,CNRS], Stephen Duncan [University of Oxford], Thomas Lathuiliere [University of Oxford], Giorgio Valmorbida.

An important aspect of nonlinear systems is the fact that stability might only be a local property. This means that associated to a stable equilibrium point or periodic trajectory, there is a region of attraction. Such a region is formed by points of trajectories converging to the stable sets. An important task of practical interest is then to estimate these regions via numerical methods that rely on the model of the system. As an illustration, it might be of interest to know the region of safe operation of an electric motor in order to preserve its integrity or, in the case of an autonomous vehicle, limit the operating condition for safety purposes.

For the particular class of Lurie systems, namely systems defined by the interconnection of a linear system and a static nonlinearity, it is possible to compute estimates based on sector inequalities characterizing the nonlinearities in the system. If further information, such as the slope of the nonlinearity is available, one can better characterize local properties such as regions of stability, and input-output relations such as reachable sets and local nonlinear gains.

To obtain these characterizations we rely on numerical methods based on convex optimization. These methods are based on the solution of Lyapunov inequalities yielding Lyapunov functions that are quadratic on both the states and the nonlinearity and has an integral term on the nonlinearity [39].

Moreover, whenever a more precise characterization of the nonlinearity is at hand as for instance nonlinearities having rational Jacobian, one can generalize the local analysis methods using polynomial optimization. This includes the case of standard Lurie systems by considering the interconnection of a polynomial system with static sector nonlinearities that have rational Jacobian. In this setting we have proposed conditions that relax the requirement on the candidate Lyapunov function [17], which serve as stability certificates, from being sum-of-squares of polynomial with respect to the nonlinearities and the Lurie-Postnikov terms from being non-negative.

Further to the stability analysis we were interested in another important phenomenon and its analysis through numerical methods : the existence of limit cycles on nonlinear systems. Such a phenomenon is relevant since it can be used as a method to design stable oscillators with known amplitude and frequency but also to evaluate and suppress undesirable oscillations in engineered systems. In order to proceed with this analysis we have limited our attention to a particular class of systems defined by a Liénard systems and formulate sufficient conditions for existence and uniqueness of limit cycles for systems with a non-differentiable vector field. As an application we consider the example of a linear system with saturation [24]. Moreover, for planar saturating systems we present sufficient conditions for the existence of periodic orbits and we characterize inner and outer sets bounding the periodic orbits. A method to build these bounds, based on the solution to a convex optimization problem is proposed and numerical examples optimizing the region bounding the limit cycle illustrate the technique [25].

6.8. New advances on backstepping

Participants: Frederic Mazenc, Michael Malisoff [LSU], Laurent Burlion [ONERA Toulouse], Jerome Weston [LSU].

We worked on the problem of improving a fundamental control design technique for nonlinear systems called backstepping by using a fundamentally new approach which consists in introducing in the control artificial delays or using dynamic extensions.

In [28], we provided backstepping results for a large class of partially linear systems with an arbitrarily large number of integrators. We proposed control laws whose size respects some constaints given a priori. The key tool is a dynamic extension that contains only one artificial delay, which is in sharp contrast with our prior contributions. We also showed that the closed-loop system is robust, in the input-to-state stability sense, with respect to a large class of model uncertainties, and robust with respect to delays in the measurements. We illustrated the result using an example that is beyond the scope of classical backstepping.

The paper [57] also provides a crucial backstepping result. We explained how globally asymptotically stabilizing output feedbacks can be constructed for a family of nonlinear systems using only a dynamic extension and a "Converging Input-Converging State" assumption and no additional delays. The technique presents several advantages. It provides control laws whose expressions are simple. It makes it possible to stabilize systems in the presence of uncertain terms, which are not necessarily of class C^1 and which prevent the use of the classical backstepping technique. It applies in cases where only part of the state variables can be measured.

6.9. Time-varying systems with delay and Switched Systems

Participants: Frederic Mazenc, Michael Malisoff [LSU], Saeed Ahmed [Inria], Hitay Ozbay [Blikent University, Turkey].

The family of the switched systems is frequently encountered in practice. It can be used to approximate time-varying systems to ease their stability analysis or control.

In [29] we provided theoretical results for the stability and robustness analysis of nonlinear switched time-varying systems with uncertainties and time-varying delays. The delays are allowed to be discontinuous and arbitrarily long with known upper bounds. We established the results via an adaptation of Halanay's inequality and a trajectory based technique. Also, we used the results for designing switched controllers that stabilize linear time-varying systems with time-varying delays.

The contribution [10] proposed a new technique of construction of observers making possible to stabilize by output feedback a class of continuous-time switched linear systems with a time-varying delay in the output. The motivation of this paper is strong: frequently measurements are affected by pointwise time-varying delays. For stability analysis, we developped an extension of the trajectory based approach. A stability condition is given in terms of the upper bound on the time-varying delay to ensure global exponential stability of the switched feedback systems. It is worth observing that the main result applies in cases where some of the subsystems of the switched system are not stabilizable and not detectable.

The paper [27] is also devoted to classes of nonlinear time-varying continuous-time systems with outputs. For a first family of systems, we builded an observer in the case where a state dependent disturbance affects the linear approximation. A fundamental feature of our observer is the fact that it converges after a predetermined finite time. When the disturbances are the zero functions, it provides exact values of the state and it provides an approximate estimate when there are nonzero disturbances. We used this construction to design a globally exponentially stabilizing dynamic output feedback for a second family of nonlinear systems whose outputs are only available on some finite time intervals. Our technique consists in switching between control laws. We applied the control design to the controlled Mathieu equation, which arises in the study of vibrations of an elliptic membrane.

The paper [38] is devoted to a stability analysis for a class of nonlinear systems with a time-varying delay taking both large and small values in an alternating manner, precluding the application of most of the classical control design techniques. The type of assumption we imposed is the following: we imposed on the delay to be "small" on "long" time intervals and possibly "large" on "small" time-intervals. Bearing in mind this key property, we first introduced the concept of delay-hybrid-dependent stability, which grasps the features of the delays described above and represented the studied system as a system with a switched delay. Then by using switching techniques and Lyapunov-Krasovskii functionals (LKFs), we provided a new stability criterion.

6.10. Observers

Participants: Frederic Mazenc, Michael Malisoff [LSU], Saeed Ahmed [Inria], Ali Zemouche [CRAN], Rajesh Rajamani [University of Minneapolis, USA], Maruthi Akella [University of Texas, USA].

We produced several works which pertain to the case where only a part of the state variables can be measured.

In the paper [58], we adopted a technique based on the indroduction of several observers in cascade (such a cascade is called 'sequential observer') for a class of time-varying linear systems in which the inputs and outputs containing sampling and arbitrarily long delays. The observers are of a continuous-discrete type. We used the observers to design controllers that ensure a strong robustness property with respect to uncertainties in the system and the output, under delays and sampling. A fundamental aspect of the approach is that it produces the observers and controllers without distributed terms. We have assessed the performance of the control laws through two examples, which inlcude a DC motor model that illustrates the utility of the work in engineering applications.

In two papers, we developped the theory of the finite time observers. In [53], we study a class of linear continuous-time time-varying systems with piecewise continuous disturbances and piecewise constant outputs. Under a classical assumption of observability, we designed a new type of observers to estimate the solutions of the system in a predetermined finite time. In contrast to the well-established finite time observer design techniques which estimate the system state using a continuous output, our proposed observer applies when only piecewise constant measurements are available. In [54], we construct finite-time reduced order observers for a broad family of nonlinear time-varying continuous-time systems. The motivation for this is the fact that in practice the time-varying aspect of a system may be an obstacle to the design of full-order finite-time observers, but not for the design of reduced order ones. We illustrated our results using a tracking problem for nonholonomic systems in chained form.

Two of our works present construction of asymptotic observers without delay. The paper [61] solves an H_∞ observer design problem for a class of descriptor nonlinear systems. The method we established is theoretical and can be applied to many automatic control design problems such as unknown input estimation problem, which plays an important role in control systems, namely for diagnosis and fault tolerant control. The design relies on the Linear Matrix Inequality condition (LMI) technique. We applied our resut to a model of a flexible joint robot system.

The work [16] is dedicated to the design of a smooth six-degree-of-freedom observer to estimate the incorporating linear and angular velocity, called dual angular velocity, for a rigid body. The approach is based on the dual-quaternion description and we proved that the estimation errors exhibit asymptotic convergence. Furthermore, to achieve tracking control objective, we combined the proposed observer 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. We performed numerical simulations for a prototypical spacecraft hovering mission application.

6.11. Stabilization of various systems with pointwise delays

Participants: Frederic Mazenc, Michael Malisoff [LSU], Delphine Bresch-Pietri [Mines Paris Tech.], Nicolas Petit [Mines Paris Tech.], Robledo Gonzalo [Univ. de Chile, Chile], Maruthi Akella [University of Texas, USA], Xi-Ming Sun [Dalian University of Technology, China], Xue-Fan Wang [Dalian University of Technology, China].

The presence of delays to big for being neglected is an obstacle to the design of stabilizing controllers in many cases. We have made efforts to overcome this challenge by developping several techniques.

In the paper [14], we investigated the design of a prediction-based controller for a linear system subject to a problematic time-varying input delay: the delay we considered is not necessarily "First-In/First-Out". The feedback law we proposed uses the current delay value in the prediction. It does not exactly compensate the delay in the closed-loop dynamics but does not require to predict future delay values, contrary to classical prediction techniques. Modeling the input delay as a transport Partial Differential Equation, we proved asymptotic stabilization of the system state, provided that the average L_2-norm of the first derivative of the delay over some time-window is sufficiently small and that the average time between two discontinuities (average dwell time) is sufficiently large.

In the paper [51], we adopted another type of strategy: we used a new sequential predictors approach to build uniformly globally exponentially stabilizing feedback controls for a large class of linear time-varying systems that contain an arbitrary number of different delays. This allows different delays in different components of the input. We illustrated our work in an example from identification theory, and in an Euler-Lagrange system arising from two-link manipulator systems.

The paper [31] continues our works on the chemostat model with an arbitrary number of competing species, one substrate, and constant dilution rates. We allowed delays in the growth rates and additive uncertainties. Using constant inputs of certain species, we derived bounds on the sizes of the delays that ensure asymptotic stability of an equilibrium when the uncertainties are zero, which can allow persistence of multiple species. In the presence of delays and uncertainties, we provided bounds on the delays and on the uncertainties that ensure, with respect to uncertainties, the robustness property called "input-to-state stability".

6.12. Low complexity constrained control using higher degree Lyapunov functions

Participants: Sarmad Munir [NTNU, Trondheim], Sorin Olaru, Morten Hovd [NTNU, Trondheim].

Explicit Model Predictive Control often has a complex solution in terms of the number of regions required to define the solution and the corresponding memory requirement to represent the solution in the online implementation. An alternative approach to constrained control is based on the use of controlled contractive sets. However, polytopic controlled contractive sets may themselves be relatively complex, leading to a complex explicit solution, and the polytopic structure can limit the size of the controlled contractive set. Our recent results [33] develop a method to obtain a larger controlled contractive set by allowing higher order functions in the definition of the contractive set, and explores the use of such higer-order contractive sets in controller design leading to a low complexity explicit control formulation.

6.13. Characterization of ultimate bounds for systems with state-dependent disturbances

Participants: Sorin Olaru, Hiroshi Ito [Kyushu Institute of Technology, Japan].

The work [37] pursues a framework of set characterization of dynamical systems with state-dependent disturbances. It aims to propose a new approach to analysis and design of nonlinear systems involving non-differentiability and asymmetric components which hamper application and effectiveness of local linearization methods. Several characterizations of ultimate bounds are developed. The utility of shifting the fix point is formulated as a parametrization of the ultimate bounds.

6.14. Combinatorial Approach towards Multi-Parametric Quadratic Programming based on Characterizing Adjacent Critical Regions

Participants: Parisa Ahmadi-Moshkenani [NTNU, Trondheim], Sorin Olaru, Tor Johansen [NTNU, Trondheim].

Several optimization-based control design techniques can be cast in the form of parametric optimization problems. The multi-parametric quadratic programming (mpQP) represents a popular class often related to the control of constrained linear systems. The complete solution to mpQP takes the form of explicit feedback functions with a piecewise affine structure, valid in polyhedral partitions of the feasible parameter space known as critical regions. The recently proposed combinatorial approach for solving mpQP has shown better efficiency than geometric approaches in finding the complete solution to problems with high dimensions of the parameter vectors. The drawback of this method, on the other hand, is that it tends to become very slow as the number of constraints increases in the problem. This work [9] presents an alternative method for enumerating all optimal active sets in a mpQP based on theoretical properties of adjacent critical regions and their corresponding optimal active sets. Consequently, it results in excluding a noticeable number of feasible but not optimal candidate active sets from investigation. Therefore, the number of linear programs that should be solved decreases noticeably and the algorithm becomes faster. Simulation results confirm the reliability of the suggested method in finding the complete solution to the mpQPs while decreasing the computational time compared favourably with the best alternative approaches.

6.15. Active vibration damping in a mechanical structures

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [Université Paris Sud], Thomas Vyhlidal [Czech technical university in Prague], Daniela Danciu [University of Craiova].

In the work [13], an aluminium-based flexible structure embedded in a mobile support subjected to an acceleration is considered. Such a flexible beam is equipped with two piezoelectric patches. One of them is used as an actuator and the second acts as a sensor. These patches are supposed to be rigidly bounded on the beam, one on each side, located at the clamped edge. The whole device is called a piezo-actuated beam which is generally modeled by Euler-Bernoulli equations. Finite element modeling is then applied to reduce the PDE system to a linear finite-dimensional system. Then, the peak of resonance of the first bending mode is damped by using a delayed output-feedback controller, without affecting the neglected vibrating modes in the reduced order model. The proposed controller design is based on the spectral abscissa characterization using the multiplicity property.

6.16. Landing of a civil aircraft

Participants: Frederic Mazenc, Michael Malisoff [LSU], Laurent Burlion [ONERA Toulouse], Victor Gibert [Airbus Toulouse].

In this work and the following, we applied the technique of [28] to problems arising from applications. The paper [56] is devoted to the problem of stabilizing a nonlinear system approximated in a neighborhood of the origin by a saturated chain of integrators when the variables are not accurately measured. We used our control design to solve a control problem that arises in the context of vision based landing of a civil aircraft. In [55], we solved the problem of stabilizing a nonlinear system when the variables are not accurately measured and cannot be differentiated. The proposed method was first motivated and thus finally applied to the vision based control problem of a landing airliner.

6.17. Power electronics devices

Participants: Frederic Mazenc, Alessio Iovine [Efficacity, France].

The contribution [50] is distinct from the papers mentioned above because it uses more traditional backstepping tools. It is devoted to power electronics devices. We proposed a nonlinear control law for a DC/DC boost converter dedicated to extract the maximum power from a photovoltaic (PV) array, taking into account the constraints of the control action. We performed simulations on SimPowerSystems to validate how the developed control strategy is able to properly control the converter.

6.18. Wind Farm Distributed PSO-based Control for Constrained Power Generation Maximization

Participants: Nicolo Gionfra [L2S], Guillaume Sandou, Houria Siguerdidjane [L2S], Damien Faille [EDF], Philippe Loevenbruck [EDF].

A novel distributed approach to treat the wind farm (WF) power maximization problem accounting for the wake interaction among the wind turbines (WTs) is presented. Power constraints are also considered within the optimization problem. These are either the WTs nominal power or a maximum allowed power injection, typically imposed by the grid operator. The approach is model-based. Coupled with a distributed architecture it allows fast convergence to a solution, which makes it exploitable for real-time operations. The WF optimization problem is solved in a cooperative way among the WTs by introducing a new distributed particle swarm optimization algorithm, based on cooperative co-evolution techniques. The algorithm is first analyzed for the unconstrained case, where we show how the WF problem can be distributed by exploiting the knowledge of the aerodynamic couplings among the WTs. The algorithm is extended to the constrained case employing Deb's rule. Simulations are carried out on different WFs and wind conditions, showing good power gains and fast convergence of the algorithm. To appear in Rnewable Energy, 2019.

6.19. Wind Farm Distributed PSO-based Control for Constrained Power Generation Maximization

Participants: Sophie Frasnedo [Safran Electronics and Defense], Guillaume Sandou, Gilles Duc [L2S], Philippe Feyel [Safran Electronics and Defense], Cedric Chapuis [Safran Electronics and Defense].

The inertial stabilisation of the line of sight of an imager fixed on a mobile carrier is considered in order to acquire good quality images despite the disturbances generated by the carrier.

A double stage mechanical stabilisation architecture is proposed, where a second stabilisation stage, based on a piezoelectric actuator, is added to the usual structure. The piezoelectric actuator transfer function and hysteresis are characterized through experiments.

In order to design the controllers of both stages, a high-level image quality criterion (the Modulation Transfer Function MTF) is considered, together with design constraints on the main variables of interest. The criterion and the constraints are evaluated by realistic simulations based on some input and noise profiles measured on a real-life system. The MTF evaluation being time-consuming, a Bayesian optimisation method specially dedicated to expensive-to-evaluate functions is used to obtain the parameters of the controllers. The obtain experimental results are displayed and their performances discussed. To appear in the International Journal of Systems and Sciences in 2019.

6.20. Model Identification for Demand-Side Management of District Heating Substations

Participants: Nadine Aoun [L2S, CEA-LITEN, ADEME], Roland Baviere [CEA-LITEN], Mathieu Vallee [CEA-LITEN], Guillaume Sandou.

Demand-Side Management (DSM) strategies, such as load shifting and nighttime set-back, exploit the thermal inertia of buildings to make the operation of District Heating Systems (DHSs) more efficient. The control strategy requires a building model to assess the flexibility of buildings in handling demand modulation, without jeopardizing the thermal comfort. Reduced Order Models (ROMs) with few parameters are often used for this end; in many previous works their parameters have been identified using time-series data including indoor temperature measurements. However, at a city scale and due to privacy rights, such internal signals are usually unavailable. Thereby, identifying the ROM shall rely solely on measurements available at the substation level.

In our work, we develop and demonstrate a method respecting this practical constraint to identify a first and a second order building model. In literature, a rather simplified approach had been proposed to derive a first order building model from substation measurements. We compare the performance of our methodology with respect to the latter, using the same model structure. As for the second order model, its structure is more relevant to account for different dynamics in buildings equipped with hydronic heating systems or featuring important internal thermal inertia. Data used for the identification is restricted to the heat flux delivered from the DHS, both supply and return water temperatures, mass flowrate across the substation's heat-exchangers and the outdoor temperature. Validation of the proposed approach is carried out using a representative white-box model of a building and its substation written in the Modelica language. Implementation of advanced control strategies for DHSs based on this model identification is in prospect.

6.21. Mathematical Modelling of Acute Myeloid Leukemia

Participants: Catherine Bonnet, Jean Clairambault [MAMBA project-team], François Delhommeau [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Walid Djema, Emilia Fridman [Tel-Aviv University], Pierre Hirsch [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Frédéric Mazenc, Hitay Özbay [Bilkent University].

Our project is about the modeling and analysis of healthy and unhealthy cell population dynamics, with a particular focus on hematopoiesis, which is the process of blood cell production and continuous replenishment. We point out that medical research is now looking for new combined targeted therapies able to overcome the challenge of cancer cells (e.g. to stop overproliferation, to restore normal apoptosis rates and differentiation of immature cells, and to avoid the high toxicity effects that characterize heavy non-selective chemotherapy). In that quest, the ultimate goal behind mathematical studies is to provide some inputs that should help biologists to suggest and test new treatment, and to contribute within multi-disciplinary groups in the opening of new perspectives against cancer. Thus, our research project is imbued within a similar spirit and fits the expectations of a better understanding of the behavior of healthy and unhealthy blood cell dynamics. It involve intensive collaboration with hematologists from Saint Antoine hospital in Paris, and aims to analyze the cell fate evolution in treated or untreated leukemia, allowing for the suggestion of new anti-leukemic combined chemotherapy.

Cells have amazing features that allow them to guide their development paths and determine their individual and collective fates. Dedifferentiation and transdifferentiation (cell plasticity) are little understood phenomena that allow cells to regress from an advanced differentiated state to a less differentiated one, including the case where cells lose their specific function and become stem cells.

We have introduced cell plasticity into a class of mathematical models we are interested in. We explored a new model involving a dedifferentiation function in the case of two cell maturity stages (stem cells and progeny). We have highlighted the role that dedifferentiation may have in the survival of cancer cells during therapy. The latter hypothesis appears to be in line with some medical observations [48].

We have also developed and analyzed a model taking into the account the fact that few cells of the proliferating compartment may be arrested during an unlimited time [49].

6.22. Analysis of Dengue Fever SIR Model with time-varying parameters

Participants: Stefanella Boatto [Univ Feder Rio de Janeiro], Catherine Bonnet, Frédéric Mazenc, Le Ha Vy Nguyen.

Migratory fluxes of humains and of insects of various species have favoured the spreading of diseases worldwide. In particular the Ae Aegypti and Ae Albopictus mosquitoes of the Aedes family are vectors able to transmit and spead among humans a variety of diseases: Dengue, Zika, Chikungunya, Yellow fever and the newly discovered Mayaro.

We have continued to analyze SIR models with time-varying parameters to predict dengue epidemics and compared numerical simulations with real data from Dengue epidemics in Rio de Janeiro in order to estimate the infectivity rate and predict what are the periods more at risk of infection [63], [41].

GAMMA3 Project-Team

5. New Results

5.1. The meshing bible

Participants: Paul-Louis George [The Boss], Houman Borouchaki, Frédéric Alauzet, Patrick Laug, Adrien Loseille, Loïc Maréchal.

Un projet important, initié en 2017, et amené à se poursuivre l'an prochain, 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.

5.2. Realistic modeling of fractured geologic media

Participants: Patrick Laug [correspondant], Géraldine Pichot.

This study started in 2016, in collaboration with the project-team Serena, aims to model, in a realistic and efficient manner, natural fractured media. These media are characterized by their diversity of structures and organizations. Numerous studies in the past decades have evidenced the existence of characteristic structures at multiple scales. At fracture scale, the aperture distribution is widely correlated and heterogeneous. At network scale, the topology is complex resulting from mutual mechanical interactions as well as from major stresses. Geometric modeling of fractured networks combines in a non-standard way a large number of 2D fractures interconnected in the 3D space. Intricate local configurations of fracture intersections require original methods of geometric modeling and mesh generation. Significant progress has been made during this year 2018, as we are now able to make geometric models and numerical simulations with more than 1 million fractures, 2 million intersections, and 18 million triangles, in about one hour on a laptop [7], [8], [19], [20], [21].

5.3. High order geometric modeling

Participants: Patrick Laug [correspondant], Houman Borouchaki.

In the area of geometric modeling, major challenges are linked to the efficient **visualization** of CAD surfaces and to the generation of **meshes** adapted to numerical simulation. In this context, the elaboration and implementation of a **discrete geometric model** provides a simple and universal representation model, without the need for CAD. A first study has been carried out for a model of degree 1 (one) defined by a "triangulation" composed of quadrilaterals and triangles. The advantage of this model of degree 1 lies in its geometric simplicity. However, in the case of complex surfaces, it may require a very large number of elements, and besides it is not sufficiently rich to give certain essential characteristics like geometric curvatures. The main goal of this project is to extend this discrete model of degree 1 to **higher degrees**. These studies are conducted by “MODIS”, an Associate Team comprising members of research teams at Inria, UTT (France) and Polytechnique Montreal (Canada) from 2017 to 2019. This year (2018) has been mostly devoted to the software implementation of all the theoretical bases obtained last year. In particular, chapters 6 and 11 of a recent book [22] give data structures where a local numbering is recursively defined for any order of the elements.

5.4. Rendu pixel-exact de solutions d’ordre élevé

Participants: Adrien Loseille [correspondant], Rémi Feuillet.

Avec le développement des méthodes d’ordre élevé, il apparaît également important de visualiser de manière fidèle à la fois le maillage et la solution associée. L’objet de cette thématique de recherche est de mettre à profit les fonctionnalités de programmation du pipeline graphique de la bibliothèque graphique OpenGL 4.0 afin de mettre en place des techniques de rendu de solutions d’ordre élevé quasiment exactes au pixel près ainsi que des techniques rapides de visualisation d’éléments d’ordre élevé. Les premiers résultats sont très satisfaisants avec un rendu de solutions d’ordre élevé allant de l’ordre 1 à 5 et ce exact au pixel près si ces dernières sont représentées sur des maillages de degré 1. Au niveau de la représentation des éléments d’ordre élevé, la visualisation est possible jusqu’à l’ordre 4 avec visualisation d’une solution dessus. Cette dernière sera d’autant plus représentée au pixel près que la représentation de la géométrie courbe (pour des degrés plus grands que 1) sera exacte. Ce travail a fait en 2018 l’objet de deux exposés à des conférences, dont une publication [13] dans les *proceedings*: *AIAA Scitech* et *WCCM*. Les prochaines étapes vont se concentrer sur la représentation de solutions et d’éléments d’ordre élevés à travers un plan de coupe, à la représentation des iso-surfaces et enfin à l’optimisation de ce code.

5.5. Génération de maillages d’ordre élevé

Participants: Frédéric Alauzet [correspondant], Adrien Loseille, Rémi Feuillet, David Marcum.

En calcul scientifique, l’utilisation de solveurs d’ordre élevé (supérieur à deux) se fait croissante. Or ces solveurs ne sont fonctionnels que lorsqu’ils sont couplés avec des maillages d’ordre élevé, nécessaires pour une représentation d’ordre élevé de la géométrie. L’idée de cette thématique de recherche est de s’intéresser à la génération et à l’*amélioration* par modification locale de tels maillages. Dans cette optique, un générateur de maillages courbe en partant de maillages droit a été développé. Ensuite, une étude importante a été consacrée à la généralisation au degré 2 des opérateurs locaux classiques d’optimisation de maillage, à savoir la bascule d’arête/face (*swap*) et le bougé de point (*smoothing*). La généralisation de tels outils a permis d’une part de rendre la génération de maillages courbe plus robuste et d’autre part rendu possibles au degré 2 les techniques de maillage mobile avec changement local de connectivité. Ce travail a fait l’objet en 2018 de deux exposés sans *proceedings* à *ECCM-ECFD* et *ICOSAHOM* et de 2 exposés avec *peer-reviewed proceedings* à *AIAA Aviation* et à l’*International Meshing Roundtable* [9], [10]. La suite de ce travail va être de générer des maillages de couche limites directement courbes (en utilisant la technique de maillage courbe mobile) puis de se consacrer à la généralisation de ce travail à des ordres plus grands. Il sera aussi apporté un soin particulier à la génération de maillages de surface courbe à partir de modèles de CAO.

5.6. Adaptation de maillages pour des écoulements visqueux en turbomachine et aéro-externe

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

5.6.1. Calcul

Les principes d'une adaptation pour les écoulements Navier-Stokes turbulents ont été validés sur des calculs de turbomachine. Pour ce faire nous avons tout d'abord traité les particularités liées aux calculs en turbomachine:

- Les aubes présentent en général une périodicité par rotation, on ne simule donc qu'une période afin d'alléger les calculs. Il faut donc traiter cette périodicité de façon appropriée dans le code CFD et l'adaptation de maillage.
- Afin de prendre en compte la rotation des pales sans employer de maillages mobiles et simulations instationnaires on peut se placer dans le référentiel tournant de l'aube en corrigeant les équations.
- Les écoulements en turbomachine sont des écoulements clos, les conditions limites d'entrée et de sortie ont donc une influence très forte et peuvent de plus se trouver très près de la turbine afin de simuler la présence d'autres étages en amont ou en aval. Des conditions limites bien précises ont donc été développées afin de traiter correctement ces effets.

5.6.2. Adaptation

Pour l'adaptation de maillages deux particularités doivent être traitées ici, la périodicité du maillage et la couche limite turbulente. En toute dimemsion, la couche limite a donc été traitée par des techniques d'adaptation. Le maillage est adapté dans le volume en utilisant la Hessienne du Mach de l'écoulement comme senseur. La périodicité est traitée en utilisant un noyau non-manifold de logiciel de remaillage `Feflo.a`.

Ces développements ont été présentés dans plusieurs conférences internationales et sont détaillés dans la thèse de Loïc Frazza [1], et dans le cadre d'une collaboration avec Safran Tech.

5.7. Parallel mesh adaptation

Participants: Frédéric Alauzet, Adrien Loseille [correspondant].

We devise a strategy in order to generate large-size adapted anisotropic meshes $O(10^8 - 10^9)$ as required in many fields of application in scientific computing. We target moderate scale parallel computational resources as typically found in R&D units where the number of cores ranges in $O(10^2 - 10^3)$. Both distributed and shared memory architectures are handled. Our strategy is based on hierarchical domain splitting algorithm to remesh the partitions in parallel. Both the volume and the surface mesh are adapted simultaneously and the efficiency of the method is independent of the complexity of the geometry. The originality of the method relies on (i) a metric-based static load-balancing, (ii) dedicated hierarchical mesh partitioning techniques to (re)split the (complex) interfaces meshes, (iii) anisotropic Delaunay cavity to define the interface meshes, (iv) a fast, robust and generic sequential cavity-based mesh modification kernel, and (v) out-of-core storing of completing parts to reduce the memory footprint. We are able to generate (uniform, isotropic and anisotropic) meshes with more than 1 billion tetrahedra in less than 20 minutes on 120 cores.

5.8. Adaptive boundary layer mesh generation

Participants: Adrien Loseille [correspondant], Victorien Menier.

Si des méthodes traditionnelles de couches limites sont désormais matures, elles sont souvent incompatibles dans un contexte adaptatif où les tailles varient dans la couche limite. On a développé dans ce cadre une méthode d'adaptation de la couche limite à la fois dans la direction normale et dans le plan tangent basée sur un couplage entre un opérateur de cavité contraint et une adaptation de surface interne.

5.9. Améliorations des schémas pour les simulation RANS

Participants: Loïc Frazza, Frédéric Alauzet [correspondant].

Grâce à une implémentation adéquate de schémas numériques modernes, nous avons montré qu'il est possible de réaliser des simulations RANS sur des maillages tétraédriques non structurés. Nous avons ainsi pu réaliser des calculs sur des maillages adaptés pour différentes applications industrielles complexes. A cette fin, nous avons réalisé l'analyse mathématiques nécessaire au développement des senseurs d'erreurs turbulents efficaces et précis. Nous avons également été amenés à étendre la résolution des variables adjointes aux modèles RANS. En comparant les performances de cette stratégie d'adaptation, nous avons pu montrer la supériorité des résultats obtenus en comparaison des méthodes hessiennes et traditionnelles sur différentes applications. Tous ces développements ont été validés dans le solveur `Wolf`, présentés et publiés dans [12], [6], [15] et ont été développés dans le cadre des collaborations avec Boeing et Safran Tech.

5.10. Deterministic smoothing parallelization

Participants: Lucille-Marie Tenkès, Frédéric Alauzet [correspondant].

On élabore des solutions algorithmiques pour paralléliser un opérateur géométrique d'optimisation de maillage, le bougé de points : une solution non-dynamique et une solution dynamique.

Le but est de paralléliser les méthodes de bougé de points de manière déterministe. En effet, avec les algorithmes actuels, le résultat de l'optimisation dépend de l'ordre dans lequel les points sont traités, qui n'est pas prévisible en parallélisation multi-thread asynchrone. Cela devient problématique lorsqu'on insère cette étape dans un processus global. S'il survient une erreur, on ne pourra pas reproduire les cas invalides pour apporter des corrections. Une première idée a été de rendre les calculs d'optimisation déterministes en implémentant une méthode non dynamique, qui prend comme référence pour le calcul des positions optimales la configuration initiale et non la configuration en cours d'optimisation. Une relaxation est effectuée une fois toutes les positions optimales calculées, et elle est globale. Cela permet d'avoir un bougé de points vraiment indépendant de l'ordre dans lequel les points sont traités. Cette méthode est bien déterministe, mais l'algorithme est moins efficace et plus lent que les méthodes de bougé de points dynamiques. L'alternative dynamique consiste à agir directement sur la parallélisation, en regroupant les points de manière à ne pas laisser les calculs interférer. L'idée est de créer une partition des nœuds en mettant dans une même classe ceux qui ne sont pas reliés entre eux par une arête. Ainsi, si l'un d'entre eux bouge lors du processus d'optimisation, il n'impactera pas ceux de sa classe. Cela revient donc à colorier ces sommets, de sorte que deux nœuds reliés par une arête n'aient pas la même couleur. L'algorithme choisi effectue un coloriage de proche en proche (approche frontale). La couleur 1 est attribuée au premier sommet, les points de sa boule sont coloriés par élimination, et ainsi de suite. Ces algorithmes ont été testés sur des maillages 2D et 3D pour caractériser leurs performances. Il en ressort que la méthode dynamique est assez efficace et rapide pour être appliquée à des maillages 3D de grande taille. De plus, l'étape de partition a été elle-même parallélisée et optimisée.

5.11. Opérateurs d'optimisation de maillage alignés et maillages quad-dominants

Participants: Lucille-Marie Tenkès, Frédéric Alauzet [correspondant].

On se base ici sur les méthodes de maillage par alignement des éléments sur la métrique. C'est-à-dire que les éléments du maillage, en plus de présenter une taille adaptée à la solution, suivent une direction prescrite. Une des difficultés ressortant de cette méthode est l'optimisation par bougé de points, car cela rompt l'alignement. On veut donc ici mettre en place une technique de bougé de points permettant de corriger, sans en détruire la structure, un maillage généré par alignement sur la métrique. Les modifications apportées à l'optimiseur sont un opérateur de réduction d'arête, une procédure d'appariement en quadrilatères, et un opérateur de bougé de points utilisant ces quadrilatères.

5.12. Multi-physic mesh adaptation

Participants: Frédéric Alauzet [correspondant], Rémi Feuillet, Julien Vanharen.

A new strategy [18] 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 P1 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. The capability of treating three-dimensional complex cases is also demonstrated.

RANDOPT Team

7. New Results

7.1. Analysis of adaptive Stochastic Optimizers

7.1.1. New ODE method for proving the geometric convergence of adaptive Stochastic Optimizers

The ODE method is a standard technique to analyze the convergence of stochastic algorithms defined as a stochastic approximation of an ODE. In a nutshell, the convergence of the algorithms derives from the stability of the ODE and the control of the error between the solution of the ODE and the trajectory of the stochastic algorithm. We have been developing a new ODE method to be able to prove the geometric convergence of stochastic approximation algorithms that derive from the family of adaptive stochastic optimization algorithms. Standard theory did not apply in this context as the state variable adapted typically converge to the boundary of the state-space domain where an infinite number of points are equilibrium points for the ODE [7].

7.1.2. Convergence and convergence rate analysis of the (1+1)-ES with one-fifth success rule

When analyzing adaptive stochastic optimizers, one is typically interested to prove the linear convergence and investigate the dependency of the convergence rate with respect to the dimension. We have greatly simplified the analysis of the convergence and convergence rate of the (1+1)-ES with one-fifth success rule on the sphere function. We have shown that the analysis derives from applying a simple "drift" theorem and consequently shown a hitting time to reach an ϵ-ball of the optimum of $\Theta(\frac{1}{d}\log(1/\epsilon))$ akin to linear convergence with a convergence rate scaling linearly with the dimension [4].

7.1.3. Quality-gain Analysis on Convex-quadratic functions

We have analyzed the expected function value decrease (related to the convergence rate) of Evolution Strategies with weighed recombination on convex-quadratic functions. We have derive different bounds and limit expression that allow to derive optimal recombination weights and the optimal step-size, and found that the optimal recombination weights are independent of the Hessian of the objective function. We have moreover shown the dependencies of the optimal parameters in the dimension and population size [1].

7.2. Benchmarking Methodology

7.2.1. Single-Objective Benchmarking

Benchmarking optimization algorithms seems trivial at first sight but is quite involved in practice and little decisions on the experimental setup can have a large effect on the displayed algorithm performance.

We have investigated some of these effects in the context of the Black-Box Optimization Benchmarking (`bbob`) test suite of the COCO platform and the well-known quasi-Newton BFGS algorithm, default in MATLAB's `fminunc` and in Python's `scipy.optimize` module [5]. We realized in particular that the instance instantiation in the COCO platform has little impact while the initial search point has a larger one. The largest performance differences, however, stem from implementation details that are typically not documented and not exposed to the user via internal algorithm parameters. For example is the MATLAB implementation of the BFGS algorithm significantly worse than the Python implementation and the MATLAB 2017 version is worse than the MATLAB 2009 implementation.

Additionally, Nikolaus Hansen gave a hands-on tutorial on good benchmarking practice at the GECCO-2018 conference in Kyoto [11].

7.2.2. Multi-Objective Benchmarking

In terms of multiobjective benchmarking, our contributions are two-fold. Firstly, we wrote a scientific article on the scientific methodology for defining our new multiobjective benchmark suite. In [10] we introduce two new bi-objective test suites on the basis of the above mentioned, well-known 24 `bbob` test functions and propose a generic test suite generator for an arbitrary number of objectives. The former are implemented in our COCO platform and extensively documented in terms of search and objective space plots for each function.

Secondly, we realized with the proposal of the biobjective `bbob` test suites that there is a need for more theoretical analyses of simple test functions that still test for practical challenges such as ill-conditioning or search space rotations. In our upcoming EMO conference paper [3] we therefore characterize theoretically Pareto sets and Pareto fronts of combinations of two convex quadratic functions with arbitrary search space dimension. Based on this theoretical analysis, we suggest a wide set of new biobjective test functions.

7.3. Large-scale Optimization

We have been studying different large-scale variants of the CMA-ES algorithm and tested them thoroughly empirically on a set of scalable large-scale testbed. The study includes comparison with the large-scale quasi-Newton algorithm, namely L-BFGS [6].

7.4. Constrained Optimization

In the context of constrained optimization, A. Atamna studied invariance properties of Augmented Lagrangian approaches and showed the relation between invariance to strictly increasing affine transformations of the objective function and the scaling of the constraints and linear convergence [2]. Progress were made towards a methodology to define scalable constrained problems with control optimum and the implementation of a new constrained testbed within the COCO platform. In her internship, E. Marescaux studied the connection between augmented Lagrangian approaches and a previously proposed adaptive constrained handling mechanism. She also studied a new idea to turn a constrained problem into an unconstrained one.

SELECT Project-Team

6. New Results

6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, Pascal Massart, Sylvain Arlot, Jean-Michel Poggi, Kevin Bleakley.

In collaboration with Damien Garreau, Sylvain Arlot studied the kernel change-point algorithm (KCP) proposed by Arlot, Celisse and Harchaoui (2012), which aims at locating an unknown number of change-points in the distribution of a sequence of independent data taking values in an arbitrary set. The change-points are selected by model selection with a penalized kernel empirical criterion. We provide a non-asymptotic result showing that, with high probability, the KCP procedure retrieves the correct number of change-points, provided that the constant in the penalty is well-chosen; in addition, KCP estimates the change-points location at the optimal rate. As a consequence, when using a characteristic kernel, KCP detects all kinds of change in the distribution (not only changes in the mean or the variance), and it is able to do so for complex structured data (not necessarily in Rd). Most of the analysis is conducted assuming that the kernel is bounded; part of the results can be extended when we only assume a finite second-order moment.

The well-documented and consistent variable selection procedure in model-based cluster analysis and classification that Cathy Maugis (INSA Toulouse) designed during her PhD thesis in SELECT, makes use of stepwise algorithms which are painfully slow in high dimensions. In order to circumvent this drawback, Gilles Celeux, in collaboration with Mohammed Sedki (Université Paris XI) and Cathy Maugis, have recently submitted an article where variables are sorted using a lasso-like penalization adapted to the Gaussian mixture model context. Using this ranking to select variables, they avoid the combinatory problem of stepwise procedures. The performances on challenging simulated and real data sets are similar to the standard procedure, with a CPU time divided by a factor of more than a hundred.

In collaboration with Benjamin Charlier and Jean-Michel Marin (Université de Montpellier), Gilles Celeux has started research aiming to propose a rapid Bayesian algorithm to estimate simply the mode of a posterior distribution for hidden structure models. This Bayesian procedure is of interest for two reasons. First, it leads to regularised estimation, which is useful for poorly posed problems. Second, it is an interesting alternative to variational approximation.

6.2. Estimator selection and statistical tests

Participant: Sylvain Arlot.

Sylvain Arlot wrote a book chapter about cross-validation in 2018. This text defines all classical cross-validation procedures, and studies their properties for two different goals: estimating the risk of a given estimator, and selecting the best estimator among a given family. For the risk estimation problem, it computes the bias (which can also be corrected) and the variance of cross-validation methods. For estimator selection, it first provides a first-order analysis (based on expectations). Then, it explains how to take into account second-order terms (from variance computations, and by taking into account the usefulness of over-penalization). This allows, in the end, to provide some guidelines for choosing the best cross-validation method for a given learning problem.

6.3. Statistical learning methodology and theory

Participants: Gilles Celeux, Serge Cohen, Christine Keribin, Michel Prenat, Sylvain Arlot, Benjamin Auder, Jean-Michel Poggi, Neska El Haouij, Kevin Bleakley, Matthieu Lerasle.

Sylvain Arlot wrote a book chapter about supervised statistical learning, from the mathematical point of view in 2018. This text describes the general prediction problem and the two key examples of regression and binary classification. Then, it studies two kinds of learning rules: empirical risk minimizers, which naturally lead to convex risks in classification, and local averaging rules, for which a universal consistency result can be obtained. Finally, it identifies the limits of learning in order to underline its challenges. The text ends with some useful probabilistic tools and some exercises.

Gilles Celeux and Serge Cohen have started research in collaboration with Agnès Grimaud (UVSQ) to perform clustering of hyperspectral images which respects spatial constraints. This is a one-class classification problem where distances between spectral images are given by the χ^2 distance, while spatial homogeneity is associated with a single link distance. This year they have developed a hybrid hierarchical clustering procedure in which sub-clusters respecting spatial consistency are constructed. Then, these sub-clusters are merged without taking spatial constraints into account. This strategy leads to a more realistic segmentation of spectral images.

Gilles Celeux continued his collaboration with Jean-Patrick Baudry on model-based clustering. Last year, they started work on assessing model-based clustering methods on cytometry data sets. The interest of these is that they involve combining clustering and classification tasks in a unified framework. This year, this work was completed, and performed well in comparison with state-of-the-art procedures.

Gillies Celeux has continued research on missing data for model-based clustering in collaboration with Christophe Biernacki (Modal team, Inria Lille) and Julie Josse (École Polytechnique). This year, they implemented several algorithms to estimate their logistic model for mixture analysis involving not missing-at-random mixtures.

In the framework of MASSICCC, Benjamin Auder and Gilles Celeux have started research on the graphical representation of model-based clusters. The aim of this is to better-display proximity between clusters.It leads to a simple procedure to represent the proximity between clusters without any additional assumptions.

After having proved the consistency and asymptotic normality of Latent Block Model estimators with V. Brault and M. Mariadassou, Christine Keribin has worked on the behavior of the ICL and BIC model criteria in this model, and in particular on their probable asymptotic equivalence.

Christine Keribin has started a new collaboration with Christophe Biernacki (Inria Modal Team) to study the ability for co-clustering to be a good regularized method for clustering in HD, which was presented at the CMStatistics 2018 conference.

J-M. Poggi (with R. Genuer), published a survey paper dedicated to “Arbres CART et Forêts aléatoires, Importance et sélection de variables”, as a book chapter published in: “Apprentissage Statistique et Données Massives” by Technip.

J.-M. Poggi and N. El Haouij (with R. Ghozi, S. Sevestre Ghalila and M. Jaïdane) provide a random forest-based method for the selection of physiological functional variables in order to classify the stress level during real-world driving experience. The contribution of this study is twofold: on the methodological side, it considers physiological signals as functional variables and offers a procedure of data processing and variable selection. On the applied side, the proposed method provides a “blind” procedure of driver’s stress level classification that does not depend on the expert-based studies of physiological signals. This work has been published in Statistical Methods & Applications.

J.-M. Poggi and N. El Haouij (with R. Ghozi, S. Sevestre Ghalila and M. Jaïdane provide a system and database to assess driver’s attention, called aAffectiveROAD. A paper presenting it has been published in the proceedings of the 33rd ACM Symposium on Applied Computing SAC’18.

6.4. Statistical analysis of genomic data

Participant: Kevin Bleakley.

In collaboration with Benno Schwikowski, Iryna Nikolayeva and Anavaj Sakuntabhai (Pasteur Institute, Paris), Kevin Bleakley worked on using 2-d isotonic regression to predict dengue fever severity at hospital arrival using high-dimensional microarray gene expression data. Important marker genes for dengue severity have been detected, some of which now have been validated in external lab trials, and an article on this was published in the Journal of Infectious Diseases in 2018.

Kevin Bleakley has also collaborated with Inserm/Paris-Saclay researchers at Kremlin-Bicêtre hospital on cyclic transcriptional clocks and renal corticosteroid signaling, and has developed novel statistical tests for detecting synchronous signals. This work was published in the FASEB journal in 2018.

Kevin Bleakley worked as part of a consortium on a crowdsourced Dream Challenge in 2018 on using molecular signatures to predict susceptibility to viral infection. Essentially, many teams of researchers from around the world used machine learning (statistical learning) algorithms to learn on training data then test on unseen real data. In the final stage, methods from several teams were combined to improve overall prediction performance. The article "A crowdsourced analysis to identify ab initio molecular signatures predictive of susceptibility to viral infection" was published in Nature Communications in 2018.

6.5. Reliability

Participants: Gilles Celeux, Florence Ducros, Patrick Pamphile.

From June 2015 until June 2018 when she defended it, in the framework of a CIFRE convention with Nexter, Florence Ducros researched a thesis on the modeling of aging of vehicles, supervised by Gilles Celeux and Patrick Pamphile. This thesis should lead to designing an efficient maintenance strategy according to vehicle use profiles. Moreover, warranty cost calculations are made in the context of heterogeneous usages. This required estimations of mixtures and competing risk models in a highly-censored setting.

This year, Patrick Pamphile and Florence Ducros have published an article which proposes a two-component Weibull mixture model for modelling unobserved heterogeneity in heavily censored lifetime data collection. Performance of classical estimation methods (maximum of likelihood, EM, full Bayes and MCMC) are poor due to the high number of parameters and the heavy censoring. Thus, a Bayesian bootstrap method called Bayesian Restoration Maximization, was used. Sampling from the posterior distribution was obtained thanks to an importance sampling technique. Simulation results showed that, even with heavy censoring, BRM is effective both in term of estimate's precision and computation times.

6.6. Dynamical systems

Participant: Sylvain Arlot.

In collaboration with Stefano Marmi and Duccio Papini, Sylvain Arlot proposed a new model for the time evolution of livestock commodities which exhibits endogenous deterministic stochastic behaviour. The model is based on the Yoccoz-Birkeland integral equation, a model first developed for studying the time-evolution of single species with high average fertility, a relatively short mating season and density dependent reproduction rates. This equation is then coupled with a differential equation describing the price of a livestock commodity driven by the unbalance between its demand and supply. At its birth the cattle population is split into two parts: reproducing females and cattle for butchery. The relative amount of the two is determined by the spot price of the meat. We prove the existence of an attractor and we investigate numerically its properties: the strange attractor existing for the original Yoccoz-Birkeland model is persistent but its chaotic behaviour depends also from the price evolution in an essential way.

6.7. Soccer forecasting

Participants: Gilles Celeux, Jean-Louis Foulley.

In collaboration with Jean-Louis Foulley (Montpellier University), Gilles Celeux has proposed a penalty criterion for assessing correct score forecasting in soccer matches. They have defined the subject of a Masters internship for next year to predict scores of soccer matches via Poisson models using maximum likelihood and Bayesian inference.

6.8. Electricity load forecasting and clustering

Participants: Jean-Michel Poggi, Benjamin Auder, Benjamin Goehry.

B. Auder, J-M. Poggi (with J. Cugliari, Y. Goude) are interested in hierarchical time-series for bottom-up forecasting. The idea is to disaggregate the signal in such a way that the sum of disaggregated forecasts improves the direct prediction. The 3-steps strategy defines numerous super-consumers by curve clustering, builds a hierarchy of partitions and selects the best one minimizing a forecast criterion. Using a nonparametric model to handle forecasting, and wavelets to define various notions of similarity between load curves, this disaggregation strategy applied to French individual consumers leads to a gain of 16% in forecast accuracy. Then the upscaling capacity of this strategy facing massive data is explored and different proposals using R are experimented. The proposed solutions to make the algorithm scalable combines data storage, parallel computing and double clustering step to define the super-consumers. This has been published in the journal Energies.

Benjamin Goehry is completing a thesis co-supervised by P. Massart and J-M. Poggi, aiming at extending this scheme by introducing the use of random forests as time series forecasting models adapted to each cluster.

J.-M. Poggi (with J. Cugliari) published in Wiley StatsRef-Statistics Reference Online, a paper entitled Electricity demand forecasting. the focus is on short-term demand forecasting at some aggregate level (e.g., zone or nationwide demands) from data with at least hourly sampled data. The main salient features of the load curve are first highlighted. Some of the common covariates used in the prediction task are also discussed. Then, some basic or now classical methodological approaches for electricity demand forecasting are detailed.

TAU Team

7. New Results

7.1. Toward Good AI

7.1.1. Causal Modeling

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

The search for **causal models** relies on quite a few hardly testable assumptions, e.g. causal sufficiency [152]; 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 [107] 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 [109]. An edited book is in preparation [64].

In D. Kalainathan's PhD and O. Goudet's postdoc, the search for causal models has been tackled in the framework of generative networks [44], 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. However, due to the shortage of real-world variable pairs for which the causation type is known, the CEP challenge has been enriched using artificial pairs (e.g. considering variations on pairs of entities involved in biological regulatory networks), biasing the causation training process. On-going studies investigate how the use of such artificial pairs (the so-called Mother Distribution) to train a causation model aimed at real pairs can be cast as a domain adaptation problem [97], [78].

An attempt to circumvent the need for a large dataset of variable pairs, sampled for the Mother Distribution, we proposed the Structural Agnostic Model approach [57]. Working directly on the observational data, this global approach implements a variant of the popular adversarial game [97] 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 inpu variables, yielding a sparse causal graph. SAM obtains state-of-the-art performances on synthetic data.

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.

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 [29] 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 first impressions analysis [56].

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, and to provide understandable explanations on its results.

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

7.1.3. Experimental Validation of the Autonomous Vehicle

Participants: Guillaume Charpiat, Marc Schoenauer; **PhD and Engineers**: Marc Nabhan, Nizham Makhoud, Raphaël Jaiswal
Collaboration: Hiba Hage, Philippe Reynaud, and Yves Tourbier (Renault)

As said (Section 3.1.2 , TAU is considering two directions of research related to the certification of MLs. The first direction, toward experimental validation, focuses on the coverage of the datasets (more particularly here, used to train an autonomous vehicle controller), and is the subject of this section, while the second one, related to formal approaches, has just started with the beginning of Julien Girard's PhD and has not yet lead to results.

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 steps i) (topic of a one-year POC) and ii) (Marc Nabhan's CIFRE PhD). In both cases, the current target scenario is the insertion of a car on a motorway, the "drosophila" of autonomous car scenarios.

Note that another approach toward experimental robustness is investigated in Nizam Makdoud's PhD (CIFRE Thalès), started in March 2018, where Reinforcement Learning is used to find ways to fool some security system.

Clustering of scenarios A first one-year Proof of Concept (ending Oct. 2018) has demonstrated the feasibility and the usefulness of scenario clustering, assuming the availability of data describing the scenarios, i.e., the trajectories of all vehicles involved. Publicly available datasets (e.g., NGSIM were used in a first step. The difficulties met are the following. Firstly, trajectories are varying-length time series, requiring the use of recurrent NNs or LSTMs. Secondly, a scenario is invariant under permutations of the different vehicles involved; neural architectures are taking inspiration from *social LSTMs* [67]. Lastly, most recorded real-world scenarios are uninteresting (all vehicles drive on in their lanes).

The results of this POC have been duly delivered to Renault, but will remain internal at this point. The follow-up collaboration will explore metrics (in the latent space, or learned via Siamese networks), to complete the clustering in a semi-supervised setting (exploiting human feedback to select "typical" scenarios).

Detection of controller flaws Marc Nabhan's PhD (CIFRE Renault) is concerned with 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.

A key difficulty, beside that of getting actual data, is the very low probability of failure.On-going work builds upon TAU expertise in active learning using Monte-Carlo Tree Search [140] and evolutionary optimization, in particular taking inspiration from Novelty Search [121] to focus the exploration on unexplored regions of the scenario space, as well as portfolio optimization and instance-based algorithm selection (see Section 3.3.1).

7.2. Learning to Learn

7.2.1. Auto-*

Participants: Guillaume Charpiat, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, François Gonard, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun, Pierre Wolinski
Collaboration: Vincent Renault (SME Artelys); Olivier Bousquet (Google Zurich), Yann Ollivier (Facebook)

TAU is an active player in the Auto-☆ field, having organized the sixth COSEAL workshop in Paris in September 2018. Furthermore, Auto-☆ studies at TAU investigate several directions.

As discussed in Section 3.3 , the most widely used approach is based on meta-features describing datasets, and builds upon past work in the team, such as Nacim Belkhir's PhD defended in 2017 [71], who won a GECCO competition in 2018 (Section 5.1.1), and François Gonard's PhD [11], defended in May 2018: an empirical performance model is built from the meta-features, and used to choose the best algorithm and its parameter configuration for unknown datasets. One key difficulty is to design useful meta-features: taking inspiration from equivariant learning [136] and learning from distributions [124], on-going work aims to learn such meta-features, based on the OpenML archive [153]. This extensive archive reports on the test predictive accuracy obtained by a few hundred algorithm configurations over a few thousand datasets.

Also mentioned in Section 3.3 , another popular approach for algorithm selection is collaborative filtering. Active learning was used on top of the CofiRank algorithm for matrix factorization [156], improving the results and the time to solution of the recommendation algorithm [62].

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 algorithm yields promising results comparatively to AutoSklearn. A difficulty consists in managing the exploration together with the resource allocation (considering subsampled datasets and/or limited computational resources in the early MCTS stages, akin [91]).

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. An extension of AutoSklearn was proposed, part of Lisheng Sun's PhD, that detects concept drifts and corrects the current model accordingly [38].

Two on-going works focus on the specific adjustment of hyper-parameters for neural nets, deriving rules for the network architecture (Pierre Wolinski's PhD), or (Leonard Blier's PhD) attaching fixed learning rates to each neuron and calibrating the learning rate distribution in such a way that neurons are sequentially active, learning in an optimally agile manner during a given learning phase, and being stable in later phases.

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 [42], and continuously contributes to the organization of new challenges (Section 7.6).

7.2.2. Deep Learning: Practical 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)

Even though a full mathematical understanding of deep learning is not available today, theoretical insights from information theory or from dynamical systems can bring significant improvements to practical deep learning algorithms or offer strong explanations for the success of some architectures compared to others.

In [32] we fully derive the LSTM structure from first axiomatic principles, using an axiom of *robustness to temporal deformation (warpings) in the data*. The LSTM architecture, introduced in the 90's, has become the currently dominant architecture for modeling temporal sequences (such as text) in deep learning. But the LSTM architecture itself is quite complex and appears very much ad hoc at first sight. We prove that LSTMs necessarily arise if one wants the model to be able to handle time warpings in the data (such as arbitrary accelerations or decelerations in the signal). In fact, LSTM-like structures are the only way to provide robustness to such deformations: their complex equations can be derived axiomatically.

In [28] (long oral presentation at ICML) we tackle the problem of mode loss in generative models via information theory. The problem is to find generative models to produce more samples similar to samples in a dataset (eg, realistic images). The standard GAN approach is to couple a generative network and an adversary network whose job is to tell the differences between generated and genuine images. This suffers from mode loss: the generator focuses on doing some images well, rather than covering a full variety of images. Instead we propose to have the discriminator predict the proportion of true and fake images in a set of images, via an information theory criterion. This makes the discriminator work at the level of the *overall distribution* of images from the generator rather than individual images. By working on sets of images, the discriminator can detect statistical imbalances between different types of images created by the generator, thus reducing mode loss. An adapted architecture is derived for this, provably able to detect (in principle) all permutation-invariant statistics in a set of images.

In [43] we tackle the problem of recurrent network training via the theory of dynamical systems. Recurrent networks deal with temporal data sequences exhibiting temporal dependencies. Then backpropagation becomes backpropagation through time: for every new data point, training must rewind the network's computations backward in time on all past data to update the model parameters. This is unrealistic in any real-time application where the data arrive online. Two years ago we presented a fully online solution avoiding this "time rewind" step, based on real-time, noisy but unbiased approximations of model gradients. Our previous solution was mathematically well motivated but extremely complex to implement for standard models such as LSTMs. We now have a simpler variant which can be implemented easily in a black-box fashion on top of any recurrent model, and which is just as well-justified mathematically. The price to pay is more variance. In the long run, this could quite extend the applicability range of recurrent model to real-time situations.

In [31][0], 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.

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).

The information content of a trained restricted Boltzmann machine (RBM) for instance can be analyzed by comparing the singular values/vectors of its weight matrix, referred to as data modes, to that of a random RBM (typically following a Marchenko-Pastur distribution) [83]. The general strategy here is to replace the analysis of the learning process of a single instance by that of a well chosen statistical 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 [15]. While the mean-field analysis conducted in closed form requires simplifying assumptions, it suggests some simple heuristics to speed up the convergence and to simplify the models. Ongoing works

[0] to be presented at ICLR 2019

concern extensions of these considerations to settings with missing input on the practical side and to the analysis of exactly solvable RBM - i.e. non-linear RBM for which the contrastive divergence can be computed in closed forms - on the theoretical side. Additionnally, we are collaborating with J. Rocchi, working at the LPTMS (Univ. Paris Sud), to investigate the landscape of RBMs learned from different initial conditions and to characterized it as a function of the number of parameters (hidden nodes) of the system.

A long standing application of our aforementioned mean-field inference methods based on probabilistic modelling concerns road traffic forecasting. In [49] we wrap up some of the techniques developed in these past works and perform, thanks to PTV-SISTeMA comprehensive experimental tests on various real world Urban traffic dataset in order to illustrate in various conditions the effectiveness of our method. As a by-product we show to some extent how to disentangle the model bias from errors caused by corrupted data and shed some light on the nature of the data themselves.

An emerging research topic, that we started to investigate thanks to exchanges with Lenka Zdeborova's group [96], is to revisit the Information Bottleneck framework [151] and analyze on non-toy NNs the gradual distillation of the mutual information (MI) along the NN layers, minimizing the MI with the input while preserving the MI with the sought output (the labels). More generally, information theory concepts could also be used to analyze the behavior of the network, for instance to detect adversarial attacks through unusual neural activity mapping.

As mentioned earlier, the use of ML to address fundamental physics problems is quickly growing. 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 could then help identifying "computational order parameters", that would advance the understanding of physical phenomena, on the one hand, and support the development of more complex models, on the other hand. Furthermore, this problem is new to the ML community and could provide 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. But while the simultaneous advent of massive data and massive computational power has opened exciting new avenues, it has also raised new questions and challenges.

Almost ten years after the first enthusiasms for "big data" in social science, P. Tubaro has undertaken a reflective effort to look back at progress made so far and at directions for the near future. She edited a special issue of *Revue Française de Sociologie* on the effects of data both on society itself and on the scientific disciplines that engage with it [46], of which she co-authored the introduction [13].

Meanwhile, four data-based studies are being conducted in TAU, about labor (hiring, working on Internet, 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
Post-docs; PhDs: Olivier Goudet; François Gonard, Diviyan Kalainathan, Thomas Schmitt
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Antonio Casilli (Telecom); Thierry Weil (Mines); Jean-Luc Bazet (RITM)

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 Our first study in the domain of job markets (Th. Schmitt's and F. Gonard's PhDs [12], [11]) tackled the matching of job ads and CVs. This study, funded by the Lidex *Institut de la Société Numérique* (ISN) at Univ. Paris-Saclay, was conducted in collaboration with EHESS, on data provided by the hiring Web agency Qapa (for blue-collars and temporary jobs) and by Association Bernard Gregory (for scientists in industry). Among other difficulties, this study revealed that for both qualified and unqualified job sectors, job seekers and recruiters do not speak the same language [143]. This first study will be continued and extended along two directions: counterfactual analysis (*What would be my options if I had this additional skill ?*DATAIA project Vadore, coll. ENSAE and Pôle Emploi), and the recommendation of vocational training (BPI-PIA contract JobAgile, coll. EHESS and Qapa). Both projects start end 2018.

The platform economy and digital labor Another topic concerns the digital economy and the transformations of labor that accompany the current developments of AI. P. Tubaro has researched the so-called "sharing economy" and ideals of social change associated to the economic model of the platform [33]. However, the platform economy is also disrupting traditional industries. CNRS's MITI office has funded a research on the effects of online services for the restaurant sector (such as La Fourchette, Trip Advisor, Yelp) on working conditions and quality of service. This project involves P. Tubaro, P. Caillou and partners at Telecom ParisTech and Paris Dauphine University.

Ongoing research is exploring online platform labor and its linkages to the development of AI. In collaboration with A.A. Casilli (Telecom ParisTech), P. Tubaro has received funding to conduct research on this topic from the Union Force Ouvrière (OPLa project), from France Stratégie (a Prime Minister's service), and from MSH Paris-Saclay (DiPLab project). A recent grant from DARES (French Ministry of Labor) will enable exploring labor changes in B2B platforms (with O. Chagny of IRES, a unions-funded think-tank).

Quality of life at work. A study, funded by ISN, examined the relationship between the quality of life at work (QLW), and the economic performance of companies [113]. The management and economics literature has already established a correlation between QLW and economic performance [76]. The question that we are currently addressing regards the direction of causality: do profitable companies pay more attention to the QLW ? Or do companies paying attention to QLW tend to be more profitable ? This project (coll. RITM Univ. Paris-Sud, SES Telecom ParisTech, Ecole des Mines, La Fabrique de l'Industrie) combines data at the individual level (DARES, Ministère du Travail) and at the company level (Secafi); cutting-edge causality algorithms are applied to address the question, and handle confounder variables such as the sector of activity.

7.3.2. Health, food, and socio-demographic issues

Participants: Philippe Caillou, Michèle Sebag, Paola Tubaro
Post-docs; PhDs: Nayat Sanchez-Pi
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 (noting that general recommendations such as *Eat 5 fruit and vegetable per day* are hardly effective on the targeted populations. 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, or a consequence of obesity, or both.

Previous research in this area included the study of eating disorders and their relationship to people's social network and usages of technology [18].

7.3.3. Scientific Information System and Visual Querying

Participants: Philippe Caillou, Michèle Sebag
Engineer: Anne-Catherine Letournel, Jonas Renault
Collaboration: Jean-Daniel Fekete (AVIZ, Inria Saclay)

A third area of activity concerns the 2D visualisation and querying of the scientific expertise in an institute/university, based on their scientific production, given as a set of articles (authors, title, abstract). 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 extension proposals, in collaboration with the department of bibliometry from Univ. Paris-Saclay, are under submission at the time of writing.

This project was initially devised as an open-source platform, aimed to answer burning questions, as the growth of academic organization prevents anyone from having a precise knowledge of who does what in the organization: Who is expert in a topic (described as a bag of words)? How are topics related? What are the rising topics? (see also Section 6.3)

Its development and the interaction with the beta-user scientists using it, increasingly raises new questions at the crossroad of human-centered computing, data visualization and machine learning: How to deal with poly-thematic researchers? How to take advantage of the fact that researchers have ideas about their relevant scientific neighborhood, and learn person-dependent metric?

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 1.8 version of the platform[20] brings new capabilities required for social science research, such as High Performance Computing to explore the simulation, Co-Modeling to link projects, advanced agent architectures to model complex behaviors and advanced visualization to display nice 3D representations for exploration and presentations.

7.4. Energy Management

7.4.1. Power Grids Daily Management

Participants: Isabelle Guyon, Marc Schoenauer
PhDs: Benjamin Donnot, Balthazar Donon, Herilalaina Rakotoarison
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Olivier Teytaud (Facebook)

In the context of the Power Grid safety (Benjamin Donnot's CIFRE PhD with RTE, to be defended in February 2019), the goal is to assess in real time the so-called "(n-1)" safety (see Section 4.2) of possible recovery actions after some problem occurred somewhere on the grid. However, the 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. A simplified simulator is also available, but its accuracy is too poor to give any good result. Deep surrogate models can be trained off-line, based on the results of the slow simulator, with high0enough 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. An original "guided dropout" approach was proposed [24], in which the topology directly acts on the connections of the deep network: a missing line suppresses some connections. However, 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 experimentaly validated against the above-mentionned approaches on small subsets of the French grid (up to 308 lines). Interestingly, and rather suprisingly, 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 [23] 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.

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.

Provided accurate predictions of consumption (see below), off-the-shelf graph optimization algorithms can be used. Berna Batu is gathering different approaches, while Herilalaina Rakotoarison's PhD is concerned with the automatic tuning of their parameters (see Section 7.2.1 , and his original approach, at the moment applied to standard benchmarks [40], as well as to Artelys' home optimizer at large Knitro, 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.

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 [25] 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 [66]. 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 is the subject of A. Pol 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. [60] 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, compared either to production solution or classical anomaly detection (one-class or I-Forest). The result has been included in the production suite of the CMS experiment at CERN.

The highly visible TrackML challenge 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).

This year, 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 [127] and, soon after, larger ones by GAFAM). A still ongoing issue is the ability to generalize across datasets (as urban and rural areas look different in different parts of the world, or even within the same country, e.g. roof types in France).

The task of segmenting satellite images comes together with the one of their registration with cadastral maps. Indeed, the ground truth in remote sensing benchmarks (cadastral maps) is often imperfect, due to spurious deformations. We tackle this issue by *learning* how to register images of different modalities (RGB pictures vs. binary cadastral maps). If one tries to predict, given an RGB photography and an associated cadastral map, the deformation that warps one onto the other, by outputting a 2D vector field indicating the predicted displacement of each pixel (which can be as large as ± 32 px), then the problem considered is too hard (32×32 possibilities for each pixel 2D displacement vector). Instead, we simplifly the problem by decomposing it in a cascade of increasing resolutions. The idea is that if one zooms out by a factor 32, while knowing that the maximum possible displacement is of magnitude 32 px, then at this low resolution one has to move pixels by at most 1 pixel. Learning the task at this low resolution is thus easy. When it is done, if we zoom in by a factor 2, thus reaching a resolution lower than the original one by a factor 16, then the maximum displacement is again of 1 pixel (since larger displacements have been dealt with at the previous scale). And so on. In the end, we train a multi-scale chain of neural networks (double U-nets) [34], and later combine it with a segmentation task [27] in order to benefit from multi-task training, known to improve results.

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 project is extremely timely, as the huge amount of (freely available) space missions data has not yet been systematically exploited in the current computational methods for space weather. Specifically, 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). The project is very ambitious: the accurate prediction of e.g., geomagnetic storms, or solar wind speed from solar images, would represent a giant leap in the field. 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*. Concerning the prediction of solar wind impacting earth magnetosphere from solar images, 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 and provided a solution tested on synthetic data.

7.5.4. Genomic Data and Population Genetics

Participants: Guillaume Charpiat, Flora Jay
PhD: Théophile Sanchez
Collaboration: TIMC-IMAG (Grenoble), Estonian Biocentre (Institute of Genomics, Tartu, Estonia)

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.

On-going work at TAU, around Théophile Sanchez' PhD, co-supervised by G. Charpiat and Flora Jay, aims at extracting information from genomic data using deep neural networks; the key difficulty is to build flexible problem-dependent architectures, supporting transfer learning and in particular handling data with variable size. In collaboration with the Bioinfo group at LRI, 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 [141]. In the short-term these architectures can be used for demographic inference; the longer-term goal is to integrate them in various systems handling genetic data (e.g., epidemiological statistics) or other biological sequence data. In collaboration with the Estonian Biocentre (Tartu, Estonia), applications will consider thousands of sequenced human genomes, and expand our knowledge of the past human history. To this aim Burak Yelmen (PhD student at the Estonian Biocentre) will visit the lab from February to April 2019. Indeed, TAU expertise regarding the methodologies of exploiting missing and noisy data, and the resulting modeling biases, can contribute to enhance these novel population genetics methods, particularly so for methods heavily relying on simulated data (thus potentially suffering from the *reality gap*).

[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.

We also contributed to tess, a method for fast inference of population genetic structure, through a collaboration with TIMC-IMAG. This method analyses SNP data and estimates the admixture coefficients (that is, the probability that an individual belongs to different groups given the genetic data) via matrix factorization. The observed high dimensional genetic data are reduced automatically via the rank-k approximation of the matrix factorization and thereby highlight the latent structure of the data: the matrix factorization scores correspond to the admixture coefficients while the loadings give the genetic characteristics of each cluster. This method is faster than the hierarchical Bayesian models that we had previously developed and hence well suited for large NGS data. We participated in the tess3 R package, that implements this algorithm, facilitates the visualization of population genetic structure and the projection on maps [14]. We are currently adapting closely related algorithms to enable dimension reduction of temporal data with an application to paleogenomics.

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. 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. Among the possible options are i) learning a parameterization of the local, low-dimensional manifold and performing a geometric extrapolation of the molecule trajectories; ii) learning a coarse description of the system and its dynamics, supporting a fast prediction of its evolution. In both cases, the states estimated from the time- or configuration-simplified models will be used for steering large scale simulations, thus accelerating the sampling of stable molecular conformations.

This task will be tackled by combining manifold learning (to find a relevant low-dimensional representation space) and reinforcement learning (for the efficient exploration of the space), taking inspiration from Graph Neural Networks [86]. On-going studies use Graph Auto-encoders to extract a meaningful representation of the conformation of molecules and to predict dynamics.

7.5.6. Storm trajectory prediction

Participants: Mo Yang, Guillaume Charpiat
Collaboration: Claire Monteleoni, Sophie Giffard-Roisin (LAL / 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 [160]. 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. On-going studies, conducted in collaboration with S. Giffard-Roisin and C. Monteleoni (now Univ. Boulder), outperform the state-of-the-art in many cases [26], [36], [35].

7.5.7. Analyzing Brain Activity

Participants: Guillaume Charpiat
Collaboration: Hugo Richard, Bertrand Thirion (Parietal team, Inria Saclay / CEA)

With the goal of understanding brain functional architecture, the brain activity of ten subjects is recorded by an fMRI scanner, while they are watching movies (sequences of short pieces of real movies). The analysis of the ensuing complex stimulation streams proceeds by extracting relevant features from the stimuli and correlating the occurrence of these features with brain activity recorded simultaneously with the presentation of the stimuli. The analysis of video streams has been carried in [87] or [108] using a deep convolutional network trained for image classification. The question is then to build good descriptors of videos, possibly involving motion.

We consider a deep neural network trained for action recognition on the largest dataset available [115], and use its activations as descriptors of the input video. This provides deep representations of the watched movies, from an architecture that relies either on optical flow, or on image content, or both simultaneously. We then train a linear model to predict brain activity from these features. From the different layers of the deep neural networks, we build video representations that allow us to segregate (1) occipital and lateral areas of the visual cortex (reproducing the results of [108] and (2) foveal and peripheric areas of the visual cortex. We also introduce an effi- cient spatial compression scheme for deep video features that allows us to speed up the training of our predictive algorithm [41]. We show that our compression scheme outperforms PCA by a large margin.

7.6. Challenges

Participants: Cécile Germain, Isabelle Guyon, Michèle Sebag
PhD: Zhengying Liu, Lisheng Sun
Collaboration: D. Rousseau (LAL), Andre Elisseeff (Google Zurich), Jean-Roch Vilmant (CERN)

Following the highly successful ChaLearn **AutoML** Challenges (NIPS 2015 – ICML 2016 [106] – PKDD 2018 [45]), the **AutoDL** challenge [37], to be run in 2019, addresses the problem of tuning the hyperparameters of Deep Neural Networks, including the topology of the network itself. Co-sponsored by Google Zurich, it will require participants to upload their code on the Codalab platform.

In conjunction with AutoDL, we will organize a challenge in computer vision called **AutoCV**, to promote automatic machine learning for video processing, in collaboration with University of Barcelona. This will make use of the TAU GPU cluster.

Part of the HEP activities of the team, **TrackML** [30], [61] first phase was run and co-sponsored by Kaggle, until September 2018. The second phase is presently running on Codalab, and will end in March 2019. The challenge has been presented at WCCI [61] and NIPS [30]. 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.

Beyond the LAP (Looking At People) series of challenges (see details and references in Section 3.4), the domain of autonomous analysis of human behavior from multimodal information has recently gained momentum. We have been involved in two Special Issues dedicated to these topics, *The Computational Face*, in PAMI [17], and *Apparent Personality Analysis*, in IEEE Trans. on Affective Computing [16]. Two other challenges were organized at ICPR 2018, one about the information fusion task in the context of multi-modal image retrieval in social media, the other one regarding the inference of personality traits from written essays, including textual and handwritten information [29].

The **HADACA** project (EIT Health) aims to run a series of challenges to promote and encourage innovations in data analysis and personalized medicine. The data challenges will gather transdisciplinary instructors (researchers and professors), students, and health professionals (clinicians). The outcome of the data challenges should provide: i) analytical frameworks to bridge the gap between large dataset and personalized medicine in disease treatments and ii) innovative pedagogical methods to sensitize students to big data analysis in health. 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.

The **L2RPN** (Learning to Run a Power Network) project (coll. RTE) [39] addresses the difficult problem of using Reinforcement Learning to assist human operator in their daily tasks of maintaining the French Ultra-High Voltage grid safety while routing power without interruption. We are collaborating with O. Pietquin (Google Brain) to firm up the challenge protocol, largely inspired by AlphaGo and other RL challenges, like the NIPS 2017 “Learning to run” challenge.

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: 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. Along similar line, F. Landes proposed a challenge in the context of S. Mallat’s course, at Collège de France.

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, we apply 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 [14], 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 [36], 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 [91].

In [15], we provide a representation theorem for "payment free" Shapley operators, showing that these are characterized by monotonicity and homogeneity axioms [15]. This extends to the two-player case known representation theorems for risk measures.

7.1.2. Nonlinear fixed point methods to compute joint spectral raddi of nonnegative matrices

Participants: Stéphane Gaubert, Nikolas Stott.

In [29], 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). The situation in which the matrices are not nonnegative is amenable to a similar approach [94].

7.1.3. Probabilistic and max-plus approximation of Hamilton-Jacobi-Bellman equations

Participants: Marianne Akian, Eric Fodjo.

The PhD thesis of Eric Fodjo concerns stochastic control problems obtained in particular in the modelisation of portfolio selection with transaction costs. The dynamic programming method leads to a Hamilton-Jacobi-Bellman partial differential equation, on a space with a dimension at least equal to the number of risky assets. The curse of dimensionality does not allow one to solve numerically these equations for a large dimension (greater to 5). We propose to tackle these problems with numerical methods combining policy iterations, probabilistic discretisations, max-plus discretisations, in order to increase the possible dimension.

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 [46], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [103], [109] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [82] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [32], [33], we improve 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 study the convergence and obtain error estimates when the parameters and the value function are bounded. The more general quadratic growth case has been studied in the PhD manuscript [12].

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 [110], [111], the stochastic max-plus scheme proposed by Zheng Qu [118], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [116], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [61], the probabilistic numerical method of Fahim, Touzi and Warin [82]. We propose to associate and compare these methods in order to solve more general structures.

In a first work [35], 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.

7.1.5. Parametrized complexity of optimal control and zero-sum game problems

Participants: Marianne Akian, Stéphane Gaubert, Omar Saadi.

As already said above, the dynamic programing approach to optimal control and zero-sum game problems suffers of the curse of dimensionality. The aim of the PhD thesis is to unify different techniques to bypass this difficulty, in order to obtain new algorithms and new complexity results.

As a first step, we worked to extend an algorithm proposed by Sidford et al. in [126]. There, they proposed a randomized value iteration algorithm which improves the usual complexity bounds of the value iteration for *discounted* Markov Decision Problems (discrete time stochastic control problems). In a joint work with Zheng Qu (Hong Kong University), we are extending this algorithm to the ergodic (mean payoff) case, exploiting techniques from non-linear spectral theory [48]; this extension covers as well the case of two players (zero-sum).

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 open cones, particularly ones that preserve or reverse the order structure associated to the cone. A bijective map that preserves the order in both directions is called an order isomorphism. Those that reverse the order in both directions are order antimorphisms. These are closely related to the isometries of the Hilbert and Thompson metrics on the cone.

Previously, we have shown [133] that if there exists an antimorphism on a finite-dimensional open cone that is homogeneous of degree -1, then the cone must be a symmetric cone, that is, have a transitive group of linear automorphisms and be self-dual. This result was improved in [44], where we showed that the homogeneity assumption is not actually necessary: every antimorphism on a cone is automatically homogeneous of degree -1.

The study of the order isomorphisms of a cone 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 linear 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 cone is the convex hull of its extreme rays, which is overly restrictive in infinite dimension. Using different techniques more suited to infinite dimension, we have been developing a necessary and sufficient criterion on the geometry of a cone for all its isomorphisms to be linear.

7.2.2. Horofunction compactifications of symmetric spaces

Participant: Cormac Walsh.

This work is in collaboration with Thomas Haettel (Montpellier), Anna-Sofie Schilling (Heidelberg), Anna Wienhard (Heidelberg).

The symmetric spaces form a fascinating class of geometrical space. These are the spaces in which there is a point reflection through every point. An example is the space $\mathrm{Pos}(\mathbb{C}, n)$ of positive definite $n \times n$ Hermitian matrices.

The interesting metrics on such spaces are the ones that are invariant under all the symmetries, in particular the invariant Finsler metrics. When the symmetric space is non-compact, as in the example just referred to, it is profitable to study the horofunction boundary of such metrics.

An important technique in trying to understand symmetric spaces is to look at their *flats*. These are subspaces that are, as their name suggests, flat in some sense. Because of the abundance of symmetries, there are many flats; indeed, every pair of points lies in a flat. Furthermore, given any two flats, there is a symmetry taking one to the other, and so they are all alike. It turns out that the restriction of an invariant Finsler metric to a single flat determines the metric everywhere, and gives the flat the geometry of a normed space.

Symmetric spaces can be compactified by means of the Satake compactification. In fact, there are several such compactifications, one associated to each irreducible faithful representation of the invariance group of the space. In [41], we show that each Satake compactification can be constructed as a horofunction compactification by choosing an appropriate invariant Finsler metric. In fact, the metrics we construct have polyhedral balls on the flat.

An important step in the proof is to show that the closure of a flat in the horofunction compactification of the symmetric space is the same as the horofunction compactification of the flat viewed as a metric space in its own right. This is not true for every metric space, since in general one might not be able to distinguish horofunctions by looking at a subspace.

7.2.3. The set of minimal upper bounds of two matrices in the Loewner order

Participant: Nikolas Stott.

A classical theorem of Kadison shows that the space of symmetric matrices equipped with the Loewner order is an anti-lattice, meaning that two matrices have a least upper bound if and only if they are comparable. In [24], we refined this theorem by characterizing the set of minimal upper bounds: we showed that it is homeomorphic to the quotient space $O(p) \setminus O(p,q)/O(q)$, where $O(p,q)$ denotes the orthogonal group associated to the quadratic form with signature (p,q), and $O(p)$ denotes the standard pth orthogonal group.

7.2.4. Generalization of the Hellinger distance

Participant: Stéphane Gaubert.

In [64] (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.

7.2.5. Spectral inequalities for nonnegative tensors and their tropical analogues

Participant: Stéphane Gaubert.

In [39] (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

Participants: Xavier Allamigeon, Ricardo Katz [Conicet, Argentine].

In [20], 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.

7.3.2. Tropical totally positive matrices

Participant: Stéphane Gaubert.

In [22] (joint work with Adi Niv) we investigate 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 show 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.

7.3.3. Tropical compound matrix identities

Participants: Marianne Akian, Stéphane Gaubert.

A number of polynomial identities in tropical semirings can be derived from their classical analogues by application of a transfer principle [49], [51]. In [16], joint with Adi Niv, we prove identities on compound matrices in extended tropical semirings, which cannot be obtained by transfer principles, but are rather obtained by combinatorial methods. Such identities include analogues to properties of conjugate matrices, powers of matrices and $\mathrm{adj}\,(A)\,\mathrm{det}\,(A)^{-1}$, all of which have implications on the eigenvalues of the corresponding matrices. A tropical Sylvester-Franke identity is provided as well.

7.3.4. Group algebra in characteristic one and invariant distances over finite groups

Participant: Stéphane Gaubert.

In [21] (joint work with Dominique Castella), we investigated a tropical analogue of group algebras. We studied tropical characters and related them to invariant distances over groups.

7.3.5. Volume and integer points of tropical polytopes

Participant: Stéphane Gaubert.

We investigate in [40] (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 P = NP.

7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

7.4.1. Tropicalization of the central path and application to the complexity of interior point methods

Participants: Xavier Allamigeon, Stéphane Gaubert.

This work is in collaboration with Pascal Benchimol (EDF Labs) and Michael Joswig (TU Berlin).

In optimization, path-following interior point methods are driven to an optimal solution along a trajectory called the central path. The *central path* of a linear program $\mathrm{LP}(A, b, c) \equiv \min\{c \cdot x \mid Ax \leq b,\ x \geq 0\}$ is defined as the set of the optimal solutions (x^μ, w^μ) of the barrier problems:

$$\begin{array}{ll} \text{minimize} & c \cdot x - \mu\left(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i\right) \\ \text{subject to} & Ax + w = b,\ x > 0,\ w > 0 \end{array}$$

While the complexity of interior point methods is known to be polynomial, an important question is to study the number of iterations which are performed by interior point methods, in particular whether it can be bounded by a polynomial in the dimension (mn) of the problem. This is motivated by Smale 9th problem [128], on the existence of a strongly polynomial complexity algorithm for linear programming. So far, this question has been essentially addressed though the study of the curvature of the central path, which measures how far a path differs from a straight line, see [77], [76], [79], [78]. In particular, by analogy with the classical Hirsch conjecture, Deza, Terlaky and Zinchencko [78] proposed the “continuous analogue of the Hirsch conjecture”, which says that the total curvature of the central path is linearly bounded in the number m of constraints.

In a work of X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig [17], we prove that primal-dual log-barrier interior point methods are not strongly polynomial, by constructing a family of linear programs with $3r+1$ inequalities in dimension $2r$ for which the number of iterations performed is in $\Omega(2^r)$. The total curvature of the central path of these linear programs is also exponential in r, disproving the continuous analogue of the Hirsch conjecture.

Our method is to tropicalize the central path in linear programming. The tropical central path is the piecewise-linear limit of the central paths of parameterized families of classical linear programs viewed through logarithmic glasses. We give an explicit geometric characterization of the tropical central path, as a tropical analogue of the barycenter of a sublevel set of the feasible set induced by the duality gap. We study the convergence properties of the classical central path to the tropical one. This allows us to show that that the number of iterations performed by interior point methods is bounded from below by the number of tropical segments constituting the tropical central path.

7.4.2. Tropicalization of semidefinite programming and its relation with stochastic games

Participants: Xavier Allamigeon, Stéphane Gaubert, Mateusz Skomra.

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.

We address 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 first study 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 [60], with further results in the PhD thesis [13].

We show in [18] 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, [124] disproved this conjecture. In [19], 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 [60] and [18].

In [27] and [13], we exploit 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.

7.4.3. Tropical polynomial systems and colorful interior of convex bodies

Participants: Marianne Akian, Marin Boyet, Xavier Allamigeon, Stéphane Gaubert.

The starting PhD thesis work of Marin Boyet, deals with the solution of 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 are currently investigated.

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 ([71]) gave a spectral interpretation of the zeroes of the Riemann zeta function involving the action of $\mathbb{R}_+^*$ on the sector $X = \mathbb{Q}_+^\times \smallsetminus \mathbb{A}_\mathbb{Q}/\widehat{\mathbb{Z}}^\times$ of the adele class space $\mathbb{A}_\mathbb{Q}/\mathbb{Q}^*$ of the field of rational numbers. In [72], [74], 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 $\mathbb{Q}(\imath\sqrt{3})$. These results are presented in the submitted article [121]. In a further work, developed this year, I extended this construction, dealing now with number fields K with narrow class number 1. In fact, if we denote $\mathcal{U}_{\mathcal{O}_K}^+$ the totally positive units of $\mathcal{O}_K$, $\mathcal{O}_K^+$ the totally positive integers, $\widehat{\mathcal{O}_K^+}$ the topos of sets with a multiplicative action of totally positive integers of $\mathcal{O}_K^+$, $D_K = \text{Conv}(\mathcal{U}_{\mathcal{O}_K}^+)$ and $\mathcal{C}_{\mathcal{O}_K} = \text{Semiring}(\{\lambda D_K/\lambda \in \mathcal{O}_K^+\}) \cup \{\varnothing, \{0\}\}$, we consider the semiringed topos $(\widehat{\mathcal{O}_K^+}, (\mathcal{C}_{\mathcal{O}_K}, \text{Conv}(\bullet \cup \bullet), +))$ and show for it similar properties as the one shown in my PhD thesis for the arithmetic sites associated to imaginary quadratic fields with class number 1 by adapting to this case the technics used in my PhD thesis, Shintani units theorem, and some remarks A.Connes made on my PhD which appear as an appendix of the article [121]. Here again tropical algebra play a crucial role in the geometrical constructions.

7.5.2. Tropical tensor products

Participants: Stéphane Gaubert, Aurélien Sagnier.

Tensors products of modules over semifields of characteristic one, like the Boolean or tropical semifields, have appeared recently, with motivations from arithmetics, in work by Connes and Consani, towards an intersection theory for arithmetic and scaling sites (spaces they have built and which are closely related to the zeroes of the Riemann zeta function). Algebraic and topological tropical tensors products were constructed in a different way by Litvinov and collaborators: here, tropical tensors are sums of "rank one" expressions, similar to the ones used in the approximation of large data sets or of functions of many parameters. We show that the canonical notion of tropical tensor product, defined in terms of the usual universal problem, differs from the definition arising from approximation theory, but that the latter can be recovered from the former by a certain "reduction" operation. We illustrate these results by computing several basic examples of categorical tensors products, including spaces of convex sets and functions.

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 [83], 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 $\chi \ : \ PX = X^I \rightarrow X \times X$ 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 $s_{F_i} \ : \ F_i \rightarrow PX$ 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. [97]). 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 a recent prepublication [84], 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 an emergency call center

Participants: Xavier Allamigeon, 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 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 [55], [56], [65]. In 2018, we performed specific case studies, with several students of École polytechnique: Laetitia de Coudenhove, Julie Poulet, Céline Moucer and Julia Escribe.

7.6.2. Tropical models of fire propagation in urban areas

Participants: Stéphane Gaubert, Daniel Jones.

As part of the team work in the ANR project Democrite, we developed a model of fire propagation in urban areas, involving a deterministic analogue of first passage percolation. We showed that the fire tends to propagate according to a polyhedral shape, and derived metric limit theorems, exploiting discrete convexity results à la Shapley-Folkman. We validated this approach by simulations, on the fire following Kobe earthquake in 1995. The polyhedral shape is also apparent in historical fires, like the great fire of London (1666). These results are announced in [28].

7.6.3. Smart Data Pricing

Participants: Marianne Akian, Jean-Bernard Eytard, Stéphane Gaubert.

This work is in collaboration with Mustapha Bouhtou (Orange Labs) and with Gleb Koshevoy (Russian academy of Science).

The PhD work [81] of Jean-Bernard Eytard concerns the optimal pricing of data trafic in mobile networks. We developed a bilevel programming approach, allowing to an operator to balance the load in the network through price incentives. We showed that a subclass of bilevel programs can be solved in polynomial time, by combining methods of tropical geometry and of discrete convexity. This work is presented in [80] and also in [34]. In a followup work, presented in [81], we managed to extend these results to wider classes of bilevel problems, and to relate them to competitive equilibria problems.

7.6.4. Game theory models of decentralized mechanisms of pricing of the smart grid

Participants: Stéphane Gaubert, Paulin Jacquot.

This work is in collaboration with Nadia Oudjane, Olivier Beaude and Cheng Wan (EDF Labs).

The PhD work of Paulin Jacquot concerns the application of game theory techniques to pricing of energy. We are developing a game theory framework for demand side management in the smart grid, in which users have movable demands (like charging an electric vehicle). We compared in particular the daily and hourly billing mechanisms. The latter, albeit more complex to analyse, has a merit as it incitates the user to move his or her consumption at off peak hours. We showed the Nash equilibrium is unique, under some assumptions, and gave theoretical bounds of the price of anarchy of the game with a hourly billing, showing this mechanism remains efficient while being more “fair” than the daily billing. We proposed and tested decentralized algorithms to compute the Nash equilibrium. These contributions are presented in [102], [23].

Another work, by Paulin Jacquot and Cheng Wan, deals with limit theorems for atomic games with a large number of players [30], [42].

GALEN-POST Team

7. New Results

7.1. Invertible Deep Networks

Participant: Edouard Oyallon (in collaboration with J.H. Jacobsen and A. Smeulders, Instituut voor Informatica)

It is widely believed that the success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand. This is supported empirically by the difficulty of recovering images from their hidden representations, in most commonly used network architectures. In this paper we show via a one-to-one mapping that this loss of information is not a necessary condition to learn representations that generalize well on complicated problems, such as ImageNet. Via a cascade of homeomorphic layers, we build the i-RevNet, a network that can be fully inverted up to the final projection onto the classes, i.e. no information is discarded. Building an invertible architecture is difficult, for one, because the local inversion is ill-conditioned, we overcome this by providing an explicit inverse. An analysis of i-RevNet's learned representations suggests an alternative explanation for the success of deep networks by a progressive contraction and linear separation with depth. To shed light on the nature of the model learned by the i-RevNet we reconstruct linear interpolations between natural image representations [28].

7.2. Compression of CNNs inputs

Participant: Edouard Oyallon (in collaboration with E. Belilovsky, DIRO, Montréal, S. Zagoruyko, WILLOW, Inria Paris and M. Valko, SEQUEL, Inria Lille)

Typical inputs of CNNs are highly redundant and could be potentially reduced. We study the first-order scattering transform as a candidate for reducing the signal processed by a convolutional neural network (CNN). We study this transformation and show theoretical and empirical evidence that in the case of natural images and sufficiently small translation invariance, this transform preserves most of the signal information needed for classification while substantially reducing the spatial resolution and total signal size. We show that cascading a CNN with this representation performs on par with ImageNet classification models commonly used in downstream tasks such as the ResNet-50. We subsequently apply our trained hybrid ImageNet model as a base model on a detection system, which has typically larger image inputs. On Pascal VOC and COCO detection tasks we deliver substantial improvements in the inference speed and training memory consumption compared to models trained directly on the input image [34].

7.3. Interstitial lung disease segmentation

Participants: Guillaume Chassagnon, Norbert Bus, Rafael Marini Silva, Evangelia Zacharaki, Maria Vakalopoulou (in collaboration with Marie-Pierre Revel and Nikos Paragios: AP-HP - Hopital Cochin Broca Hotel Dieu; Therapanacea)

Interstitial lung diseases (ILD) encompass a large spectrum of diseases sharing similarities in their physiopathology and computed tomography (CT) appearance. In the work [42], we propose the adaption of a deep convolutional encoder-decoder (CED) that has shown high accuracy for image segmentation. Such architectures require annotation of the total region with pathological findings. This is difficult to acquire, due to uncertainty in the definition and extent of disease patterns and the need of significant human effort, especially for large datasets. Therefore, often current methods use patch-based implementations of convolutional neural networks, which however tend to produce spatially inhomogeneous segmentations due to their local contextual view. We exploit the advantages of both architectures by using the output of a patch-based classifier as a prior to a CED.

Moreover, in order to deal with the limited available datasets that are available, in [41], we introduce a novel multi-network architecture that exploits domain knowledge to address those challenges. The proposed architecture consists of multiple deep neural networks that are trained after co-aligning multiple anatomies through multi-metric deformable registration. This multi-network architecture can be trained with fewer examples and leads to better performance, robustness and generalization through consensus. Comparable to human accuracy, highly promising results on the challenging task of interstitial lung disease segmentation demonstrate the potential of our approach.

7.4. Image Registration with 3D Convolutional Neural Networks

Participants: Stergios Christodoulidis, Mihir Sahasrabudhe, Guillaume Chassagnon, Maria Vakalopoulou (in collaboration with Stavroula Mougiakakou and Marie-Pierre Revel and Nikos Paragios: University of Bern; AP-HP - Hopital Cochin Broca Hotel Dieu; Therapanacea)

Image registration and in particular deformable registration methods are pillars of medical imaging. Inspired by the recent advances in deep learning, we propose in this paper, [25] we proposed a new deep learning based and unsupervised method for image registration. In partucular, a novel convolutional neural network architecture that couples linear and deformable registration within a unified architecture endowed with near real-time performance. Our framework is modular with respect to the global transformation component, as well as with respect to the similarity function while it guarantees smooth displacement fields. We evaluate the performance of our network on the challenging problem of MRI lung registration, and demonstrate superior performance with respect to state of the art elastic registration methods. The proposed deformation (between inspiration & expiration) was considered within a clinically relevant task of interstitial lung disease (ILD) classification and showed promising results.

7.5. Radiomics for response to immunotherapy

Participants: Roger Sun, Maria Vakalopoulou (in collaboration with Elaine Johanna Limkin, Laurent Dercle, Stéphane Champiat, Shan Rong Han, Loic Verlingue, David Brandao, Andrea Lancia, Samy Ammari, Antoine Hollebecque, Jean-Yves Scoazec, Aurélien Marabelle, Christophe Massard, Jean-Charles Soria, Charlotte Robert, Nikos Paragios, Eric Deutsch, Charles Ferté: Institute Gustave Roussy; Therapanacea)

Because responses of patients with cancer to immunotherapy can vary in success, innovative predictors of response to treatment are urgently needed to improve treatment outcomes. In this retrospective multicohort work [17], we used four independent cohorts of patients with advanced solid tumours to develop and validate a radiomic signature predictive of immunotherapy response by combining contrast-enhanced CT images and RNA-seq genomic data from tumour biopsies to assess CD8 cell tumour infiltration. To develop the radiomic signature of CD8 cells, we used the CT images and RNA sequencing data of 135 patients with advanced solid malignant tumours who had been enrolled into the MOSCATO trial between May 1, 2012, and March 31, 2016, in France (training set). The genomic data, which are based on the CD8B gene, were used to estimate the abundance of CD8 cells in the samples and data were then aligned with the images to generate the radiomic signatures. The concordance of the radiomic signature (primary endpoint) was validated in a Cancer Genome Atlas [TGCA] database dataset including 119 patients who had available baseline preoperative imaging data and corresponding transcriptomic data on June 30, 2017. From 84 input variables used for the machine-learning method (78 radiomic features, five location variables, and one technical variable), a radiomics-based predictor of the CD8 cell expression signature was built by use of machine learning (elastic-net regularised regression method). Two other independent cohorts of patients with advanced solid tumours were used to evaluate this predictor. The immune phenotype internal cohort (n=100), were randomly selected from the Gustave Roussy Cancer Campus database of patient medical records based on previously described, extreme tumour-immune phenotypes: immune-inflamed (with dense CD8 cell infiltration) or immune-desert (with low CD8 cell infiltration), irrespective of treatment delivered; these data were used to analyse the correlation of the immune phenotype with this biomarker. Finally, the immunotherapy-treated dataset (n=137) of patients recruited from Dec 1, 2011, to Jan 31, 2014, at the Gustave Roussy Cancer Campus, who had been treated with anti-PD-1 and anti-PD-L1 monotherapy in phase 1 trials, was used to assess the predictive value of this biomarker in terms of clinical outcome.

7.6. Semantic Segmentation Techniques for Brain Tumor Patients

Participants: Siddhartha Chandra, Théo Estienne, Roger Sun, Enzo Battistella, Maria Vakalopoulou (in collaboration with Charlotte Robert, Nikos Paragios, Eric Deutsch: Institute Gustave Roussy; Therapanacea)

In this work [23] we propose a novel deep learning based pipeline for the task of brain tumor segmentation. Our pipeline consists of three primary components: (i) a preprocessing stage that exploits histogram standardization to mitigate inaccuracies in measured brain modalities, (ii) a first prediction stage that uses the V-Net deep learning architecture to output dense, per voxel class probabilities, and (iii) a prediction refinement stage that uses a Conditional Random Field (CRF) with a bilateral filtering objective for better context awareness. Additionally, we compare the V-Net architecture with a custom 3D Residual Network architecture, trained on a multi-view strategy, and our ablation experiments indicate that V-Net outperforms the 3D ResNet-18 with all bells and whistles, while fully connected CRFs as post processing, boost the performance of both networks. We report competitive results on the BraTS 2018 validation and test set as also summarized on [52].

7.7. Demystification of AI-driven medical image interpretation

Participants: Maria Vakalopoulou (in collaboration with P. Savadjiev, J. Chong, A. Dohan, C. Reinhold, B. Gallix: McGill University; Therapanacea)

The recent explosion of 'big data' has ushered in a new era of artificial intelligence (AI) algorithms in every sphere of technological activity, including medicine, and in particular radiology. However, the recent success of AI in certain flagship applications has, to some extent, masked decades-long advances in computational technology development for medical image analysis. In this work [16], we provide an overview of the history of AI methods for radiological image analysis in order to provide a context for the latest developments. We review the functioning, strengths and limitations of more classical methods as well as of the more recent deep learning techniques. We discuss the unique characteristics of medical data and medical science that set medicine apart from other technological domains in order to highlight not only the potential of AI in radiology but also the very real and often overlooked constraints that may limit the applicability of certain AI methods. Finally, we provide a comprehensive perspective on the potential impact of AI on radiology and on how to evaluate it not only from a technical point of view but also from a clinical one, so that patients can ultimately benefit from it.

7.8. Semantic Segmentation for Remote Sensing Data

Participants: Maria Papadomanolaki, Maria Vakalopoulou (in collaboration with Christina Karakizi, Georgia Antoniou, Konstantinos Karantzalos, Nikos Paragios; National Technical University of Athens, Therapanacea)

Detailed, accurate and frequent land cover mapping is a prerequisite for several important geospatial applications and the fulfilment of current sustainable development goals. This work [9] introduces a methodology for the classification of annual high-resolution satellite data into several detailed land cover classes. In particular, a nomenclature with 27 different classes was introduced based on CORINE Land Cover (CLC) Level-3 categories and further analysing various crop types. Without employing cloud masks and/or interpolation procedures, we formed experimental datasets of Landsat-8 (L8) images with gradually increased cloud cover in order to assess the influence of cloud presence on the reference data and the resulting classification accuracy. The performance of shallow kernel-based and deep patch-based machine learning classification frameworks was evaluated. Quantitatively, the resulting overall accuracy rates differed within a range of less than 3%; however, maps produced based on Support Vector Machines (SVM) were more accurate across class boundaries and the respective framework was less computationally expensive compared to the applied patch-based deep Convolutional Neural Network (CNN). Further experimental results and analysis indicated that employing all multitemporal images with up to 30% cloud cover delivered relatively higher overall accuracy rates as well as the highest per-class accuracy rates. Moreover, by selecting 70% of the top-ranked features after applying a feature selection strategy, slightly higher accuracy rates were achieved. A detailed discussion of the quantitative and qualitative evaluation outcomes further elaborates on the performance of all considered classes and highlights different aspects of their spectral behaviour and separability.

Moreover, semantic segmentation is a mainstream method in several remote sensing applications based on very-high-resolution data, achieving recently remarkable performance by the use of deep learning and more specifically, pixel-wise dense classification models. In this work [36], we exploit the use of a relatively deep architecture based on repetitive downscale upscale processes that had been previously employed for human pose estimation. By integrating such a model, we are aiming to capture low-level details, such as small objects, object boundaries and edges. Experimental results and quantitative evaluation has been performed on the publicly available ISPRS (WGIII/4) benchmark dataset indicating the potential of the proposed approach.

7.9. BRANE Clust: Cluster-Assisted Gene Regulatory Network Inference Refinement

Participants: Jean-Christophe Pesquet (in collaboration with Aurélie Pirayre, IFP Energies nouvelles, Camille Couprie, Facebook Research, Laurent Duval, IFP Energies nouvelles)
Discovering meaningful gene interactions is crucial for the identification of novel regulatory processes in cells. Building accurately the related graphs remains challenging due to the large number of possible solutions from available data. Nonetheless, enforcing a priori on the graph structure, such as modularity, may reduce network indeterminacy issues. BRANE Clust (Biologically-Related A priori Network Enhancement with Clustering) refines gene regulatory network (GRN) inference thanks to cluster information. It works as a post-processing tool for inference methods (i.e. CLR, GENIE3). In BRANE Clust, the clustering is based on the inversion of a system of linear equations involving a graph-Laplacian matrix promoting a modular structure. Our approach [14] is validated on DREAM4 and DREAM5 datasets with objective measures, showing significant comparative improvements. We provide additional insights on the discovery of novel regulatory or co-expressed links in the inferred Escherichia coli network evaluated using the STRING database. The comparative pertinence of clustering is discussed computationally (SIMoNe, WGCNA, X-means) and biologically (RegulonDB).

7.10. Proximity Operators of Discrete Information Divergences

Participants: Jean-Christophe Pesquet (in collaboration with Mireille El Gheche, EPFL, Giovanni Chierchia, ESIEE Paris)
Information divergences allow one to assess how close two distributions are from each other. Among the large panel of available measures, a special attention has been paid to convex ϕ-divergences, such as Kullback-Leibler, Jeffreys-Kullback, Hellinger, Chi-Square, Renyi, and I_α divergences. While ϕ-divergences have been extensively studied in convex analysis, their use in optimization problems often remains challenging. In this regard, one of the main shortcomings of existing methods is that the minimization of ϕ-divergences is usually performed with respect to one of their arguments, possibly within alternating optimization techniques. In this paper, we overcome this limitation by deriving new closed-form expressions for the proximity operator of such two-variable functions. This makes it possible to employ standard proximal methods for efficiently solving a wide range of convex optimization problems involving ϕ-divergences. In addition, we show that these proximity operators are useful to compute the epigraphical projection of several functions of practical interest. The proposed proximal tools are numerically validated in the context of optimal query execution within database management systems, where the problem of selectivity estimation plays a central role. Experiments are carried out on small to large scale scenarios [6].

7.11. Stochastic quasi-Fejèr block-coordinate fixed point iterations with random sweeping

Participants: Jean-Christophe Pesquet (in collaboration with Patrick Combettes, North Caroline State University)

Our previous work 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 present paper establishes results on the mean-square and linear convergence of the iterates. Applications to monotone operator splitting and proximal optimization algorithms are presented.

7.12. Rational optimization for nonlinear 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 [53].

7.13. Representation Learning on Real-World Graphs

Participants: Fragkiskos Malliaros, Abdulkadir Çelikkanat (in collaboration with Duong Nguyen, UC San Diego)

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 BiasedWalk, an unsupervised Skip-gram-based network embedding algorithm which can preserve higher-order proximity information, as well as capture both the homophily and role equivalence relationships between nodes [33]. BiasedWalk relies on a novel node sampling procedure based on biased random walks, that can behave as actual depth-first-search and breath-first-search explorations – thus, forcing the sampling scheme to capture both role equivalence and homophily relations between nodes. Furthermore, BiasedWalk is scalable on large scale graphs, and is able to handle different types of networks structures, including (un)weighted and (un)directed ones.

Furthermore, we have introduced TNE (Topical Node Embeddings), a general framework to enhance node embeddings acquired by means of the random walk-based approaches [45]. Similar to the notion of *topical word embeddings* in the domain of Natural Language Processing, the proposed framework assigns each vertex to a topic with the favor of various statistical models and community detection methods, and then generates enhanced community representations.

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 the biased random walks as well as the incorporation of vertex and topic embeddings outperform widely-known baseline NRL methods.

7.14. Anonymity on Directed Networks

Participants: Fragkiskos Malliaros (in collaboration with Jordi Casas-Roma and Julián Salas, Universitat Oberta de Catalunya; Michalis Vazirgiannis, École Polytechnique)

In recent years, a huge amount of social and human interaction networks have been made publicly available. Embedded within this data, there is user's private information that must be preserved before releasing the data to third parties and researchers. In this work, we have considered the problem of anonymization on directed networks. Although there are several anonymization methods for networks, most of them have explicitly been designed to work with undirected networks and they can not be straightforwardly applied when they are directed. Moreover, ignoring the direction of the edges causes important information loss on the anonymized networks in the best case. In the worst case, the direction of the edges may be used for reidentification, if it is not considered in the anonymization process. Here, we have proposed two different models for k-degree anonymity on directed networks, and we also present algorithms to fulfill these k-degree anonymity models [4]. Given a network G, we construct a k-degree anonymous network by the minimum number of edge additions. Our algorithms use multivariate micro-aggregation to anonymize the degree sequence, and then they modify the graph structure to meet the k-degree anonymous sequence. We apply our algorithms to several real datasets and demonstrate their efficiency and practical utility.

7.15. Influence Maximization in Complex Networks

Participants: Fragkiskos Malliaros (in collaboration with Michalis Vazirgiannis, George Panagopoulos, Maria-Evgenia Rossi, Bowen Shi, Christos Giatsidis, École Polytechnique; Nikolaos Tziortziotis, Université Paris-Sud)

Influence maximization in complex networks has attracted a lot of attention due to its numerous applications, including diffusion of social movements, the spread of news, viral marketing and outbreak of diseases. The objective is to discover a group of users that are able to maximize the spread of influence across a network. The seminal *greedy* algorithm developed by Kempe, Kleinberg and Tardos progressively adds new nodes to the seed set, maximizing the expected influence spread; the algorithm gives a solution to the influence maximization problem while having a good approximation ratio.

Nevertheless, one of the bottlenecks of the greedy algorithm is that it does not scale well on large scale datasets. In our work, we have proposed Matrix Influence (MATI), an efficient algorithm that can be used under both the Linear Threshold and Independent Cascade diffusion models [15]. MATI is based on the precalculation of the influence by taking advantage of the simple paths in the node's neighborhood. An extensive empirical analysis has been performed on multiple real-world datasets showing that MATI has competitive performance when compared to other well-known algorithms with regards to running time and expected influence spread.

Furthermore, the previously described greedy algorithm focuses solely on static networks. However, with the emergence of several complementary data, such as the network's temporal changes and the diffusion cascades taking place over it, novel methods have been proposed with promising results. In our work, we have introduced a simple yet effective algorithm (called DiffuGreedy) that combines the algorithmic methodology of the greedy approach with diffusion cascades [35]. We have compared it with four different prevalent influence maximization approaches, on a large scale Chinese microblogging dataset. More specifically, for comparison, we have employed methods that derive the seed set using the static network, the temporal network, the diffusion cascades, and their combination. A set of diffusion cascades from the latter part of the dataset is set aside for evaluation. The experimental evaluation has shown that the proposed DiffuGreedy outperforms widely used baseline methods in both quality of the seed set and computational efficiency.

7.16. Graph-based Text Analytics

Participants: Fragkiskos Malliaros (in collaboration with Konstantinos Skianis and Michalis Vazirgiannis, École Polytechnique)

Text categorization is a core task in a plethora of text mining applications. In our work, contrary to the traditional *Bag-of-Words* approach, we have considered the *Graph-of-Words* model in which each document is represented by a graph that encodes relationships between the different terms. Based on this formulation, we treat the term weighting task as a node ranking problem; the importance of a term is determined by the importance of the corresponding node in the graph, using node centrality criteria. We have also introduced novel graph-based weighting schemes by enriching graphs with word-embedding distances, in order to reward or penalize the importance of semantically close terms [39]. Our methods produce more discriminative feature weights for text categorization, outperforming existing frequency-based criteria – highlighting also the importance of graph-based methods in text analytics and natural language processing in general.

7.17. Auxiliary Variable Method for MCMC Algorithms in High Dimension

Participants: Emilie Chouzenoux, Jean-Christophe Pesquet (Collaboration: Yosra Marnissi, SAFRAN TECH, and Amel Benazza-Benyahia, SUP'COM Tunis)

In this work, we are interested in Bayesian inverse problems where either the data fidelity term or the prior distribution is Gaussian or driven from a hierarchical Gaussian model. Generally, Markov chain Monte Carlo (MCMC) algorithms allow us to generate sets of samples that are employed to infer some relevant parameters of the underlying distributions. However, when the parameter space is high-dimensional, the performance of stochastic sampling algorithms is very sensitive to existing dependencies between parameters. In particular, this problem arises when one aims to sample from a high-dimensional Gaussian distribution whose covariance matrix does not present a simple structure. Another challenge is the design of Metropolis–Hastings proposals that make use of information about the local geometry of the target density in order to speed up the convergence and improve mixing properties in the parameter space, while not being too computationally expensive. These two contexts are mainly related to the presence of two heterogeneous sources of dependencies stemming either from the prior or the likelihood in the sense that the related covariance matrices cannot be diagonalized in the same basis. In this work, we address these two issues. Our contribution consists of adding auxiliary variables to the model in order to dissociate the two sources of dependencies. In the new augmented space, only one source of correlation remains directly related to the target parameters, the other sources of correlations being captured by the auxiliary variables. Experimental results conducted on two practical image restoration problems indicate that adding the proposed auxiliary variables makes the sampling problem simpler, and thus the computational cost of each iteration of the Gibbs sampler is significantly reduced while ensuring good mixing properties [11].

7.18. Generation of patient-specific cardiac vascular networks

Participant: Hugues Talbot (in collaboration with C. Jaquet, L. Najman, ESIEE Paris; L. Grady, M. Schaap, B. Spain, H. Kim, C. Taylor, HeartFlow; I. Vignon-Clementel, REO)

In this work, we have proposed a blood-vessel generation procedure for extending known patient vasculature over and within the heart ventricle [8]. 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.

7.19. Curvilinear structure analysis using path operators

Participant: Hugues Talbot (in collaboration with O. Merveille, N. Passat, CRESTIC, and L. Najman, ESIEE Paris)

In this work, we propose mathematical morphology based operators that use paths as families of structuring elements [12]. Structuring elements are like the windows of linear operators, they define the extent of the related operators (convolutions in the linear case, openings and closings in the morphology case). When dealing with thin objects (e.g. fibres, blood vessels, textures, etc), a compact, isotropic window is usually inappropriate because no such window can fit in these objects. This is more critical for morphology, which is concerned with preserving shapes, than with linear operators. Thin windows must therefore be devised, but there are a large number of potentially interesting thin windows at each point in an image. In this article, we leverage the definition of noise-resistant, path operators to define a non-linear notion of vesselness, that can be used for thin object detection, filtering and segmentation in 2D and 3D.

7.20. High throughput automated detection of axial malformations in fish embryo

Participant: Hugues Talbot (in collaboration with D. Genest, M. Léonard, N. De Crozé, L'Oréal, and E. Puybareau, J. Cousty, LIGM)

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 tail malformation in fish embryo, based on image analysis and machine learning [5]. 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.

LIFEWARE Project-Team

7. New Results

7.1. Graphical Requirements for Multistationarity in CRNs and their Verification in BioModels

Participants: Adrien Baudier, François Fages, Sylvain Soliman.

Thomas's necessary conditions for the existence of multiple steady states in gene networks have been proved by Soulé with high generality for dynamical systems defined by differential equations. When applied to (protein) reaction networks however, those conditions do not provide information since they are trivially satisfied as soon as there is a bimolecular or a reversible reaction. Refined graphical requirements have been proposed to deal with such cases. In [1], we present for the first time a graph rewriting algorithm for checking the refined conditions given by Soliman, and evaluate its practical performance by applying it systematically to the curated branch of the BioModels repository. This algorithm analyzes all reaction networks (of size up to 430 species) in less than 0.05 second per network, and permits to conclude to the absence of multistationarity in 160 networks over 506. The short computation times obtained in this graphical approach are in sharp contrast to the Jacobian-based symbolic computation approach. We also discuss the case of one extra graphical condition by arc rewiring that allows us to conclude on 20 more networks of this benchmark but with a high computational cost. Finally, we study with some details the case of phosphorylation cycles and MAPK signalling models which show the importance of modelling the intermediate complexations with the enzymes in order to correctly analyze the multistationarity capabilities of such biochemical reaction networks.

7.2. Influence Networks compared with CRNs: Semantics, Expressivity and Attractors

Participants: François Fages, Thierry Martinez [former member], David Rosenblueth [former member], Sylvain Soliman, Denis Thieffry.

Biochemical reaction networks are one of the most widely used formalism in systems biology to describe the molecular mechanisms of high-level cell processes. However modellers also reason with influence diagrams to represent the positive and negative influences between molecular species and may find an influence network useful in the process of building a reaction network. In [4], we introduce a formalism of influence networks with forces, and equip it with a hierarchy of Boolean, Petri net, stochastic and differential semantics, similarly to reaction networks with rates. We show that the expressive power of influence networks is the same as that of reaction networks under the differential semantics, but weaker under the discrete semantics. Furthermore, the hierarchy of semantics leads us to consider a (positive) Boolean semantics without test for absence, that we compare with the (negative) Boolean semantics with test for absence of gene regulatory networks à la Thomas. We study the monotonicity properties of the positive semantics and derive from them an algorithm to compute attractors in both the positive and negative Boolean semantics. We illustrate our results on models of the literature about the p53/Mdm2 DNA damage repair system, the circadian clock, and the influence of MAPK signaling on cell-fate decision in urinary bladder cancer.

As an application, in [11] methods are shown to add dynamics to large molecular influence maps.

7.3. Reducing CRNs by Tropicalization

Participants: Eléonore Bellot, François Fages, Aymeric Quesne, Sylvain Soliman, Eliott Suits.

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 with constraint programming or SAT solving techniques. However this approach does not allow us to actually reduce models. In the framework of the ANR-DFG SYMBIONT project [10] we are investigating model reduction methods based on tropicalization and constraint programming techniques [0] together with correctness conditions based on Tikhonov theorem.

7.4. Compiling mathematical functions and programs in CRNs

Participants: Auriane Cozic, Elisabeth Degrand, François Fages, Mathieu Hemery, Wei-Chih Huang, Lena Le Quellec, Sylvain Soliman.

In a previous paper, we have proven that any computable function over the reals in the sense of computable analysis (i.e. computable with finite yet arbitrary precision by a Turing machine) is computable by a continuous CRN over a finite set of molecular species. In this approach, the real-valued molecular concentrations are the information carriers and computation can be purely analog. We have derived from the proof of this result a compiler of real functions (of either time or input concentrations) specified by polynomial initial value problems (PIVP) in elementary CRNs. This compiler makes it possible to automate the design of abstract CRNs for implementing arbitrary computable functions over the reals presented by PIVPs, in particular arithmetic, trigonometric, sigmoid and logical functions. The compilation of sequentiality, program control flows and mixed analog-digital imperative programs lead us however to consider more efficient implementations of Heavyside functions with simple CRNs that have no simple mathematical expression as input/output functions. Our goal is to develop a compiler of high-level mixed analog-digital programs in efficient abstract CRNs amenable to practical implementation with real enzymes in DNA-free vesicles, as illustrated in Section 7.8 .

7.5. Evolving CRNs from data time series

Participants: Elisabeth Degrand, François Fages, Jérémy Grignard [former&future Member], Mathieu Hemery, Sylvain Soliman.

Another approach to CRN design is by evolutionary algorithms. Given a function given by its graph with a finite set of points, and using the same framework based on PIVPs as above, we have designed a genetic algorithm which interleaves the evolution of a population of PIVPs with parameter optimization using CMA-ES for fitting the input curve. On the cosine function, this algorithm recovers PIVPs equivalent to the standard PIVP for cosine, while on Heavyside functions, the algorithm finds (mathematically mysterious) CRNs that are much simpler than Hill functions of high order for instance.

7.6. Learning CRNs from data time series

Participants: François Fages, Jérémy Grignard [former&future Member], Nicolas Levy, Julien Martinelli, Sylvain Soliman.

The problem of learning a mechanistic model from observed data is more difficult than learning a blackbox model fitting the data, due to the difference between causal relationships and correlations. In a biological context, learning a mechanistic model from experimental data would help understanding the underlying biological processes. To that end, considering multiple time series data generated by a hidden CRN from different initial states (by either stochastic or differential simulation), we develop a clustering-based algorithm for the inference of biological reaction networks. The output is a set of reactions which can be used to generate new traces. A model selection method is derived from these newly generated traces. We evaluate the performance of this algorithm on a range of models from Biomodels.

[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.

7.7. Optimizing CRN robustness

Participants: François Fages, Lucia Nasti, Sylvain Soliman.

In [7] we present two complementary notions of robustness of a system with respect to a property of its behaviour expressed in temporal logic: first the statistical notion of model robustness to parameter perturbations, defined as its mean functionality; and second, a metric notion of formula satisfaction robustness, defined as the penetration depth in the validity domain of the temporal logic constraints. We show how the formula robustness can be used in BIOCHAM-4 with no extra cost as an objective function in the parameter optimization procedure, to actually improve CRN robustness. We illustrate these unique features with a classical example of the hybrid systems community and provide some performance figures on a model of MAPK signalling with 37 parameters.

7.8. Robust biochemical programming of synthetic microreactors

Participants: Auriane Cozic, François Fages, Wei-Chih Huang, Lena Le Quellec, Lucia Nasti, Sylvain Soliman.

Biological systems have evolved efficient sensing and decision-making mechanisms to maximize fitness in changing molecular environments. Synthetic biologists have exploited these capabilities to engineer control on information and energy processing in living cells. While engineered organisms pose important technological and ethical challenges, de novo assembly of non-living biomolecular devices could offer promising avenues towards various real-world applications. However, assembling biochemical parts into functional information processing systems has remained challenging due to extensive multidimensional parameter spaces that must be sampled comprehensively in order to identify robust, specification compliant molecular implementations. In [3], we introduce a systematic methodology based on automated computational design and microfluidics enabling the programming of synthetic cell-like microreactors embedding biochemical logic circuits, or protosensors, to perform accurate biosensing and biocomputing operations in vitro according to temporal logic specifications. We show that proof-of-concept protosensors integrating diagnostic algorithms detect specific patterns of biomarkers in human clinical samples. Protosensors may enable novel approaches to medicine and represent a step towards autonomous micromachines capable of precise interfacing of human physiology or other complex biological environments, ecosystems or industrial bioprocesses.

7.9. Identification of individual cells from z-stacks of bright-field microscopy images

Participants: Grégory Batt, Chiara Fracassi [former Member], Jean-Baptiste Lugagne [former Member].

Obtaining single cell data from time-lapse microscopy images is critical for quantitative biology, but bottlenecks in cell identification and segmentation must be overcome. In [5], we propose a novel, versatile method that uses machine learning classifiers to identify cell morphologies from z-stack bright-field microscopy images. We show that axial information is enough to successfully classify the pixels of an image, without the need to consider in focus morphological features. This fast, robust method can be used to identify different cell morphologies, including the features of *E. coli, S. cerevisiae* and epithelial cells, even in mixed cultures. Our method demonstrates the potential of acquiring and processing Z-stacks for single-layer, single-cell imaging and segmentation.

7.10. Applying ecological resistance and resilience to dissect bacterial antibiotic responses

Participants: Virgile Andreani, Grégory Batt.

An essential property of microbial communities is the ability to survive a disturbance. Survival can be achieved through resistance, the ability to absorb effects of a disturbance without a notable change, or resilience, the ability to recover after being perturbed by a disturbance. These concepts have long been applied to the analysis of ecological systems, although their interpretations are often subject to debate. In [6], we show that this framework readily lends itself to the dissection of the bacterial response to antibiotic treatment, where both terms can be unambiguously defined. The ability to tolerate the antibiotic treatment in the short term corresponds to resistance, which primarily depends on traits associated with individual cells. In contrast, the ability to recover after being perturbed by an antibiotic corresponds to resilience, which primarily depends on traits associated with the population. This framework effectively reveals the phenotypic signatures of bacterial pathogens expressing extended-spectrum β-lactamases when treated by a β-lactamase antibiotic. Our analysis has implications for optimizing treatment of these pathogens using a combination of a β-lactamase and a β-lactamase inhibitor. In particular, our results underscore the need to dynamically optimize combination treatments based on the quantitative features of the bacterial response to the antibiotic or the Bla inhibitor.

M3DISIM Project-Team

7. New Results

7.1. Mathematical and Mechanical Modeling

7.1.1. Microscopic model of collagen fiber

Participants: Florent Wijanto, Matthieu Caruel, Jean-Marc Allain [correspondant].

Our studies on collagen tissues have shown that the collagen fibers are able to elongate inelastically under stretch. In tendon, this effect has been attributed to the non-permanent cross-bridges which connect the different collagen fibrils (to assemble a fiber). This sliding effect appears experimentally to be reversible (at least partially) if the tissue is left long enough at its initial resting length. However, this sliding is classically included as an irreversible plastic response, or as a damage of the tissue. We are building a model based on a stochastic description of the binding and unbinding of the cross-bridges. This approach will enable us to have a microscopically based picture of the sliding, which will be able to explain some alteration in case of ageing or of pathological alterations of the tissue. At the moment, we have shown the importance of the density of cross-bridges in the cooperative response of the system. A publication is in preparation on the topic.

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

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

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. This work is accepted for publication in BMMB.

7.1.3. The importance of the pericardium for cardiac biomechanics

Participant: Radomir Chabiniok [correspondant].

The human heart is enclosed in the pericardial cavity. The pericardium consists of a layered thin sac and is separated from the myocardium by a thin film of fluid. It provides a fixture in space and frictionless sliding of the myocardium. The influence of the pericardium is essential for predictive mechanical simulations of the heart. However, there is no consensus on physiologically correct and computationally tractable pericardial boundary conditions. Here we propose to model the pericardial influence as a parallel spring and dashpot acting in normal direction to the epicardium. Using a four-chamber geometry, we compare a model with pericardial boundary conditions to a model with fixated apex. The influence of pericardial stiffness is demonstrated in a parametric study. Comparing simulation results to measurements from cine magnetic resonance imaging reveals that adding pericardial boundary conditions yields a better approximation with respect to atrioventricular plane displacement, atrial filling, and overall spatial approximation error. We demonstrate that this simple model of pericardial-myocardial interaction can correctly predict the pumping mechanisms of the heart as previously assessed in clinical studies. Utilizing a pericardial model can not only provide much more realistic cardiac mechanics simulations but also allows new insights into pericardial-myocardial interaction which cannot be assessed in clinical measurements yet. The work was accepted for publication in Biomechanics and Modeling in Mechanobiology [26], and is a joint work with Technical University in Munich, Germany (group of W.A. Wall) and Bernoulli Institute for Mathematics at University of Groningen, The Netherlands (C. Bertoglio).

7.1.4. Solving 2D linear isotropic elastodynamics by means of scalar potentials: a new challenge for finite elements

Participants: Sébastien Imperiale, Patrick Joly [Poems].

In this work we present a method for the computation of numerical solutions of 2D homogeneous isotropic elastodynamics equations by solving scalar wave equations. These equations act on the potentials of a Helmholtz decomposition of the displacement field and are decoupled inside the propagation domain. We detail how these equations are coupled at the boundary depending on the nature of the boundary condition satisfied by the displacement field. After presenting the case of rigid boundary conditions, that presents no specific difficulty, we tackle the challenging case of free surface boundary conditions that presents severe stability issues if a straightforward approach is used. We introduce an adequate functional framework as well as a time domain mixed formulation to circumvent these issues. Numerical results confirm the stability of the proposed approach.

7.1.5. Lung multiscale poromechanical modeling, from breathing to pulmonary fibrosis-induced chronic remodeling

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

Pulmonary diseases are about to become the third cause of death in the world. One on them, Idiopathic Pulmonary Fibrosis (IPF), which involves thickening, stiffening and destruction the alveolar walls, remains poorly understood, diagnosed and treated. It has been hypothesized, however, that IPF involves a mechanical vicious circle, where fibrosis induces higher stresses, which in turns favors fibrosis. In this project, we intend to better understand the role of mechanics in the disease progression, in order to improve diagnosis and prognosis. We model the lung behavior during breathing at organ-scale, based on a poromechanical theory, previously established in the team. Then we estimate the regional mechanical properties of the lung, based on clinical data. In the future, the procedure can be used as a prognostic tool by the clinicians.

7.1.6. Mathematical modelling of transient shear wave elastography in the heart

Participants: Federica Caforio [correspondant], Sébastien Imperiale.

The aim of this work is to provide a mathematical model of the excitation and the resulting shear wave propagation in Acoustic Radiation Force (ARF)-based shear wave cardiac elastography. Our approach is based on asymptotic analysis; more precisely, it consists in considering a family of problems, parametrised by a small parameter inversely proportional to the excitation frequency of the probes, the viscosity and the velocity of pressure wave propagation. We derive a simplified model for the expression of the ARF by investigating the limit behaviour of the solution when the small parameter goes to zero. By formal asymptotic analysis - an asymptotic expansion of the solution is used - we show that the leading order term of the expansion is the underlying nonlinear cardiac mechanics. Subsequently, two corrector terms are computed. The first is a fast-oscillating pressure wave generated by the probes, solution of a Helmholtz equation at every time instant. The second corrector term consists in an elastic field with prescribed divergence, having a function of the first corrector as a source term. This field corresponds to the shear acoustic wave induced by the ARF. We also confirm that, in cardiac mechanics, the presence of viscosity in the model is essential to derive an expression of the shear wave propagation from the ARF, and that this phenomenon is related to the nonlinearity of the partial differential equation.

7.1.7. Analysis and calibration of a linear model for structured cell populations with unidirectional motion : Application to the morphogenesis of ovarian follicles

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

In [41], we have analyzed a multi-type age dependent model for cell populations subject to unidirectional motion, in both a stochastic and deterministic framework. Cells are distributed into successive layers; they may divide and move irreversibly from one layer to the next. We have adapted results on the large-time convergence of PDE systems and branching processes to our context, where the Perron-Frobenius or Krein-Rutman theorems cannot be applied. We have derived explicit analytical formulas for the asymptotic cell number moments, and the stable age distribution. We have illustrated these results numerically and we have applied them to the study of the morphodynamics of ovarian follicles. We have proven the structural parameter identifiability of our model in the case of age independent division rates. Using a set of experimental biological data, we have estimated the model parameters to fit the changes in the cell numbers in each layer during the early stages of follicle development.

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

Participants: Frédérique Clément [correspondant], Marie Postel [Sorbonne Universités].

Work in collaboration with Sylvie Schneider-Maunoury (Sorbonne Universités), 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. To understand 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 [43]. A special focus has been put on the population of intermediate progenitors (IPs), a transit amplifying progenitor type critically involved in the size of the final neuron pool. Our 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, has revealed a shortening of the neurogenic period associated with an increased influx of newborn IPs from apical progenitors at mid-neurogenesis. Additional information have been 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.

7.1.9. Advances in computational modeling approaches of pituitary gonadotropin signaling

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

Work in collaboration with Pascale Crépieux, Anne Poupon and Éric Reiter (INRA). We have reviewed thoroughly the state-of-the-art in computational modeling approaches of pituitary gonadotropin signaling [30]. Pituitary gonadotropins play an essential and pivotal role in the control of human and animal reproduction within the hypothalamic-pituitary-gonadal (HPG) axis. The computational modeling of pituitary gonadotropin signaling encompasses phenomena of different natures such as the dynamic encoding of gonadotropin secretion, and the intracellular cascades triggered by gonadotropin binding to their cognate receptors, resulting in a variety of biological outcomes. We have overviewed historical and ongoing issues in modeling and data analysis related to gonadotropin secretion in the field of both physiology and neuro-endocrinology. We have mentioned the different mathematical formalisms involved, their interest and limits. We have discussed open statistical questions in signal analysis associated with key endocrine issues. We have also reviewed recent advances in the modeling of the intracellular pathways activated by gonadotropins, which yields promising development for innovative approaches in drug discovery. The greatest challenge to be tackled in computational modeling of pituitary gonadotropin signaling is the embedding of gonadotropin signaling within its natural multiscale environment, from the single cell level, to the organic and whole HPG level. The development of modeling approaches of G protein-coupled receptor signaling, together with multicellular systems biology may lead to unexampled mechanistic understanding with critical expected fallouts in the therapeutic management of reproduction.

7.1.10. Structured cell population dynamics applied to the early development of ovarian follicles

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

The ovarian follicles are the basic anatomical and functional units of the ovaries, which are renewed from a quiescent pool all along reproductive life. Follicular development involves a finely tuned sequence of growth and maturation processes, involving complex cell dynamics. Understanding follicular development is a crucial issue for the management of reproduction in a clinical or breeding context, and for the preservation of endangered species. In their early stages of development, ovarian follicles are made up of a germ cell (oocyte), whose diameter increases steadily, and of surrounding proliferating somatic cells, which are layered in a globally spherical and compact structure. We have designed a modeling approach dedicated to the initiation phase of follicle development. The initiation phase is described by joint stochastic dynamics accounting for cell shape transitions (from a flattened to a cuboidal shape) and proliferation of reshaped cells. We have then derived the mean time elapsed before all cells have changed shapes and the corresponding increment in the total cell number, which is fitted to experimental data retrieved from primordial follicles (single layered follicle with only flattened cells) and primary follicles (single layered follicles with only cuboidal cells).

7.1.11. Newton-Krylov method for computing the cyclic steady states of evolution problems in non-linear mechanics

Participants: Ustim Khristenko, Patrick Le Tallec [correspondant].

This work is focused on the Newton-Krylov technique for computing the steady cyclic states of evolution problems in nonlinear mechanics with space-time periodicity conditions. This kind of problems can be faced, for instance, in the modeling of a rolling tire with a periodic tread pattern, where the cyclic state satisfies "rolling" periodicity condition, including shifts both in time and space. The Newton-Krylov method is a combination of a Newton nonlinear solver with a Krylov linear solver, looking for the initial state, which provides the space-time periodic solution. The convergence of the Krylov iterations is proved to hold in presence of an adequate preconditioner. After preconditioning, the Newton-Krylov method can be also considered as an observer-controller method, correcting the transient solution of the initial value problem after each period. Using information stored while computing the residual, the Krylov solver computation time becomes negligible with respect to the residual computation time. The method has been analyzed and tested on academic applications and compared with the standard evolution (fixed point) method. Finally, it has been implemented into the Michelin industrial code, applied to a full 3D rolling tire model.

7.1.12. Delayed feedback control method for computing the cyclic steady states of evolution problems

Participants: Ustim Khristenko, Patrick Le Tallec [correspondant].

This work is focused on fast techniques for computing the cyclic steady states of evolution problems in non-linear mechanics with space–time periodicity conditions. In industrial applications, in order to avoid the inversion of very large matrices, such a cyclic solution is usually computed as an asymptotic limit of the associated initial value problem with arbitrary initial data. However, when the relaxation time is high, convergence to the limit cycle can be very slow. In such cases nonetheless, one is not interested in the transient solution, but only in a fast access to the limit cycle. Thus, in this work we modify the problem, introducing the time-delayed feedback control, which is widely used for stabilization of unstable periodic orbits. In our framework it is applied to an initially stable system in order to accelerate its convergence to the limit cycle. Moreover, the control term, based on the space–time periodicity error, includes both shifts in time and in space. Our main result is the optimal form of the control term for a very general class of linear evolution problems, providing the fastest convergence to the cyclic solution, which has been further extended and studied in the non-linear case. Efficiency of the method increases with the problem's relaxation time. The method has been tested using academic applications and compared to the non-controlled asymptotic convergence as well as to the Newton–Krylov shooting algorithm. Finally, the method has been implemented into the Michelin industrial code, applied to a full 3D rolling tyre model.

7.2. Numerical Methods

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

Participants: Dominique Chapelle [correspondant], Philippe Moireau.

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. This work is accepted for publication in Acta Mathematicae Applicatae Sinica.

7.2.2. Efficient estimation of personalized biventricular mechanical function employing gradient-based optimization

Participant: Martin Genet [correspondant].

Individually personalized computational models of heart mechanics can be used to estimate important physiological and clinically-relevant quantities that are difficult, if not impossible, to directly measure in the beating heart. Here, we present a novel and efficient framework for creating patient-specific biventricular models using a gradient-based data assimilation method for evaluating regional myocardial contractility and estimating myofiber stress. These simulations can be performed on a regular laptop in less than 2 hours and produce excellent fit between measured and simulated volume and strain data through the entire cardiac cycle. By applying the framework using data obtained from 3 healthy human biventricles, we extracted clinically important quantities as well as explored the role of fiber angles on heart function. Our results show that steep fiber angles at the endocardium and epicardium are required to produce simulated motion compatible with measured strain and volume data. We also find that the contraction and subsequent systolic stresses in the right ventricle are significantly lower than that in the left ventricle. Variability of the estimated quantities with respect to both patient data and modeling choices are also found to be low. Because of its high efficiency, this framework may be applicable to modeling of patient specific cardiac mechanics for diagnostic purposes.

7.2.3. Equilibrated warping: Finite element image registration with finite strain equilibrium gap regularization

Participant: Martin Genet [correspondant].

In this work, we propose a novel continuum finite strain formulation of the equilibrium gap regularization for image registration. The equilibrium gap regularization essentially penalizes any deviation from the solution of a hyperelastic body in equilibrium with arbitrary loads prescribed at the boundary. It thus represents a regularization with strong mechanical basis, especially suited for cardiac image analysis. We describe the consistent linearization and discretization of the regularized image registration problem, in the framework of the finite elements method. The method is implemented using FEniCS & VTK, and distributed as a freely available python library. We show that the equilibrated warping method is effective and robust: regularization strength and image noise have minimal impact on motion tracking, especially when compared to strain-based regularization methods such as hyperelastic warping. We also show that equilibrated warping is able to extract main deformation features on both tagged and untagged cardiac magnetic resonance images.

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

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

7.2.5. A conservative penalisation strategy for the semi-implicit time discretisation of the incompressible elastodynamics equation

Participants: Federica Caforio [correspondant], Sébastien Imperiale.

The principal aim of this work is to provide an adapted numerical scheme for the approximation of elastic wave propagation in incompressible solids. We rely on high-order conforming finite element with mass lumping for space discretisation and implicit/explicit, second-order, energy-preserving time discretisation. The time step restriction only depends on the shear wave velocity and at each time step a Poisson problem must be solved to account for the incompressibility constraint that is imposed by penalisation techniques.

7.2.6. High-order discrete Fourier transform for the solution of the poisson equation

Participants: Federica Caforio [correspondant], Sébastien Imperiale.

The aim of this work is to propose a novel, fast, matrix-free solver for the Poisson problem discretised with High-Order Spectral Element Methods (HO-SEM). 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 frequency space. The solver proposed is endowed with several properties. First, it preserves the efficiency of standard FFT algorithm; then, the matrix storage is minimised; a pseudo- explicit Singular Value Decomposition (SVD) is used for the inversion of the symbols; finally, it can be easily extended to multiple dimensions and non-periodic boundary conditions. In particular, 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.

7.3. Inverse Problems

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

Participants: Sébastien Imperiale, Philippe Moireau [correspondant].

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 stabilization properties obtained from the use of the available measurements, hence allowing to still be able to reconstruct the unknown initial condition. This work is accepted with minor revision for publication in COCV.

7.4. Experimental Assessments

7.4.1. Mathematical modeling and experimental validation of flow through aortic valve

Participant: Radomir Chabiniok [correspondant].

Assessment of the valvular diseases by phase-contrast magnetic resonance imaging (MRI) has known limits due to limited spatial-temporal resolution of MRI and artifacts intrinsic to the method. This problem is addressed by the collaborative work of the Institute for Clinical and Experimental Medicine in Prague (IKEM, participants J. Tintera and R. Galabov) and the mathematical modeling group at the Czech Technical University in Prague (CTU, participants P. Paus, R. Fucik), additionally with the combined clinical cardiovascular MRI & modeling expertise of R. Chabiniok (Inria). A flow phantom was constructed at IKEM and used to perform an extensive experimental study targeted to capture the phenomena in valvular stenosis / regurgitation. The Mathematical modeling group at CTU then performed flow simulations by using the techniques of Lattice-Boltzmann method and their high-performance computing GPU implementations. This work is shedding light into possibly significant factors limiting the direct interpretation of PC MRI and opening the way into interaction of PC MRI data with mathematical model as a “smart filtering” of flow exam.

7.4.2. Skin multiscale mechanics

Participant: Jean-Marc Allain [correspondant].

Skin is a complex, multi-layered organ, with important functions in the protection of the body. The dermis provides structural support to the epidermal barrier, and thus has attracted a large number of mechanical studies. As the dermis is made of a mixture of stiff fibres embedded in a soft non-fibrillar matrix, it is classically considered that its mechanical response is based on an initial alignment of the fibres, followed by the stretching of the aligned fibres. Using a recently developed set-up combining multiphoton microscopy with mechanical assay, we imaged the fibres network evolution during dermis stretching. These observations, combined with a wide set of mechanical tests, allowed us to challenge the classical microstructural interpretation of the mechanical properties of the dermis: we observed a continuous alignment of the collagen fibres along the stretching. All our results can be explained if each fibre contributes by a given stress to the global response. This plastic response is likely due to inner sliding inside each fibre. The non-linear mechanical response is due to structural effects of the fibres network in interaction with the surrounding non-linear matrix. This multiscale interpretation explains our results on genetically-modified mice with a simple alteration of the dermis microstructure. Our previous works have led us to write this year one review article and one chapter of book on multiscale skin biomechanics, to be published next year.

7.4.3. Cornea biomechanics

Participants: Chloé Giraudet, Jean-Marc Allain [correspondant], Patrick Le Tallec.

Cornea is the outer part of the eye. It is a curved transparent organ, which gives 2/3 of the focalisation capacity of the eye. Microscopically, it is made mostly of collagen fibres (as skin) organised in cristal-like lamellae of few micrometers of height and a hundred micrometers in length and width. The lamellae are piled up in a plywood structure, creating a millimetre-thick tissue. Between the lamellae, some cells are present to repair and regenerate the tissue. However, this simple image of the organisation of the collagen is in fact too simple and a more complex heterogeneous organisation has been recently described, with in particular some striae (called the Vogt striae). In C. Giraudet’s PhD, we propose to explore the link between microstructure organisation of the collagen in the cornea and mechanical properties. To do so, we will first start by proposing an extension of classical mechanical models (such as Holzapfel’s law or others) to the specific case of the cornea. This model will be tested against mechanical assays made under advanced optical microscopes to test first if the model can correctly predict the strain field in volume, and secondly if it correctly predicts the evolution of the lamellae microstructure at different stretch levels. At the moment, we have developed the tools to mechanically test the cornea, but also to build a finite element simulation using the real shape of the cornea we are looking at.

7.4.4. Multiscale properties of the passive cardiac muscle

Participants: Nicole Tueni, Jean-Marc Allain [correspondant], Martin Genet.

We are interested in understanding the effect of the remodelling of cardiac tissues after a disease. Cardiac tissues are mostly made of muscle cells. They can remodel themselves in response to an alteration of their normal response by modifying the sizes and the geometries of the cells in the tissue. Nowadays, we are able to describe the active and passive response of a cardiac tissue, assuming we know the main orientation of the cells inside. However, we do not have models which include explicitly the microstructural cellular organization. Such complex models will be strongly beneficial to determine the consequences of local alterations of the muscle behaviour. In N. Tueni's PhD, we are investigating this multi-scale relationship. To do so, we are imaging the organization at the microscale, while measuring the mechanical properties. These results will be the building block to test and develop mechanical models of the cardiac tissues.

7.4.5. Mechano-perception at the cell level

Participant: Jean-Marc Allain [correspondant].

All cells and organisms experience mechanical forces. Plants along their life are submitted from their environment to long lasting sustained stresses and to recurrent cyclic loading/unloading due to wind or water stream. Mechanical stimulations induce short-term cellular responses, leading to mechanoresponsive gene activation followed by long-term responses permitting structural reinforcement at the whole-plant level. We show that the Mechanosensitive channel Small conductance-Like 10 (MSL10) contributes to oscillation perception at the cell level. This channel responds to pulsed membrane stretching with rapid activation and relaxation. Furthermore, oscillatory pressure stimulation modulates its activity, with increased open probability upon oscillatory than during sustained stimulation. Combined with the adequate localization of MSL10 in plant shoot and leaves, its ability to detect oscillatory deformation at the molecular-scale is relevant for a function of this channel in oscillatory perception in plant.

7.5. Clinical Applications

7.5.1. Exploring kinetic energy as a new marker of cardiac function in the single ventricle circulation

Participants: Radomir Chabiniok [correspondant], Tarique Hussain [ToFMOD].

Ventricular volumetric ejection fraction (VV EF) is often normal in patients with single ventricle circulations despite them experiencing symptoms related to circulatory failure. We sought to determine if kinetic energy (KE) could be a better marker of ventricular performance. KE was prospectively quantified using four-dimensional flow MRI in 41 patients with a single ventricle circulation (aged 0.5-28 yr) and compared with 43 healthy volunteers (aged 1.5-62 yr) and 14 patients with left ventricular (LV) dysfunction (aged 28-79 yr). Intraventricular end-diastolic blood was tracked through systole and divided into ejected and residual blood components. Two ejection fraction (EF) metrics were devised based on the KE of the ejected component over the total of both the ejected and residual components using 1) instantaneous peak KE to assess KE EF or 2) summating individual peak particle energy (PE) to assess PE EF. KE metrics are markers of healthy cardiac function. PE EF may be useful in grading dysfunction. The work was published in Journal of Applied Physiology (J Appl Physiol 125: 889-900, 2018), [29]. The work represents a collaboration with King's College London (J. Wong, K. Pushparajah, R. Razavi) and with UT Southwestern Dallas (T. Hussain, the member of Inria Associate team ToFMOD).

7.5.2. Using a patient-specific biomechanical cardiovascular model to estimate continuously Left Ventricular Pressure Volume Loop: A proof of concept study

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

Pressure Volume loops (PV loops) could contribute to optimise haemodynamic managements. While the invasiveness of PV loop acquisition prevents it from being routinely used during surgery, cardiovascular modelling could represent an alternative. Using continuous recording of aortic pressure and flow, we aimed at calibrating a patient-specific model and at interpreting the simulated PV loop during administration of noradrenaline (NOR). This study is the first to allow continuous PV loop monitoring during general anaesthesia. The work was pursued in the collaboration with Lariboisiere Hospital in Paris (A. Le Gall and F. Vallée, both dually affiliated at Inria and at AP-HP, "poste d'accueil").

7.5.3. Augmenting the interpretation of cardiac MRI by biomechanical modeling: Application to Tetralogy of Fallot

Participants: Marija Gusseva, Philippe Moireau, Tarique Hussain [ToFMod], Gerald Greil [ToFMod], Animesh Tandon [ToFMOD], Dominique Chapelle, Radomir Chabiniok [correspondant].

The particularity of the mixed-valve disease – pulmonary regurgitation often combined with a stenosis – requested to extend our model-representation of the valve to allow the backflow during the heart relaxation. For each patient, biomechanical models of their left and right ventricles (LV, RV) were set up. These models then allowed to investigate the functional properties of dilated right ventricles (RV) with incompetent pulmonary valves and of the pulmonary circulation, properties not directly visible in the clinical data. In particular, immediately after deploying the new valve we could observe a decrease of RV contractility by 15%, while the output of RV into pulmonary circulation has increased. This suggests a positive immediate outcome, as the energy needs for function of RV will decrease. The higher cardiac output also suggests an increase of the filling of LV (preload), which could contribute to an improvement of LV function. The model also uncovered a decrease of resistance in the pulmonary circulation. This very preliminary result might suggest some pathophysiological changes, which are typically not thought of in clinics.

This work is pursued under the objectives of the Inria Associate Team ToFMod (T. Hussain, G. Greil, A. Tandon are members of ToFMOD and affiliated at UT Southwestern Medical Center Dallas, USA), the work was accepted for a conference of International Society of Magnetic Resonance in Medicine 2018 and is in preparation for publication.

7.5.4. Longitudinal study of ventricular remodeling and reverse-remodeling in tetralogy of Fallot patients using CMR coupled with biomechanical modelling

Participants: Marija Gusseva, Tarique Hussain [ToFMod], Animesh Tandon [ToFMod], Dominique Chapelle, Radomir Chabiniok [correspondant].

A preliminary study was performed with the patient-specific models for RV and pulmonary circulations set up from three datasets including the 6-months post-PVR follow-up exams obtained in late 2018 from King's College London. Clinical data analyses show a positive result of pulmonary replacement therapy (PVR) and normalization of the RV size, i.e. the so-called reverse-remodeling of the pathologically dilated RV, in all three patients. The biomechanical modeling suggests a further reduction of the active stress needed to be developed by RV (contractility), i.e. a long-term unloading of the previously overloaded ventricle.

This work is pursued under the objectives of the Inria Associate Team ToFMOD (T. Hussain, A. Tandon are members of ToFMOD and affiliated at UT Southwestern Medical Center Dallas, USA). The main partner in this task is King's College London ("Other Participant" in the ToFMOD Associate team, K. Pushparajah, M. Jones, S. Qureshi) who provided unique clinical data of patients with a long-term follow-up after PVR. The work was submitted to the conference of International Society of Magnetic Resonance in Medicine 2019 – the world-wide major scientific & clinical event when MR data are involved.

7.5.5. Optical flow-based non-rigid registration of cardiac MR images

Participant: Radomir Chabiniok [correspondant].

This work deals with non-rigid registration of cardiac MR images, particularly the MOLLI sequences. MOLLI sequence consists of 11 heart images acquired over 17 cardiac cycles. The images of MOLLI sequence are used for pixel-wise estimation of T1 relaxation time values. In this case the registration is necessary to correct the deformations that occur because of the patient's imperfect breath-holding during the acquisition. The main characteristics of the MOLLI sequence is the evolving intensity of the tissues and also large variations of the image contrast. This characteristics of the sequence make the registration process challenging and make the use of intensity-based registration method impossible. For this purpose, we propose a method based on optical flow, using information obtained by image segmentation. The first step of the registration process, is segmentation of the regions of interest, using the level set method. The segmented objects are represented by distance maps. The transformation between original images is determined by applying the optical flow method to the distance maps. The registration process is independent of the varying intensity and takes into account only the shape and position of the segmented areas, such as the myocardium or the ventricles. The implementation of the proposed method is described and the method is tested on several MOLLI sequences. The results are compared to the results of methods based on maximisation of mutual information, and the proposed method performs better for the images with significant changes in intensity.

The work represents a collaborative project with Institute for Clinical and Experimental Medicine (IKEM) Prague (J. Tintera) and with Czech Technical University in Prague (K. Solovska, T. Oberhuber).

7.5.6. *Quantification of biventricular strains in heart failure with preserved ejection fraction using hyperelastic warping method*

Participant: Martin Genet.

Heart failure (HF) imposes a major global health care burden on society and suffering on the individual. About 50% of HF patients have preserved ejection fraction (HFpEF). More intricate and comprehensive measurement-focused imaging of multiple strain components may aid in the diagnosis and elucidation of this disease. Here, we describe the development of a semi-automated hyperelastic warping method for rapid comprehensive assessment of biventricular circumferential, longitudinal, and radial strains that is physiological meaningful and reproducible. We recruited and performed cardiac magnetic resonance (CMR) imaging on 30 subjects [10 HFpEF, 10 HF with reduced ejection fraction patients (HFrEF) and 10 healthy controls]. In each subject, a three-dimensional heart model including left ventricle (LV), right ventricle (RV), and septum was reconstructed from CMR images. The hyperelastic warping method was used to reference the segmented model with the target images and biventricular circumferential, longitudinal, and radial strain–time curves were obtained. The peak systolic strains are then measured and analyzed in this study. The ROC analysis indicated LV peak systolic circumferential strain to be the most sensitive marker for differentiating HFpEF from healthy controls. Our results suggest that the hyperelastic warping method with the CMR-derived strains may reveal subtle impairment in HF biventricular mechanics, in particular despite a “normal” ventricular ejection fraction in HFpEF.

7.5.7. *Extra corporeal life support for cardiac arrest patients with post-cardiac arrest syndrome: the ECCAR study*

Participant: Arthur Le Gall.

Purpose: Post-Cardiac Arrest Shock (PCAS) occurring after resuscitated cardiac arrest (CA), is a main cause of early death. Extra-Corporeal Life Support (ECLS) could be useful pending recovery of myocardial failure. We aimed to describe our PCAS population, and factors associated with ECLS initiation. Materials and Methods: This analysis included 924 patients admitted in two intensive care units (ICU) between 2005 and 2014 for CA and PCAS, and, of those patients, 43 patients for whom an ECLS was initiated. Neurological and ECLS-related outcomes were gathered retrospectively. Conclusions: ECLS, as a salvage therapy for PCAS, could represent an acceptable alternative for highly selected patients.

7.5.8. *Evaluation of cardiac output variations with the peripheral pulse pressure to mean arterial pressure ratio.*

Participant: Arthur Le Gall.

Cardiac output (CO) optimisation during surgery reduces post-operative morbidity. Various methods based on pulse pressure analysis have been developed to overcome difficulties to measure accurate CO variations in standard anaesthetic settings. Several of these methods include, among other parameters, the ratio of pulse pressure to mean arterial pressure (PP/MAP). The aim of this study was to evaluate whether the ratio of radial pulse pressure to mean arterial pressure (ΔPPrad/MAP) could track CO variations (Δ CO) induced by various therapeutic interventions such as fluid infusions and vasopressors boluses [phenylephrine (PE), norepinephrine (NA) or ephedrine (EP)] in the operating room. Trans-oesophageal Doppler signal and pressure waveforms were recorded in patients undergoing neurosurgery. CO and PPrad/MAP were recorded before and after fluid challenges, PE, NA and EP bolus infusions as medically required during their anaesthesia. ΔPPrad/MAP tracked ΔCO variations during PE and NA vasopressor challenges. However, after positive fluid challenge or EP boluses, ΔPPrad/MAP was not as performant to track ΔCO which could make the use of this ratio difficult in current clinical practice.

7.5.9. *Perioperative management of patients with coronary artery disease undergoing non-cardiac surgery: Summary from the French Society of Anaesthesia and Intensive Care Medicine 2017 convention*

Participant: Arthur Le Gall.

This review summarises the specific stakes of preoperative, intraoperative, and postoperative periods of patients with coronary artery disease undergoing non-cardiac surgery. All practitioners involved in the perioperative management of such high cardiac risk patients should be aware of the modern concepts expected to decrease major adverse cardiac events and improve short- and long-term outcomes. A multidisciplinary approach via a functional heart team including anaesthesiologists, cardiologists and surgeons must be encouraged. Rational and algorithm-guided management of those patients should be known and implemented from preoperative to postoperative period.

PARIETAL Project-Team

7. New Results

7.1. Reducing the number of samples in spatiotemporal dMRI acquisition design

Acquisition time is a major limitation in recovering brain white matter microstructure with diffusion magnetic resonance imaging. The aim of this work is to bridge the gap between growing demands on spatio-temporal resolution of diffusion signal and the real-world time limitations. We introduce an acquisition scheme that reduces the number of samples under adjustable quality loss. Finding a sampling scheme that maximizes signal quality and satisfies given time constraints is NP-hard. Therefore, a heuristic method based on genetic algorithm is proposed in order to find sub-optimal solutions in acceptable time. The analyzed diffusion signal representation is defined in the $q\tau$ space, so that it captures both spacial and temporal phenomena. The experiments on synthetic data and in vivo diffusion images of the C57Bl6 wild-type mouse corpus callosum reveal the superiority of the proposed approach over random sampling and even distribution in the $q\tau$ space. The use of genetic algorithm allows to find acquisition parameters that guarantee high signal reconstruction accuracy under given time constraints. In practice, the proposed approach helps to accelerate the acquisition for the use of q-dMRI signal representation.

More information can be found in [12]

7.2. Robust EEG-based cross-site and cross-protocol classification of states of consciousness

Determining the state-of-consciousness in patients with disorders-of-consciousness (DOC) is a challenging practical and theoretical problem. Recent findings suggest that multiple markers of brain activity extracted from the electroencephalogram (EEG) may index the state of consciousness in the human brain. Furthermore, machine learning has been found to optimize their capacity to discriminate different states of consciousness in clinical practice. However, it is unknown how dependable these EEG-markers are in the face of signal variability due to different EEG-configurations, EEG-protocols and subpopulations from different centers encountered in practice. In our recent paper [11] we addressed the following questions: What is the impact of the EEG configuration (selection of sensors, duration of EEG used)? Do models based on current EEG-markers achieve prospective generalization on independent data from other EEG protocols and other hospitals? Are single markers sufficiently powerful and when does multivariate classification provide the clearest advantage? For summary of methods and approahc see Figure4 . Our results highlight the effectiveness of classical well-studied EEG-signatures such as alpha [8-12Hz] and theta [5-7Hz] frequency band oscillations for detecting consciousness when combined with machine learning. While univariate predictive models achieved good performance, multivariate models showed better generalization capacity and increased robustness to different types of noise while mitigating the impact of the EEG-configuration. Our findings suggest that pooling data over multiple centers for predictive modeling of DOC is a concrete possibility and can become a promising alley for the field of cognitive neurology.

7.3. A deep learning architecture for temporal sleep stage classification using multivariate and multimodal time series

Sleep stage classification constitutes an important preliminary exam in the diagnosis of sleep disorders. It is traditionally performed by a sleep expert who assigns to each 30 s of signal a sleep stage, based on the visual inspection of signals such as electroencephalograms (EEG), electrooculograms (EOG), electrocardiograms (ECG) and electromyograms (EMG). We introduce here the first deep learning approach for sleep stage

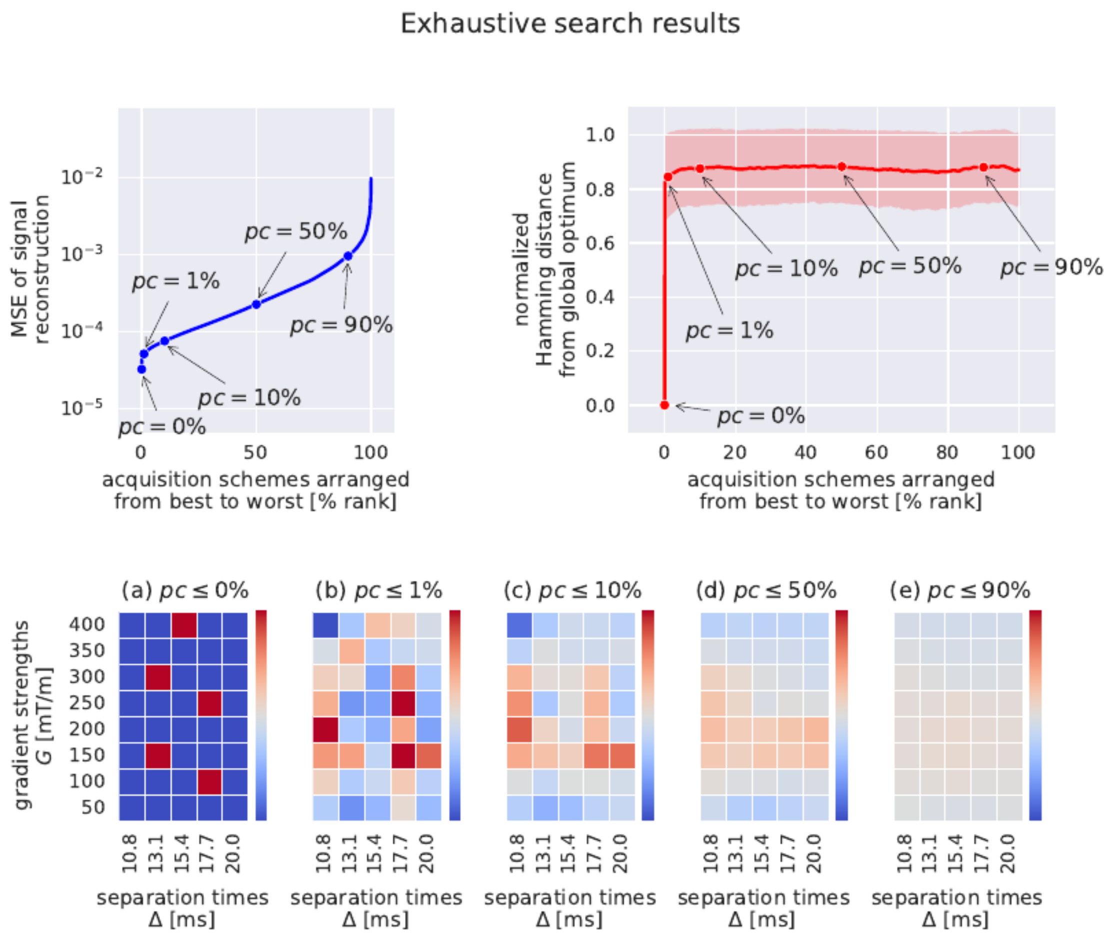


Figure 3. Exhaustive search results of the optimization by shells for the in silico experiment with nmax = 100. The plots at the top present all the 658,008 feasible acquisition schemes arranged from best to worst, illustrating the mean squared errors (MSEs) of signal reconstruction (top-left plot) and the normalized Hamming distances from the global optimum ± 1 standard deviation (top-right). In order to visualize the analyzed (G, Δ) parameter space, the percentiles pc = 0%, 1%, 10%, 50%, 90% are annotated on both plots, showing respectively the global optimum, the top 1% solutions, the top 10% solutions, etc. The corresponding cumulative averages of acquisition schemes are depicted in the heat maps at the bottom. The colors reflect the likelihood of a given (G, Δ) pair in the scheme. The heat maps for pc ≤ 0% and pc ≤ 1% represent, respectively, the global optimum and its proximity. The interval between pc = 10% and pc = 90% contains a huge spectrum of schemes with similar MSEs and almost equally large distances from the global optimum.

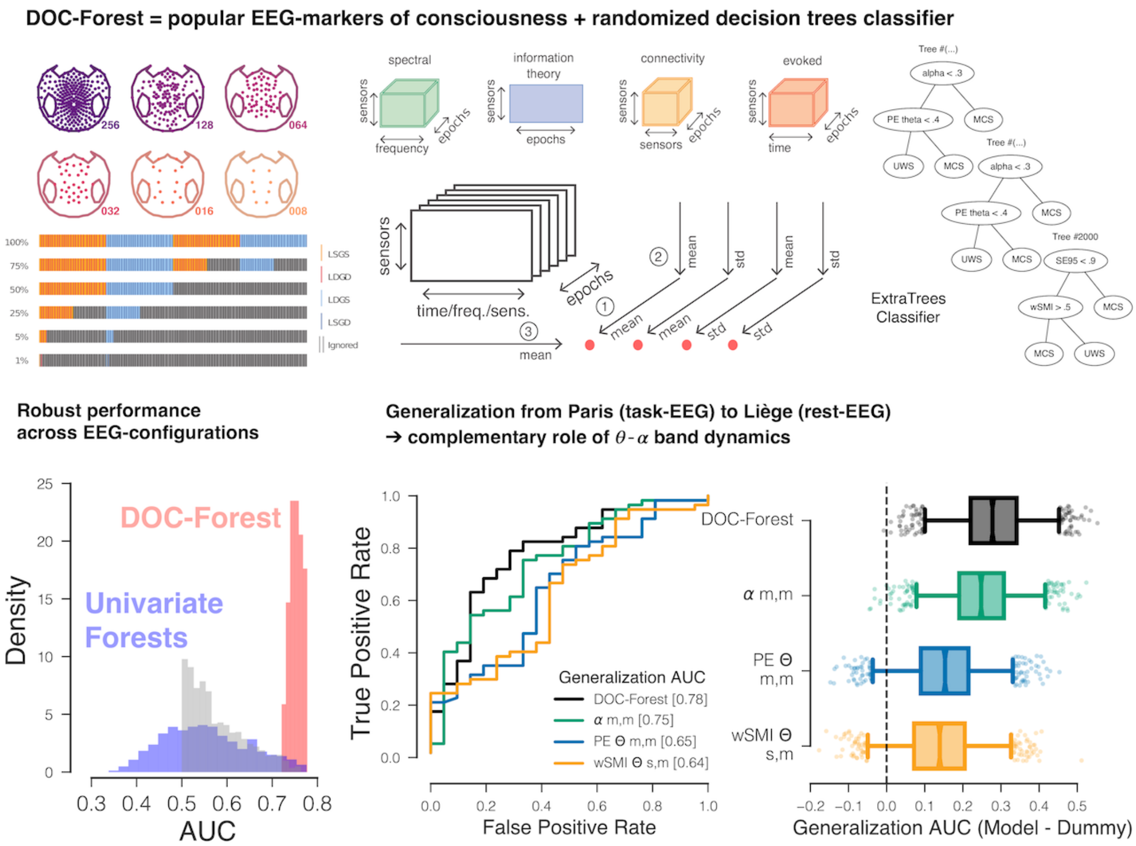


Figure 4. We probed the robustness and validity of EEG-markers of consciousness. Using the robust Extra-Trees algorithm (Geurts, Ernst, & Wehenkel, 2006) we developed a classifier trained to differentiate UWS from MCS patients. This classifier (named "DOC-forest") was trained and tested using 28 potential EEG-markers of consciousness (112 features) from 249 patients recorded at the Paris Pitié-Salpêtrière and 78 patients from the University Hospital of Liège. We used the MNE-Python software for EEG processing and the scikit-learn package for machine learning. Our results show that optimally combining multiple EEG-markers of states of consciousness using machine learning enables robust generalization across EEG-configurations, EEG-protocols and sites. Our recipe for extracting biomarkers is available on Github: https://nice-tools.github.io/nice. For a neuroscientific discussion of our work see the accompanying commentary article by Sokoliuk and Cruse (https://doi.org/10.1093/brain/awy267).

classification that learns end-to-end without computing spectrograms or extracting hand-crafted features, that exploits all multivariate and multimodal Polysomnography (PSG) signals (EEG, EMG and EOG), and that can exploit the temporal context of each 30 s window of data. For each modality the first layer learns linear spatial filters that exploit the array of sensors to increase the signal-to-noise ratio, and the last layer feeds the learnt representation to a softmax classifier. Our model is compared to alternative automatic approaches based on convolutional networks or decisions trees. Results obtained on 61 publicly available PSG records with up to 20 EEG channels demonstrate that our network architecture yields state-of-the-art performance. Our study reveals a number of insights on the spatio-temporal distribution of the signal of interest: a good trade-off for optimal classification performance measured with balanced accuracy is to use 6 EEG with 2 EOG (left and right) and 3 EMG chin channels. Also exploiting one minute of data before and after each data segment offers the strongest improvement when a limited number of channels is available. As sleep experts, our system exploits the multivariate and multimodal nature of PSG signals in order to deliver state-of-the-art classification performance with a small computational cost.

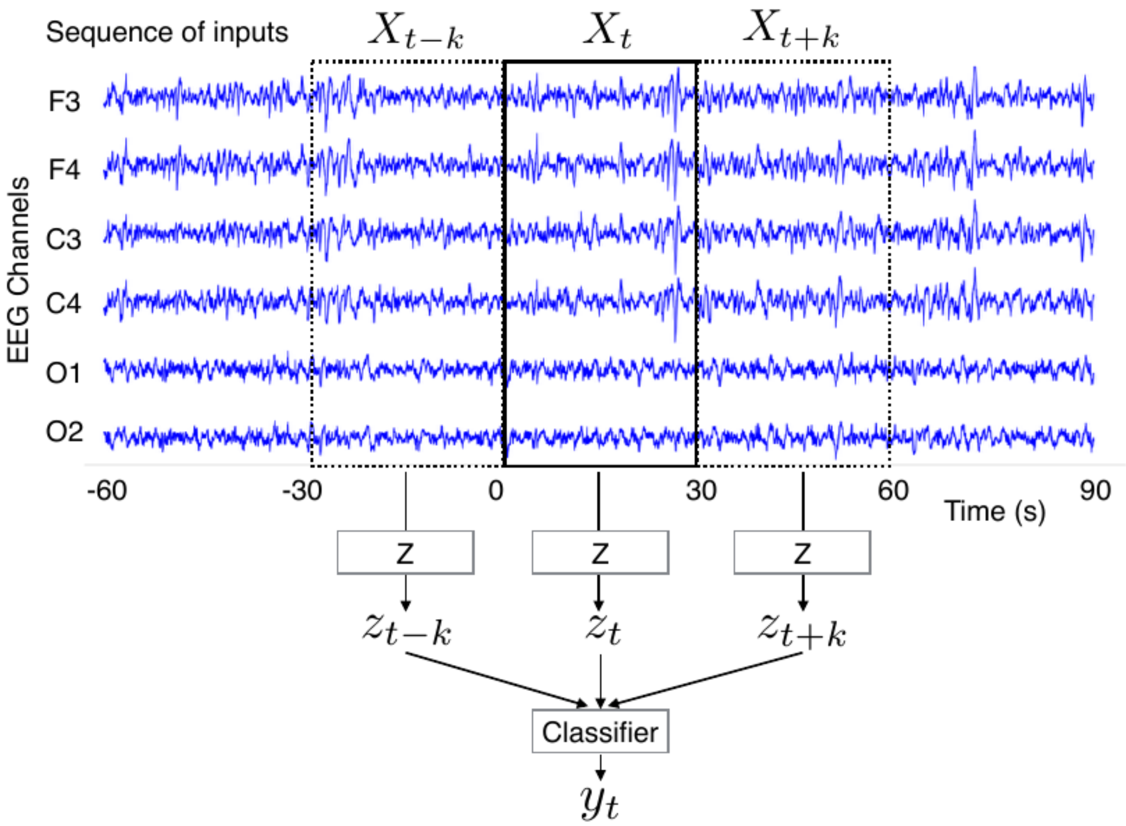


Figure 5. Time distributed architecture to process a sequence of inputs $S_t^k = \{X_{t-k}, \cdots, X_t, \cdots, X_{t+k}\}$ with k = 1. X_k stands for the multivariate input data over 30 s that is fed into the feature extractor Z. Features are extracted from consecutive 30 s samples: X_{t-k}, ..., X_t, ..., X_{t+k}. Then the obtained features are aggregated $[z_{t-k}, \cdots, z_t, \cdots, z_{t+k}]$. The resulting aggregation of features is finally fed into a classifier to predict the label y_t associated with the sample X_t.

More information can be found in [8].

7.4. Individual Brain Charting, a high-resolution fMRI dataset for cognitive mapping

Functional Magnetic Resonance Imaging (fMRI) has furthered brain mapping on perceptual, motor, as well as higher-level cognitive functions. However, to date, no data collection has systematically addressed the functional mapping of cognitive mechanisms at a fine spatial scale. The Individual Brain Charting (IBC) project stands for a high-resolution multi-task fMRI dataset that intends to provide the objective basis toward a comprehensive functional atlas of the human brain. The data refer to a cohort of 12 participants performing many different tasks. The large amount of task-fMRI data on the same subjects yields a precise mapping of the underlying functions, free from both inter-subject and inter-site variability. The present article gives a detailed description of the first release of the IBC dataset. It comprises a dozen of tasks, addressing both low- and high-level cognitive functions. This openly available dataset is thus intended to become a reference for cognitive brain mapping.

More information can be found in [25]

7.5. Atlases of cognition with large-scale brain mapping

To map the neural substrate of mental function, cognitive neuroimaging relies on controlled psychological manipulations that engage brain systems associated with specific cognitive processes. In order to build comprehensive atlases of cognitive function in the brain, it must assemble maps for many different cognitive processes, which often evoke overlapping patterns of activation. Such data aggregation faces contrasting goals: on the one hand finding correspondences across vastly different cognitive experiments, while on the other hand precisely describing the function of any given brain region. Here we introduce a new analysis framework that tackles these difficulties and thereby enables the generation of brain atlases for cognitive function. The approach leverages ontologies of cognitive concepts and multi-label brain decoding to map the neural substrate of these concepts. We demonstrate the approach by building an atlas of functional brain organization based on 30 diverse functional neuroimaging studies, totaling 196 different experimental conditions. Unlike conventional brain mapping, this functional atlas supports robust reverse inference: predicting the mental processes from brain activity in the regions delineated by the atlas. To establish that this reverse inference is indeed governed by the corresponding concepts, and not idiosyncrasies of experimental designs, we show that it can accurately decode the cognitive concepts recruited in new tasks. These results demonstrate that aggregating independent task-fMRI studies can provide a more precise global atlas of selective associations between brain and cognition.

More information can be found in [28].

7.6. Celer: a Fast Solver for the Lasso with Dual Extrapolation

Convex sparsity-inducing regularizations are ubiquitous in high-dimensional machine learning, but solving the resulting optimization problems can be slow. To accelerate solvers, state-of-the-art approaches consist in reducing the size of the optimization problem at hand. In the context of regression, this can be achieved either by discarding irrelevant features (screening techniques) or by prioritizing features likely to be included in the support of the solution (working set techniques). Convex duality comes into play at several steps in these techniques. Here, we propose an extrapolation technique starting from a sequence of iterates in the dual that leads to the construction of improved dual points. This enables a tighter control of optimality as used in stopping criterion, as well as better screening performance of Gap Safe rules. Finally, we propose a working set strategy based on an aggressive use of Gap Safe screening rules. Thanks to our new dual point construction, we show significant computational speedups on multiple real-world problems compared to alternative state-of-the-art coordinate descent solvers.

More information can be found in [54]. Code can be found at https://mathurinm.github.io/celer/.

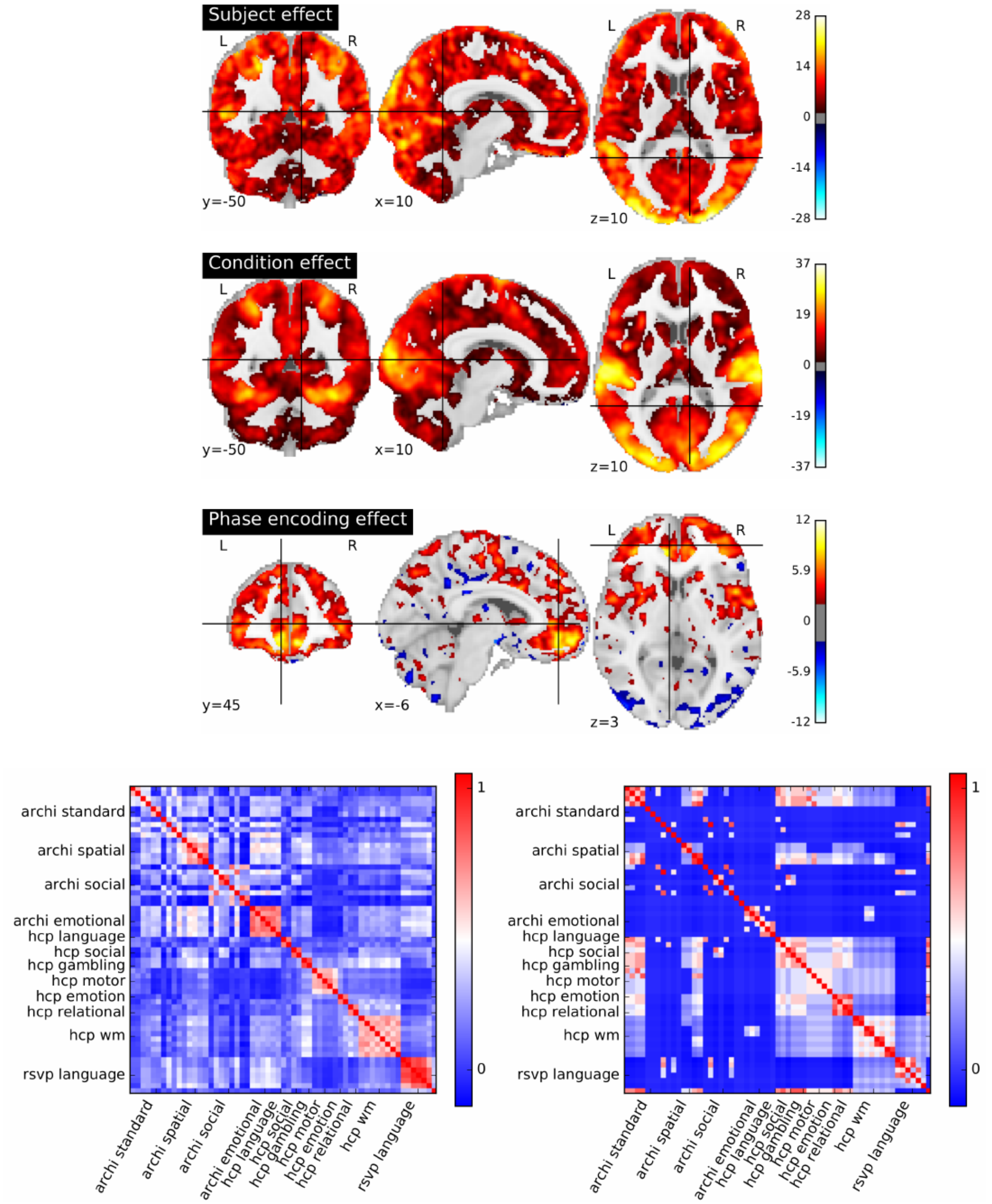


Figure 6. Overview of information conveyed by activation maps resulting from a first-level analysis. (top) Global effects of experimental subject condition, and phase-encoding direction. A per-voxel ANOVA breaks the variance of the set of brain maps into subject, experimental condition, and phase-encoding direction values. All maps are given in z-scale and thresholded at an FDR level of 0.05. (Bottom) Focusing on condition effect, the similarity between condition-related maps, averaged across subjects (left) is clearly related to the dissimilarity of the conditions, when these are characterized in terms of the Cognitive Atlas (right).

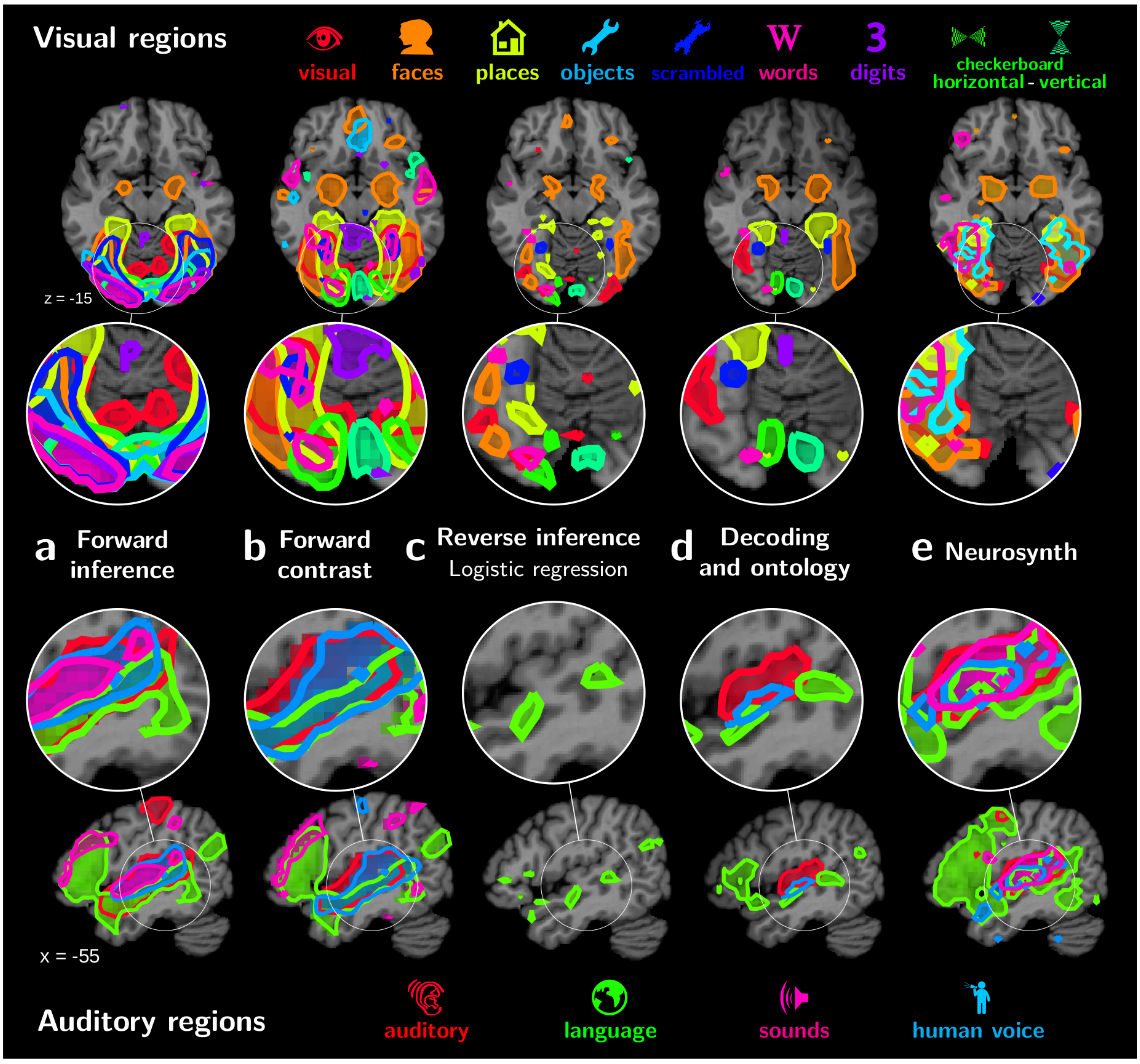


Figure 7. Different functional atlases – Regions outlined using different functional mapping approaches, from left to right: a. forward term mapping; b. forward inference with ontology contrasts (standard analysis); c. reverse inference with logistic regression; d. NeuroSynth reverse inference; and e. our approach, mapping with decoding and an ontology. The top part shows visual regions, and the lower one auditory regions in the left hemisphere. Forward term mapping outlines overlapping regions, as brain responses capture side effects such as the stimulus modality: for visual and auditory regions every cognitive term is represented in the corresponding primary cortex. Forward mapping using contrasts removes the overlap in primary regions, but a large overlap persists in mid-level regions, as control conditions are not well matched across studies. Standard reverse inference, specific to a term, creates overly sparse regions though with little overlap. Reverse inference with Neurosynth also displays large overlap in mid-level regions. Finally, ontology-based decoding maps recover known functional areas the visual and auditory cortices.

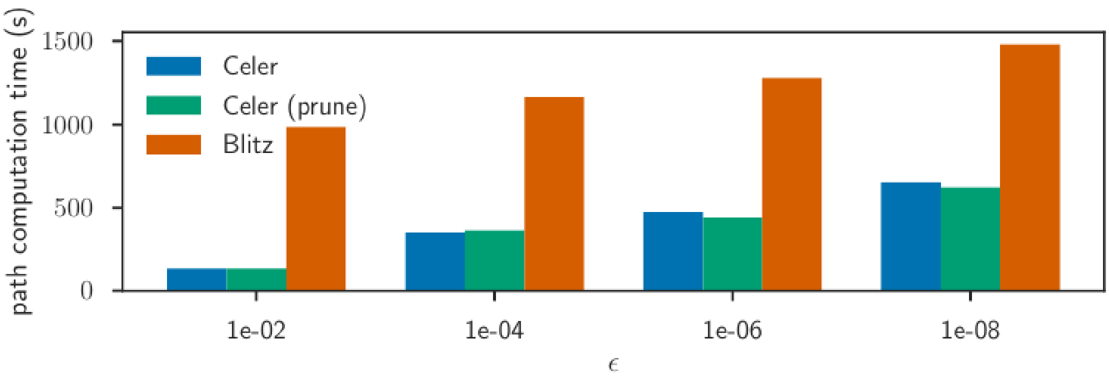


Figure 8. Times to solve the Lasso path to precision ϵ for 100 values of λ, from λ_{max} to $\lambda_{max}/100$, on the Finance data. CELER outperforms BLITZ . Both safe and prune versions behave similarly.

7.7. Multivariate Convolutional Sparse Coding for Electromagnetic Brain Signals

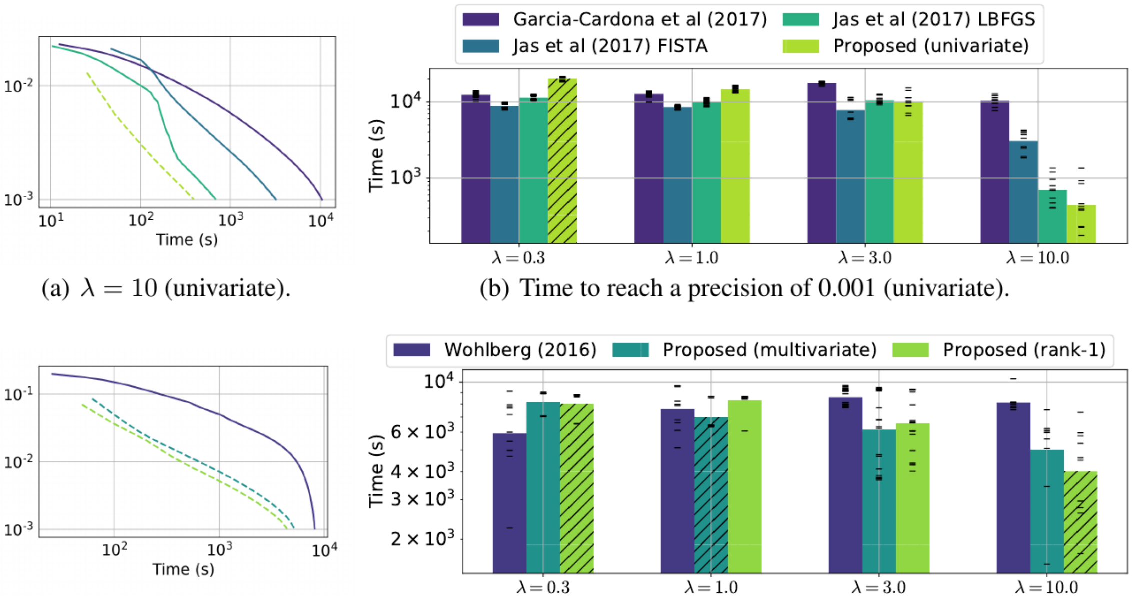
Frequency-specific patterns of neural activity are traditionally interpreted as sustained rhythmic oscillations, and related to cognitive mechanisms such as attention, high level visual processing or motor control. While alpha waves (8–12 Hz) are known to closely resemble short sinusoids, and thus are revealed by Fourier analysis or wavelet transforms, there is an evolving debate that electromagnetic neural signals are composed of more complex waveforms that cannot be analyzed by linear filters and traditional signal representations. In this work, we propose to learn dedicated representations of such recordings using a multivariate convolutional sparse coding (CSC) algorithm. Applied to electroencephalography (EEG) or magnetoencephalography (MEG) data, this method is able to learn not only prototypical temporal waveforms, but also associated spatial patterns so their origin can be localized in the brain. Our algorithm is based on alternated minimization and a greedy coordinate descent solver that leads to state-of-the-art running time on long time series. To demonstrate the implications of this method, we apply it to MEG data and show that it is able to recover biological artifacts. More remarkably, our approach also reveals the presence of non-sinusoidal mu-shaped patterns, along with their topographic maps related to the somatosensory cortex.

More information can be found in [52]. Code can be found at https://alphacsc.github.io/.

7.8. Stochastic Subsampling for Factorizing Huge Matrices

We present a matrix-factorization algorithm that scales to input matrices with both huge number of rows and columns. Learned factors may be sparse or dense and/or non-negative, which makes our algorithm suitable for dictionary learning, sparse component analysis, and non-negative matrix factorization. Our algorithm streams matrix columns while subsampling them to iteratively learn the matrix factors. At each iteration, the row dimension of a new sample is reduced by subsampling, resulting in lower time complexity compared to a simple streaming algorithm. Our method comes with convergence guarantees to reach a stationary point of the matrix-factorization problem. We demonstrate its efficiency on massive functional Magnetic Resonance Imaging data (2 TB), and on patches extracted from hyperspectral images (103 GB). For both problems, which involve different penalties on rows and columns, we obtain significant speed-ups compared to state-of-the-art algorithms.

More information can be found in [24].



(a) $\lambda = 10$ (univariate).

(b) Time to reach a precision of 0.001 (univariate).

(c) $\lambda = 10$ (multivariate).

(d) Time to reach a precision of 0.001 (multivariate).

Figure 9. Comparison of state-of-the-art univariate (a, b) and multivariate (c, d) methods with our approach. (a) Convergence plot with the objective function relative to the obtained minimum, as a function of computational time. (b) Time taken to reach a relative precision of 10^{-3}, for different regularization parameters λ. (c, d) Same as (a, b) in the multivariate setting P=5.

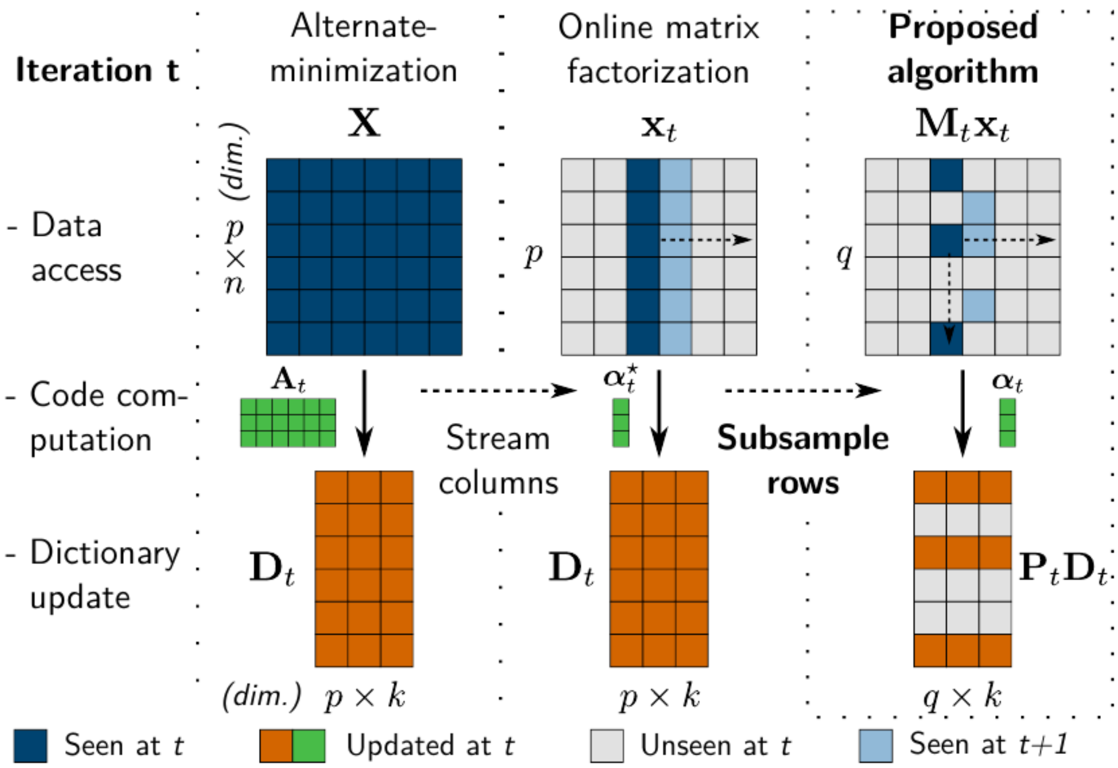


Figure 10. Stochastic subsampling further improves online matrix factorizationhandle datasets with large number of columns and rows. X is the input $p \times n$ matrix, D_t and A_t are respectively the dictionary and code at time t.

7.9. Text to brain: predicting the spatial distribution of neuroimaging observations from text reports

Despite the digital nature of magnetic resonance imaging, the resulting observations are most frequently reported and stored in text documents. There is a trove of information untapped in medical health records, case reports, and medical publications. In this paper, we propose to mine brain medical publications to learn the spatial distribution associated with anatomical terms. The problem is formulated in terms of minimization of a risk on distributions which leads to a least-deviation cost function. An efficient algorithm in the dual then learns the mapping from documents to brain structures. Empirical results using coordinates extracted from the brain-imaging literature show that i) models must adapt to semantic variation in the terms used to describe a given anatomical structure, ii) voxel-wise parameterization leads to higher likelihood of locations reported in unseen documents, iii) least-deviation cost outperforms least-square. As a proof of concept for our method, we use our model of spatial distributions to predict the distribution of specific neurological conditions from text-only reports.

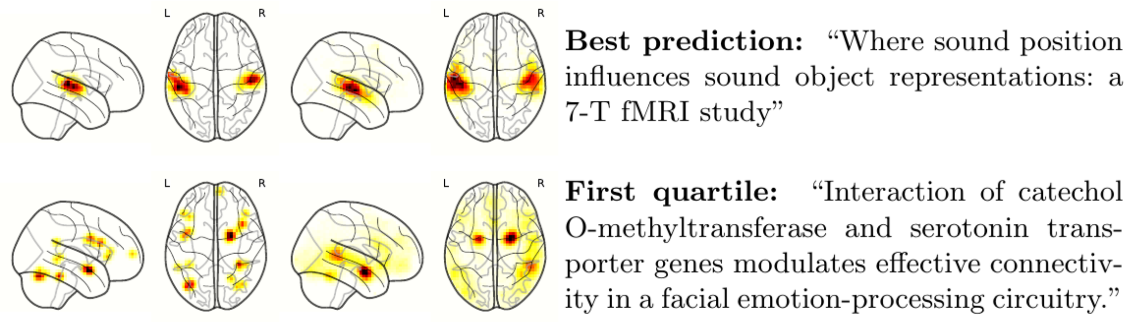


Figure 11. True probability density function (estimated with kernel density estimator) and the prediction for the articles which obtained respectively the best and the first- quartile scores.

More information can be found in [37].

7.10. Similarity encoding for learning with dirty categorical variables

For statistical learning, categorical variables in a table are usually considered as discrete entities and encoded separately to feature vectors, e.g., with one-hot encoding. "Dirty" non-curated data gives rise to categorical variables with a very high cardinality but redundancy: several categories reflect the same entity. In databases, this issue is typically solved with a deduplication step. We show that a simple approach that exposes the redundancy to the learning algorithm brings significant gains. We study a generalization of one-hot encoding, similarity encoding, that builds feature vectors from similarities across categories. We perform a thorough empirical validation on non-curated tables, a problem seldom studied in machine learning. Results on seven real-world datasets show that similarity encoding brings significant gains in prediction in comparison with known encoding methods for categories or strings, notably one-hot encoding and bag of character n-grams. We draw practical recommendations for encoding dirty categories: 3-gram similarity appears to be a good choice to capture morphological resemblance. For very high-cardinality, dimensionality reduction significantly reduces the computational cost with little loss in performance: random projections or choosing a subset of prototype categories still outperforms classic encoding approaches.

More information can be found in [7].

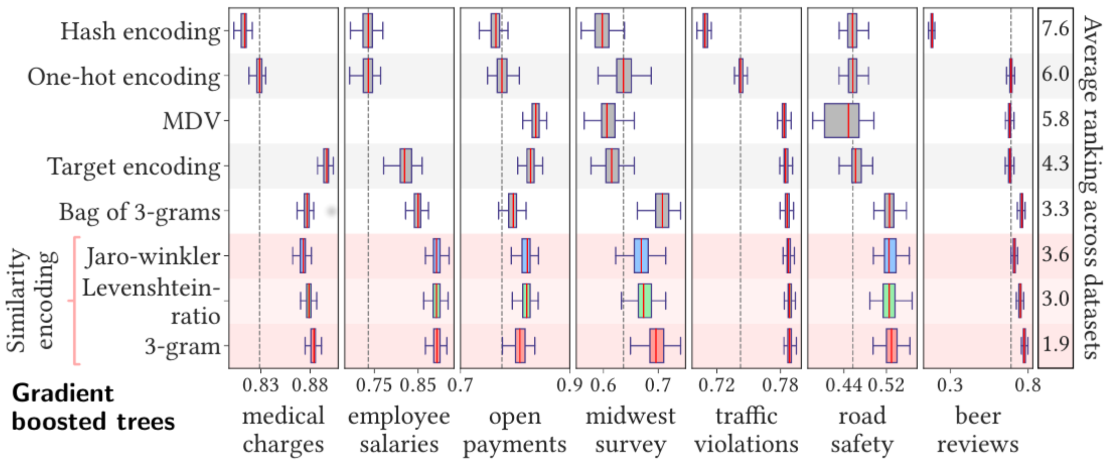


Figure 12. Performance of different encoding methods in a gradient boosting classification task. Each box-plot summarizes the prediction scores of 100 random splits (with 80% of the samples for training and 20% for testing). For all datasets, the prediction score is upper bounded by 1 (a higher score means a better prediction). The right side of the figure indicates the average ranking across datasets for each method. The vertical dashed line indicates the median value of the one-hot encoding method.

XPOP Project-Team

7. New Results

7.1. Normalizing constants of log-concave densities

We derive explicit bounds for the computation of normalizing constants Z for log-concave densities $\pi = \mathrm{e}^{-U}/Z$ w.r.t. the Lebesgue measure on $\mathbb{R}^d$. Our approach relies on a Gaussian annealing combined with recent and precise bounds on the Unadjusted Langevin Algorithm (Durmus, A. and Moulines, E. (2016). High-dimensional Bayesian inference via the Unadjusted Langevin Algorithm). Polynomial bounds in the dimension d are obtained with an exponent that depends on the assumptions made on U. The algorithm also provides a theoretically grounded choice of the annealing sequence of variances. A numerical experiment supports our findings. Results of independent interest on the mean squared error of the empirical average of locally Lipschitz functions are established.

7.2. The Tamed Unadjusted Langevin Algorithm

We consider the problem of sampling from a probability measure π having a density on $\mathbb{R}^d$ known up to a normalizing constant, $x \to \mathrm{e}^{-U(x)}/Z$. The Euler discretization of the Langevin stochastic differential equation (SDE) is known to be unstable in a precise sense, when the potential U is superlinear. Based on previous works on the taming of superlinear drift coefficients for SDEs, we introduce the Tamed Unadjusted Langevin Algorithm (TULA) and obtain non-asymptotic bounds in V-total variation norm and Wasserstein distance of order 2 between the iterates of TULA and π, as well as weak error bounds. Numerical experiments support our findings.

7.3. Development and performance of npde for the evaluation of time-to-event models

Normalised prediction distribution errors (npde) are used to graphically and statistically evaluate mixed-effect models for continuous responses. Our aim was to extend npde to time-to-event (TTE) models and evaluate their performance. We extended npde to TTE models using imputations to take into account censoring. We then evaluated their performance in terms of type I error and power to detect model misspecifications for TTE data by means of a simulation study with different sample sizes. Type I error was found to be close to the expected 5% significance level for all sample sizes tested. The npde were able to detect misspecifications in the baseline hazard as well as in the link between the longitudinal variable and the survival function. The ability to detect model misspecifications increased as the difference in the shape of the survival function became more apparent. As expected, the power also increased as the sample size increased. Imputing the censored events tended to decrease the percentage of rejections.

7.4. Low-rank Interaction with Sparse Additive Effects Model for Large Data Frames

Many applications of machine learning involve the analysis of large data frames-matrices collecting heterogeneous measurements (binary, numerical, counts, etc.) across samples-with missing values. Low-rank models are popular in this framework for tasks such as visualization, clustering and missing value imputation. Yet, available methods with statistical guarantees and efficient optimization do not allow explicit modeling of main additive effects such as row and column, or covariate effects. We introduced a low-rank interaction and sparse additive effects (LORIS) model which combines matrix regression on a dictionary and low-rank design, to estimate main effects and interactions simultaneously. We provide statistical guarantees in the form of upper bounds on the estimation error of both components. Then, we introduced a mixed coordinate gradient descent (MCGD) method which provably converges sub-linearly to an optimal solution and is computationally efficient for large scale data sets. Simulated and survey data showed that the method has a clear advantage over current practices, which consist in dealing separately with additive effects in a preprocessing step.

7.5. Diffusion approximations and control variates for MCMC

A new methodology was developed for the construction of control variates to reduce the variance of additive functionals of Markov Chain Monte Carlo (MCMC) samplers. Our control variates are defined as linear combinations of functions whose coefficients are obtained by minimizing a proxy for the asymptotic variance. The construction is theoretically justified by two new results. We first show that the asymptotic variances of some well-known MCMC algorithms, including the Random Walk Metropolis and the (Metropolis) Unadjusted/Adjusted Langevin Algorithm, are close to the asymptotic variance of the Langevin diffusion. Second, we provide an explicit representation of the optimal coefficients minimizing the asymptotic variance of the Langevin diffusion. Several examples of Bayesian inference problems demonstrate that the corresponding reduction in the variance is significant, and that in some cases it can be dramatic.

7.6. Density estimation for random walks in random environment

We consider the problem of non-parametric density estimation of a random environment from the observation of a single trajectory of a random walk in this environment. We first construct a density estimator using the beta-moments. We then show that the Goldenshluger-Lepski method can be used to select the beta-moment. We prove nonasymptotic bounds for the supremum norm of these estimators for both the recurrent and the transient to the right case. A simulation study supports our theoretical findings.

7.7. Imputation of mixed data with multilevel singular value decomposition

Statistical analysis of large data sets offers new opportunities to better understand many processes. Yet, data accumulation often implies relaxing acquisition procedures or compounding diverse sources. As a consequence, such data sets often contain mixed data, i.e. both quantitative and qualitative and many missing values. Furthermore, aggregated data present a natural multilevel structure, where individuals or samples are nested within different sites, such as countries or hospitals. Imputation of multilevel data has therefore drawn some attention recently, but current solutions are not designed to handle mixed data, and suffer from important drawbacks such as their computational cost. In this article, we propose a single imputation method for multilevel data, which can be used to complete either quantitative, categorical or mixed data. The method is based on multilevel singular value decomposition (SVD), which consists in decomposing the variability of the data into two components, the between and within groups variability, and performing SVD on both parts. We show on a simulation study that in comparison to competitors, the method has the great advantages of handling data sets of various size, and being computationally faster. Furthermore, it is the first so far to handle mixed data. We apply the method to impute a medical data set resulting from the aggregation of several data sets coming from different hospitals. This application falls in the framework of a larger project on Trauma patients. To overcome obstacles associated to the aggregation of medical data, we turn to distributed computation. The method is implemented in an R package

7.8. Logistic Regression with Missing Covariates – Parameter Estimation, Model Selection and Prediction

Logistic regression is a common classification method in supervised learning. Surprisingly , there are very few solutions for performing it and selecting variables in the presence of missing values. We develop a complete approach, including the estimation of parameters and variance of estimators, derivation of confidence intervals and a model selection procedure, for cases where the missing values can be anywhere in covariates. By well organizing different patterns of missingness in each observation , we propose a stochastic approximation version of the EM algorithm based on Metropolis-Hasting sampling, to perform statistical inference for logistic regression with incomplete data. We also tackle the problem of prediction for a new individual with missing values, which is never addressed. The methodology is computationally efficient, and its good coverage and variable selection properties are demonstrated in a simulation study where we contrast its performances to other methods. For instance, the popular multiple imputation by chained equation can lead to biased estimates while our method is unbiased. The method was applied on a dataset of severely traumatized patients from Paris hospitals to predict the occurrence of hemorrhagic shock, a leading cause of early preventable death in severe trauma cases. The aim is to consolidate the current red flag procedure, a binary alert identifying patients with a high risk of severe hemorrhage. The methodology is implemented in the R package misaem.

7.9. A fast Stochastic Approximation of the EM algorithm 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 perform such sampling, but this method is known to converge slowly for high dimensional problems, or when the joint structure of the distributions to sample is spatially heterogeneous. We propose an independent 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. Indeed, this distribution is automatically obtained thanks to a Laplace approximation of the incomplete data model. We show that such approximation is equivalent to linearizing the structural model in the case of continuous data. Numerical experiments based on simulated and real data demonstrate the good performance of the proposed methods. In particular, we show that the suggested MH algorithm can be efficiently combined with a stochastic approximation version of the EM algorithm for maximum likelihood estimation in nonlinear mixed effects models.

7.10. Incomplete graphical model inference via latent tree aggregation

Graphical network inference is used in many fields such as genomics or ecology to infer the conditional independence structure between variables, from measurements of gene expression or species abundances for instance. In many practical cases, not all variables involved in the network have been observed, and the samples are actually drawn from a distribution where some variables have been marginalized out. This challenges the sparsity assumption commonly made in graphical model inference, since marginalization yields locally dense structures, even when the original network is sparse. We developed a procedure for inferring Gaussian graphical models when some variables are unobserved, that accounts both for the influence of missing variables and the low density of the original network. Our model is based on the aggregation of spanning trees, and the estimation procedure on the Expectation-Maximization algorithm. We treat the graph structure and the unobserved nodes as missing variables and compute posterior probabilities of edge appearance. To provide a complete methodology, we also propose several model selection criteria to estimate the number of missing nodes. A simulation study and an illustration flow cytometry data reveal that our method has favorable edge detection properties compared to existing graph inference techniques. The methods are implemented in an R package.

INFINE-POST Team

5. New Results

5.1. IoT Scripting Over-The-Air

Participants: Emmanuel Baccelli, Francisco Acosta.

A large part of the Internet of Things (IoT) will consist of interconnecting low-end devices, whose characteristics include very small memory capacity (a few kBytes) and limited energy consumption (1000 times less than a RaspberryPi). IoT use-cases require the orchestration of different pieces of logic running concurrently on low-end IoT devices and elsewhere on the network (e.g. in the cloud) and communicating with one another. In a number of use-cases, the logic that needs to run on low-end IoT devices is not known upfront, before deploying the device(s). For instance, some part of the logic (e.g. pre-processing of some data) may need to be transferred on demand, from the cloud to the device, for privacy or performance reasons. Another example is the fine-tuning of some parameters of the logic running on some device, which can only be done after the deployment (e.g. the sensitivity of a distributed alarm system on-site). In such context, this paper presents a generic approach to host, run and update IoT application logic on heterogeneous low-end devices, using over-the-air scripting and small containers. Based on RIOT and Javascript, we provide a proof- of-concept implementation of this approach for a building automation IoT scenario, as well as a preliminary evaluation of this implementation running on common off-the-shelf low-end IoT hardware. Our evaluation shows the prototype runs on common off-the-shelf low-end IoT hardware with as little as 32kB of memory. Recent prior work in this domain also proposed Actinium, an approach using small, distributed runtime containers on computers proxying for low-end IoT devices, accessible as Web resources, and hosting JavaScript logic. Compared to Actinium, we eliminate the need for Web resource proxying, as runtime containers are running directly on the low-end IoT devices.

This work was published and presented at the IEEE Percom 2018 conference as ”Scripting Over-The-Air: Towards Containers on Low-end Devices in the Internet of Things”.

5.2. Information-centric IoT Robotics

Participants: Loic Dauphin, Cedric Adjih, Emmanuel Baccelli.

As IoT emerges, minibots (miniature robots) have appeared on the market. A large community emerged, designing do-it- yourself minibots, and cheap, re-programmable minibots with communication capabilities are now available. For in- stance, small wheeled robots such as the Zooid are based on a small microcontroller (8kB RAM, 64kB ROM) and communicating with a low-power radio in the 2.4 GHz ISM band. Other examples are cheap drones such as the Cheerson CX-10, which has similar hardware characteristics, and which costs under 15$. Simple robotic arms and legged robots are also available, such as the MetaBot. A current trend bases software embedded in minibots on open source frameworks. The Robot Operating System (ROS) is a software framework for robot application development which has become a de facto standard for most areas in robotics. Other open source robotics frameworks include software suite tailored for drones, some of which provide compatibility with ROS. In fact, we observe that minibots have a number of charac- teristics in common with low-end devices found in the Internet of Things (IoT). Compared to low-end IoT devices, minibots are based on similar hardware and their software follows similar trends. For instance, an IoT-enabled actuator based on a System-on-Chip (SoC) embarking a small microcontroller, and a radio communicating with a remote server, is very similar to a simple radio-controlled robot. Low-end IoT devices use similar radio modules, and software embedded in IoT devices is more and more based on a variety of open source, lightweight operating systems such as RIOT, FreeRTOS and NuttX, among others. Similarly, as for IoT embedded systems, the network com- ponent of minibots represents by itself in important part of the software (in terms of features, code/memory size, and performance). In fact, a wide variety of radio modules and communication protocols are used on minibots. The protocols used by micro-robots for (internal or external) communication range from direct motor control (pulse width modulation PWM, pulse position modulation PPM, or PCM), to serial/bus protocols, and high level protocols such as Real-time Publish- Subscribe Protocol (RTPS). In this work we thus to explored the potential of bundling open source robotics software frameworks with IoT software and network architectures, to program and control minibots. To do so, we extend our recent work by designing ROS-ready technology for a minibot based on RIOT and ROS2. We focus primarily on software and networking aspects, targeting ultra-lightweight robots based on a reprogrammable SoC with a microcontroller running at approximately 50 MHz, with 10kB RAM, 100kB Flash, and a low-power radio. Using an information-centric networking paradigm extending NDN, we design and implement the communication primitives required by RIOT-ROS2. Our prototype is able to maintain full compatibility between ROS nodes running on the minibot(s) and ROS nodes running elsewhere on the network without the use of a bridge. We show that RIOT-ROS2 fits on low-end robotics hardware such as a System-on-Chip with an ARM Cortex-M0+ microcontroller. On the software and network performance evaluation side, we illustrate that the latency incurred with our ICN approach is completely acceptable for minibot control, even on constrained radio, based on micro-benchmarks.

This work was published and presented at the IEEE PEMWN 2018 conference as ”RIOT-ROS2: Low-Cost Robots in IoT Controlled via Information-Centric Networking”.

5.3. Human Mobility completion of Sparse Call Detail Records

Participants: Guangshuo Chen, Aline Carneiro Viana, Marco Fiore [CNR - IEIIT (Italy)], Carlos Sarraute [Grandata Labs].

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.

These works have been published as invited papers at the ACM CHANTS 2016 workshop (in conjunction with ACM MobiCom 2016), at the IEEE DAWM workshop (in conjunction with IEEE Percom 2017) and at Computer Communication Elsevier journal in 2018. Another journal version (also registered as TR: hal-01675570) is in revision at the EPJ Data Science Journal.

5.4. Adaptive sampling frequency of human mobility

Participants: Panagiota Katsikouli, Aline Carneiro Viana, Marco Fiore [CNR - IEIIT (Italy)], Diego Madariaga.

The problem we address here is the design of a location sampling system for smartphones and handheld devices that reduces the energy consumed by the continuous activation of the GPS, it reduces the space required to store recorded locations, while reliably capturing the movements of the tracked user. The applications here are related to a number of fields relevant to ubiquitous computing, such as energy-efficient mobile computing, location-based service operations, active probing of subscribers’ positions in mobile networks and trajectory data compression.

To this end, we propose an adaptive sampling system without the use of any assisting sensors for the activation of GPS, such as accelerometer, or GSM information. Our system captures the mobility of a user with high accuracy and reliably adjusts the sampling frequency depending on the user's movement. During high mobility, our system densely samples the locations of the tracked user, but at a rate at most the usual rate found today in most applications (e.g., 1 sample per minute). During low mobility, we sample sparsely at much lower rate than usual. As a result, the recorded trace contains much less samples than it would contain if we sampled with the fixed pre-defined sampling rate, requiring less storage space and less energy to activate the GPS.

Our first quest for a response led to the discovery of *(i)* seemingly universal spectral properties of human mobility, and *(ii)* a linear scaling law of the localization error with respect to the sampling interval. Our findings were based on the analysis of fine-grained GPS trajectories of 119 users worldwide. This work was published at the IEEE Globecom 2017 international conference.

We have improved the published sampling approach by incorporating human behavioral features at the sampling decisions to make it more adaptive. This is an on-going work with Panagiota Katsikouli, who spent 5 months in our team working as an internship and is currently doing a Post-Doc at the AGORA Inria team, and Diego Madariaga who spent 3 months in our team working as an internship and is going to start a PhD in co-tutelle with Aline C. Viana. Diego has implemented an Android application to sample mobility data of users according to our adaptive system described here above. The application is currently under deployment and 8 volunteers are running it in their smartphones. The collected data will allow us validating the correctness and performance of our adaptive sampling system. A patent discussion is also on-going with Inria, currently performing a marked/business study.

5.5. Inference of human personality from mobile phones datasets

Participants: Adriano Di Luzio, Aline Carneiro Viana, Julinda Stefa, Katia Jaffres-Runser [INPT-ENSEEIHT - IRIT (Toulouse University)], Alessandro Mei [Sapienza University (Italy) - Dept. of Computer Science].

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. We take a ground-breaking step in (i) deeply capturing human habits in terms of movements, visits, wireless connectivity as well as some routinary actions from a crowdsourced mobility dataset and in (ii) better understanding the relationship between personality traits and individual behavior. We do so by leveraging a dataset collecting very detailed routines of individuals originating from different countries located in 2 different continents, who answered the Big Five Inventory and allowed continuous collection of data from their smartphones for research purposes for 3 years. We use this dataset to engineer a set of human-adapted features that capture three aspects of human behavior: Temporal Mobility (e.g. time at home/work or commuting), Spatial Mobility (e.g. number of most frequent places, maximum distance from home), and the Context of Use (battery charging habits, wireless hotspots availabilities). Then, we use the features that have a statistically significant correlation with the OCEAN traits to predict the personality of a test-set portion of our dataset through cross validation.

Our results attest an accurate prediction of users' personality traits when a 5-level granularity is used per trait. This brings a much higher precision to our predicted results, when compared to the usual 3-level literature granularity. In addition, our prediction methodology carefully takes advantage of engineered features that (1) are more human-adapted and consequently, allow better capturing individuals' habits in terms of movements, visits, connectivity, context, as well as actions (note that contrarily to the literature, neither calls behavior nor data content is leveraged in our analysis), and (2) are designed having in mind the differences and particularities among the Big5 traits of personality. Thus, this work has the potential to impact the way we characterise unique behaviors of individuals as well as quantify how human personality influences lives and actions. Our results show (1) a significant correlation of most of the traits with a small set of mobility-related features and (2) that we are able to predict the individuals' Big5 traits with considerable accuracy (e.g., prediction of the 5 levels of Openness trait shows an F1 score of 0.77), which is significantly outperforming a benchmark approach, when only considering a set of only 3 of our human-adapted features. Finally, we discuss the ethical concerns of our work, its privacy implications, and ways to tradeoff privacy and benefits.

This is an on-going work with Adriano di Luzio, who spent 4 months in our team working as an internship, Julinda Stefa, an invited research visitor at Infine, and two other researchers: Katia Jaffres-Runser and Alessandro Mei. A paper describing this work is under submission at ACM Mobihoc 2018, but a technical report is also registered under the name hal-01954733.

5.6. Data offloading decision via mobile crowdsensing

Participants: Emanuel Lima, Aline Carneiro Viana, Ana Aguiar [FEUP (Portugal) - Dept. of Electrical and Computer Engineering], Paulo Carvalho [FEUP (Portugal) - Dept. of Electrical and Computer Engineering].

According to Cisco forecasts [0], 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 intend to extend these works by studying human mobility from the perspective of mobile data offloading. This brings two major differences compared to the related work. First, high temporal resolution of positioning datasets is needed. In the majority of the related work, important locations have a temporal dimension representing the time spent by a user in that location, which confers its degree of importance. This time is usually in the order of several minutes which is suitable for the case of detecting important locations but not for a mobile data offloading scenario. Here, according to the amount of data traffic that needs to be offloaded, locations with a visiting temporal resolution of few seconds may be enough for data offloading. Thus, we expect to discover additional offloading opportunities, which were not visible with a coarser temporal resolution. Second, while important locations are usually limited in size, offloading locations can have any arbitrary shape and size.

In this work, offloading regions are defined as spatially aggregated locations where users have mobility suitable to offload. The main contribution of this work are: (a) the identification of offloading regions on an individual basis through unsupervised learning; (b) the characterization of these regions in terms of availability, sojourn, and transition time based on their relevance; (c) the study of the impact of the users mobility on the design of mobile offloading systems. This work was published at ACM CHANTS 2018.

We now working on the extension of this work, which will incorporate the mobility prediction of the users. Such prediction is essential to the design of the decision offloading strategy. Such strategy will be used to allow a mobile phone of a user deciding if offload or not her traffic, i.e., when, where (in which offloading region) and how (if the traffic will be offloadied to one or more Access Points). This is an on-going work with the the PhD Emanuel Lima, who spent 4 months as an intern in our team, and his advisors.

[0] https://www.cisco.com/c/en/us/solutions/collateral/service-provider/visual-networking-index-vni/mobile-white-paper-c11-520862.html

5.7. Infering friends in the crowd in Device-to-Device communication

Participants: Rafael Costa, Aline Carneiro Viana, Leobino Sampaio [UFBA (Brazil) - Institute of Mathematics], Artur Ziviani [National Laboratory for Scientific Computing (Brazil)].

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 plan to investigate how human-aspects and behavior can be useful to leverage future device-to-device communication.

This is the PhD thesis subject of Rafael Costa, aiming the design of a methodology 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. A tutorial paper is under submission to a journal (a TR is in hal-01675445) and a 4h-tutorial was presented at the SBRC 2018 conference [0] (the biggest conference on Computer and Network Science in Brazil).

The next step is then the design of forwarding strategies for data offloading through Device-to-Device (D2D) communication, 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.

5.8. Urban Computing Leveraging Location-Based Social Network Data: a Survey

Participants: Thiago H. Silva [UTFPR (Brazil) - Dept. of Computer Science], Aline Carneiro Viana, Antonio Loureiro.

Urban computing is an interdisciplinary area in which urban issues are studied using state-of-the-art computing technologies. This area is at the intersection of a variety of disciplines: sociology, urban planning, civil engineering, computer science, and economics, to name a few. More than half of the world's population today live in cities and, consequently, there is enormous pressure on providing the proper infrastructure to cities, such as transport, housing, water, and energy. To understand and partly tackle these issues, urban computing combines various data sources such as those coming from Internet of Things (IoT) devices; statistical data about cities and its population (e.g., the Census); and data from Location-Based Social Networks (LBSN), sometimes also termed as location-based social media. One fundamental difference between data from LBSNs and data from other sources is that the former offers unprecedented geographic and temporal resolutions: it reflects individual user actions (fine-grained temporal resolution) at the scale of entire world-class cities (global geographic resolution).

Urban computing with LBSN data has its particularities. For instance, users who share data in Foursquare, a popular LBSN, usually have the goal of showing to their friends where they are while also providing personalized recommendations of places they visit. Nevertheless, when correctly analyzed for knowledge extraction, this data can be used to better understand city dynamics and related social, economic, and cultural aspects. To achieve this purpose, new approaches and techniques are commonly needed to explore that data properly.

[0] http://www.sbrc2018.ufscar.br/minicurso-1-mc-1/

In order to better study such needs, we have published at ACM Computing Survey Journal (the ACM journal with highest impact factor) a survey that provides an extensive discussion of the related literature, focusing on major findings and applications. Although its richness concerning knowledge provision, LBSN data presents several challenges, requiring extra attention to its manipulation and usability, which drives future research opportunities in the field of urban computing using LBSN data. Our work is complementary to two existing surveys in the area of urban computing (i.e., by Jiang et al. and by Zheng et al.) since they only mention briefly few studies that explore LBSN data, neglecting key challenges that revolve around LBSNs. We hope that taken together, our effort and these existing ones, provide a broad perspective of urban computing studies and its development through the lens of different data-driven approaches.

5.9. Identifying how places impact each other by means of user mobility

Participants: Lucas Santos, Pedro Olmo [UFMG (Brazil) - Dept. of Computer Science], 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. In other words, how important is this POI for its neighborhood? We proposed thus a framework to measure POI influence by means of LBSN data. First, we modeled the problem using mobility graph approach where each POI is a node and the transitions of users among POI is a weighted vertex. Also, we treat the users' check-in records among POI as a measure of uncertainty, and their strength can be measured by entropy, which enabled to measure direct influence. Second, using same graph, we propose another influence measure taking account the POI importance for its one-hop vicinity in terms of incoming human transition. In addition, this mobility graph can be viewed as a collaborative filtering. We use this collaborative filter for compute the G-causality and evaluate if the transitions among POI has a causal relation and consequently, the influence among POI. Moreover, to the best of our knowledge, we are the first study which investigated POI influence by means of human mobility using LBSN data source.

This work is being prepared for a submission to an international conference.

POEMS-POST Team

7. New Results

7.1. New schemes for time-domain simulations

7.1.1. Solving the Isotropic Linear Elastodynamics Equations Using Potentials

Participant: Patrick Joly.

This work is done in collaboration with Sébastien Impériale (EPI M3DISIM) and Jorge Albella and Jeronimo Rodríguez from the University of Santiago de Compostela.

We pursue our research on the numerical solution of 2D elastodynamic equations in piecewise homogeneous media using the decomposition of the displacement fields into the sum of the gradient and the rotational (respectively) of two scalar potentials potentials. This allows us to obtain an automatic decomposition of the wave field into the sum of pressure and shear waves (respectively). The approach is expected to be efficient when the velocity of shear waves is much smaller than the velocity of pressure waves, since one can adapt the discretization to each type of waves. This appears as a challenge for finite element methods , the most delicate issue being the treatment of boundary and transmission conditions, where the two potentials are coupled..

A stable (mixed) variational formulation of the evolution problem based on a clever choice of Lagrange multipliers has been proposed as well as various finite element approximations which have been successfully implemented. The analysis of the continuous problem has been published in a long paper in the journal of Scientific computing.The numerical analysis of the discretized problem is in progress.

7.1.2. Time domain Half-Space Matching method

Participants: Sonia Fliss, Hajer Methenni.

This work is done in the framework of the PhD of Hajer Methenni (funded by CEA-LIST) and in collaboration with Sebastien Imperiale (EPI M3DISIM) and Alexandre Imperiale (CEA-LIST).

The objective of this work is to propose a numerical method to solve the elastodynamics equations in a locally perturbed unbounded anisotropic media. Let us mention that all the classical methods to restrict the computation around the perturbations are unstable in anisotropic elastic media (PMLs for instance) or really costly (Integral equations). The idea is to extend the method already developed for the corresponding time harmonic problem, called the Halfspace Matching Method. We have considered, for now, the 2D scalar wave equation but the method is constructed in order to be applied to the elastodynamic problem. The method consists in coupling several representations of the solution in half-planes surrounding the defect with a FE representation in a bounded domain including the defect. In order to ensure the stability of the method, we first semi-discretize in time the equations and apply the method to the semi-discrete problem. Thus, for each time step, by ensuring that all the representations of the solution match, in particular in the intersection of the half-planes, we end up, at each time step, with a system of equations which couples, via integral operators, the solution at this time step in the bounded domain and its traces on the edge of the half-planes, the right hand side being a convolution operator involving the solution at the previous time steps. The method has been implemented and validated with Xlife++.

We are now looking to make the method more efficient by implementing methods of acceleration. Finally, we will also seek to develop another version of the method based on the Convolution quadrature.

7.1.3. Time domain modelling for wave propagation in fractal trees

Participants: Patrick Joly, Maryna Kachanovska.

In order to simulate wave propagation in fractal trees (see section 7.4.3), which have infinite structure, it is necessary to be able to truncate the computations to a finite subtree. This was done using Dirichlet-to-Neumann (DtN) operators in our previous work in collaboration with A. Semin (TU Darmstadt). In this case a DtN operator is a convolution operator, whose kernel is not known in a closed form. Based on the results of this previous work, in 2017 we had proposed two methods for approximating these convolution operators:

- constructing an exact DtN operator for a semi-discretized system (in the spirit of convolution quadrature methods).
- truncating meromorphic expansion for the symbol (Fourier transform of the convolution kernel) of the DtN operator, which allows to approximate the DtN operator by local operators.

This year we have performed a complete convergence and stability analysis of these methods, based on the energy techniques.

In particular, for the convolution quadrature methods, we were able to obtain all the estimates using time-domain analysis, by avoiding passage to the Laplace domain.

As for the method based on the meromorphic expansion of the symbol of the DtN operator, we have shown that the error induced by truncating the expansion to L terms can be controlled by a remainder of a series, which, in particular, depends on the eigenvalues of the weighted Laplacian on the fractal trees. To obtain an explicit dependence of the error on L, we have computed Weyl bounds for the eigenvalues, based on a refinement of the ideas of [Kigami, Lapidus, Comm. Math. Phys. 158 (1993)].

Additionally, we have addressed some computational aspects of the two methods, in particular, efficient evaluation of the symbol of the DtN operator (we have an algorithm that allows to evaluate it at the frequency ω in $O(\log^k|\omega|)$ time), as well as a method for efficient computation of the poles of the symbol (based on Möbius transform and polynomial interpolation).

7.2. Integral equations and boundary element methods (BEMs)

7.2.1. Accelerated and adapted BEMs for wave propagation

Participants: Faisal Amlani, Stéphanie Chaillat.

This work is done in collaboration with Adrien Loseille (EPI Gamma3).

We extend to high-order curved elements a recently introduced metric-based anisotropic mesh adaptation strategy for accelerated boundary element methods (e.g. Fast Multipole(FM-) BEM) applied to exterior boundary value problems. This method derives from an adaptation framework for volumetric finite element methods and is based on an iterative procedure that completely remeshes at each refinement step and that leads to a strategy that is independent of discretization technique (e.g., collocation or Galerkin) and integral representation (e.g., single- or double-layer). In effect, it results in a truly anisotropic adaptation that alters the size, shape and orientation of each element according to an optimal metric based on a numerically recovered Hessian of the boundary solution. The algorithm is principally characterized by its ability to recover optimal convergence rates for both flat and curved discretizations (e.g. P_0-, P_1- or P_2-elements) of a geometry containing singularities such as corners and edges. This is especially powerful for realistic geometries that include engineering detail (whose solutions often entail severe singular behavior).

Additionally, we address — by way of introducing hierarchical ($\mathcal{H}$-) matrix preconditioning applied to fast multipole methods via a Flexible GMRES (FGMRES) routine — the computational difficulties that arise when resolving highly anisotropic (and hence highly ill-conditioned) linear systems. The new technique, which uses a very coarse $\mathcal{H}$-matrix system (constructed rapidly via high-performance parallelization) to precondition the full Fast Multipole Method system, drastically reduces the overall computation time as well as the iterative solve time, further improving the tractability of addressing even larger and more complex geometries by FM-BEM.

7.2.2. Preconditioned $\mathcal{H}$-matrix based BEMs for wave propagation

Participants: Stéphanie Chaillat, Patrick Ciarlet, Félix Kpadonou.

We are interested with fast boundary element methods (BEMs) for the solution of acoustic and elastodynamic problems.

The discretisation of the boundary integral equations, using BEM, yields to a linear system, with a fully-populated matrix. Standard methods to solve this system are prohibitive in terms of memory requirements and solution time. Thus one is rapidly limited in terms of complexity of problems that can be solved. The $\mathcal{H}$-matrix based BEMs is commonly used to address these limitations. It is a purely algebraic approach.

The starting point is that the BEM matrix can be partitioned into some blocks which can either be of low or full rank. Memory can be saved by using low-rank revealing technique such as the Adaptive Cross Approximation. We have already study the efficiency of this approach for wave propagation problems. The purpose being the applications to large scale problems, we are now interested in an efficient implementation of the solver in a high performance computing setting. Thus, a bottleneck, with an hierarchical matrix data-sparse representation, is the management of the memory and its (prior) estimation for array allocations.

The first part of our work has been devoted to the proposition of an a priori estimation of the ranks of the blocks in the hierarchical matrix. Afterwards, we have implemented a parallel construction of the $\mathcal{H}$-matrix representation and H-matrix vector product (basic operation in any iterative solver), using a multi-threading OpenMP parallelization. The solution is then computed through the GMRES iterative solver. A crucial point is then the solution time of that solver and the number of iterations as the problem complexity increases. We have developed a two-level, nested outer-inner, iterative solver strategy. The inner solver preconditioned the outer. The preconditioner is a coarse data-sparse representation of the BEM system matrix.

7.2.3. Coupling integral equations and high-frequency methods

Participants: Marc Bonnet, Marc Lenoir, Eric Lunéville, Laure Pesudo.

This theme concerns wave propagation phenomena which involve two different space scales, namely, on the one hand, a medium scale associated with lengths of the same order of magnitude as the wavelength (medium-frequency regime) and on the other hand, a long scale related to lengths which are large compared to the wavelength (high-frequency regime). Integral equation methods are known to be well suited for the former, whereas high-frequency methods such as geometric optics are generally used for the latter. Because of the presence of both scales, both kinds of simulation methods are simultaneously needed but these techniques do not lend themselves easily to coupling.

The scattering of an acoustic wave by two sound-hard obstacles: a large obstacle subject to high-frequency regime relatively to the wavelength and a small one subject to medium-frequency regime has been investigated by Marc Lenoir, Eric Lunéville and Laure Pesudo. The technique proposed in this case consists in an iterative method which allows to decouple the two obstacles and to use Geometric Optics or Physical Optics for the large obstacle and Boundary Element Method for the small obstacle. This approach has been validated on various situations using the XLife++ library developed in the lab. When the obstacles are not sticked, even if they are very close, the iterative method coupling BEM and some high-frequency methods (ray approximation or Kirchoff approximation) works very well. When the obstacle are sticked, the "natural" iterative method is no longer convergent. We are currently looking for some improved methods to deal with these cases that have a practical interest.

7.2.4. The eddy current model as a low-frequency, high-conductivity asymptotic form of the Maxwell transmission problem

Participant: Marc Bonnet.

In this work, done in collaboration with Edouard Demaldent (CEA LIST), we study the relationship between the Maxwell and eddy current (EC) models for three-dimensional configurations involving highly-conducting bounded bodies in air and sources placed remotely from those bodies. Such configurations typically occur in the numerical simulation of eddy current non destructive testing (ECT). The underlying Maxwell transmission problem is formulated using boundary integral formulations of PMCHWT type. In this context, we derive and rigorously justify an asymptotic expansion of the Maxwell integral problem with respect to the non-dimensional parameter $\gamma := \sqrt{\omega\varepsilon_0/\sigma}$. The EC integral problem is shown to constitute the limiting form of the

Maxwell integral problem as $\gamma \to 0$, i.e. as its low-frequency and high-conductivity limit. Estimates in γ are obtained for the solution remainders (in terms of the surface currents, which are the primary unknowns of the PMCHWT problem, and the electromagnetic fields) and the impedance variation measured at the extremities of the exciting coil. In particular, the leading and remainder orders in γ of the surface currents are found to depend on the current component (electric or magnetic, charge-free or not). Three-dimensional illustrative numerical simulations corroborate these theoretical findings.

7.2.5. *Modelling the fluid-structure coupling caused by a far-field underwater explosion*

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

This work, funded by Naval Group and a CIFRE PhD grant, addresses the computational modelling of the mechanical effect on ships of remote underwater explosions. We aim at a comprehensive modelling approach that accounts for the effect of the initial (fast) wave impinging the ship as well as that of later, slower, water motions. Both fluid motion regimes are treated by boundary element methods (respectively for the wave and potential flow models), while the structure is modelled using finite elements. To cater for large and geometrically complex structures, the BEM-FEM interface requires large numbers of DOFs, which entails the use of a fast BEM solver. Accordingly, the wave-like fluid motions are to be computed by means of the convolution quadrature method (CQM) implemented in the in-house fast BEM code COFFEE. This work is in progress (the thesis having started in Dec. 2017). Work accomplished so far has mainly consisted in (a) thoroughly examinating the physical modelling issues, (b) formulating the mathematical and computational model that takes relevant physical features into account, and (c) implementing and assessing the CQM under conditions similar to those of the aimed application.

7.3. Domain decomposition methods

7.3.1. *Transparent boundary conditions with overlap in unbounded anisotropic media*

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

This work is done in the framework of the PhD of Yohanes Tjandrawidjaja (funded by CEA-LIST), in collaboration with Vahan Baronian (CEA). This follows the PhD of Antoine Tonnoir (now Assistant Professor at Insa of Rouen) who developed a new approach, the Half-Space Matching Method, to solve scattering problems in 2D unbounded anisotropic media. The objective is to extend the method to a 3D plate of finite width.

In 2D, our approach consists in coupling several plane-waves representations of the solution in half-spaces surrounding the defect with a FE computation of the solution around the defect. The difficulty is to ensure that all these representations match, in particular in the infinite intersections of the half-spaces. It leads to a formulation which couples, via integral operators, the solution in a bounded domain including the defect and some traces of the solution on the edges of the half-planes. We have proven that, in presence of dissipation, this system is a Fredholm equation of the second kind, in an L2 functional framework. The truncation of the Fourier integrals and the finite element approximation of the corresponding numerical method have been also analyzed.

The method has been extended to the 3D case, for an application to non-destructive testing. The objective is to simulate the interaction of Lamb waves with a defect in an anisotropic elastic plate. The additional complexity compared to the 2D case lies in the representations which are obtained semi-analytically by decomposition on Lamb modes. In addition, the system of equations couples the FE representation in the bounded perturbed domain with not only the displacement, but also the normal stress of the solution on the infinite bands limiting the half-plates. A first numerical result has been obtained in the isotropic case.

The perspectives now concern the efficiency of the method (which could be improved by replacing the direct inversion by a preconditioned iterative inversion with an efficient product matrix-vector), the analysis of the method in the case without dissipation and the analysis of the method in the elastic case.

7.3.2. Coupling BEMs in overlapping domains when a global Green's function is not available

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

We consider in this work problems for which the Green's function is not available, so that classical Boundary Integral equation methods are not applicable. Let us mention for instance the junction of two different stratified media (tapered optical fibers in integrated optics or junction of two topographic elastic surfaces in geophysics).

To this end, we propose a generalization of the Half-Space Matching method (see section 7.3.1).

In this work, by replacing the Fourier representations by integral representations, we are able to replace the half-spaces by more general unbounded overlapping sub-domains. We choose the sub-domains in such a way that an explicit Green's function is available for each subdomain. For instance, for the configuration described above (figure 1 a), it suffices to introduce two infinite sub domains, each of them containing only one stratification (figures 1 c and 1 d) and a bounded domain containing the junction (figure 1 b). The formulation couples the solution in the bounded domain with the single and double layer potentials on each boundary of the sub-domains. The approximation relies on a FE discretisation of the volume unknown and a truncation and a discretization of the boundary/surface unknowns.

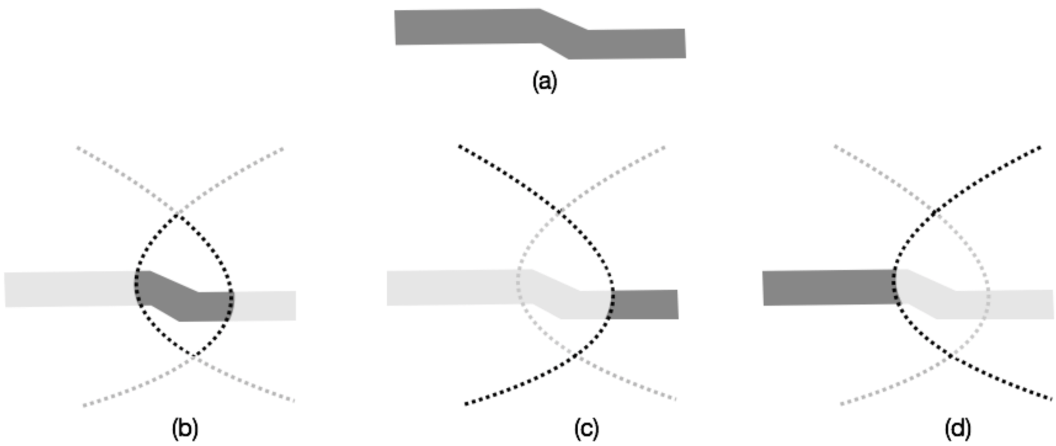


Figure 1. Coupling BEMs in overlapping domains

A study concerning the choice of the discretisation parameters and the shape of the infinite lines have to be done. The theoretical analysis of the method raises challenging open questions: for instance, a first uniqueness result has been derived, which requires the definition of a variational formulation on a Rie. Finally, we want to apply the method to the scattering by a step, i.e. the junction of two semi infinite-planes joined together by a step.

7.3.3. Domain decomposition method for acoustics with uniform exponential rate of convergence using non-local impedance operators

Participants: Patrick Joly, Francis Collino, Émile Parolin.

This work is done in the framework of the PhD of Émile Parolin (funded by ANR NonlocalDD), in collaboration with X. Clayes (EPI Alpines & LJLL).

We continued the work on non-overlapping domain decomposition methods with non-local transmission conditions for time-harmonic wave propagation. The analysis of such methods is conducted by writing them as a relaxed Jacobi algorithm. In the absence of junctions points, the continuous algorithm converges exponentially fast under suitable assumptions on the impedance operators. These assumptions cannot be satisfied using local operators and rely in practice on singular integral operators. The progress achieved is as follows.

- In the context of acoustic wave propagation, we established a new result on the robustness of the algorithm with respect to the mesh size. We have proven that for Lagrange finite element approximations the exponential rate of convergence of the algorithm is independent of the discretization parameter, hence does not deteriorate when the mesh is refined. The proof relies on the Scott-Zhang interpolator and led to the submission.
- We have been working on the extension to 3D time harmonic Maxwell's equations. The main difficulty is to design well adapted operators taking into account the specificity of the corresponding trace spaces. An adequate operator must behave like a pseudo-differential operator with opposite order on the 'curl part' and 'grad part' of a tangential field (this is related to the Helmholtz decomposition of tangential fields). Guided by potential theory for elliptic operators, we proposed two classes of suitable operators. The first one is based on Bessel potentials (fractional powers of the shifted Laplacian) and the second one relies on Riesz potentials. We have shown that the proposed operators satisfy the desired properties in the case of a sphere using modal analysis techniques. We have also been working on the design of the finite element approximation of these operators.

7.3.4. Domain decomposition method with cross-point treatment for high-frequency acoustic scattering

Participant: Axel Modave.

This work is done in collaboration with X. Antoine (IECL & EPI SPHINX) and C. Geuzaine (Université de Liège).

Solving high-frequency time-harmonic scattering problems using FE techniques is challenging, as such problems lead to very large, complex and indefinite linear systems. Optimized Schwarz domain decomposition methods (DDMs) are currently a very promising approach, where subproblems of smaller sizes are solved in parallel using direct solvers, and are combined in an iterative procedure. It is well-known that the convergence rate of these methods strongly depends on the transmission condition enforced on the interfaces between the subdomains.

Local transmission conditions based on high-order absorbing boundary conditions (HABCs) have proved well suited. They represent a good compromise between basic impedance conditions (which lead to suboptimal convergence) and the exact Dirichlet-to-Neumann (DtN) map related to the complementary of the subdomain (which is expensive to compute). However, a direct application of this approach for domain decomposition configurations with cross-points, where more than two subdomains meet, does not provide satisfactory results.

We work on improved DDMs that efficiently addresses configurations with cross-points. Noting that these points actually are corners for the subdomains, our strategy consists in incorporating a corner treatment developed for HABCs (see section 7.7.1) into the DDM procedure. We propose a cross-point treatment for HABC-based DDMs in settings with cross-points and right angles. The method is implemented and successfully tested for two-dimensional examples. The analysis of this method is currently in progress. Extensions to more complicated settings (e.g. 3D, with non-right angles, other physical waves) will be investigated in the future.

7.4. Wave propagation in complex media

7.4.1. Enriched Homogenization in presence of boundaries or interfaces

Participants: Clement Beneteau, Sonia Fliss.

This work is done in the framework of the PhD of Clement Beneteau and is done in collaboration with X. Claeys (Sorbonne & EPI Alpines).

This work is motivated by the fact that classical homogenization theory poorly takes into account interfaces or boundaries. It is particularly unfortunate when one is interested in phenomena arising at the interfaces or the boundaries of the periodic media (the propagation of plasmonic waves at the surface of metamaterials for instance). To overcome this limitation, we have constructed an effective model which is enriched near the interfaces and/or the boundaries. For now, we have treated and analysed the case of simple geometries: for instance a half-plane with Dirichlet or Neumann boundary conditions or a plane interface between two periodic half spaces. We have derived a high order approximate model which consists in replacing the periodic media by an effective one but the boundary/transmission conditions are not classical. The obtained conditions involve Laplace- Beltrami operators at the interface and requires to solve cell problems in periodicity cell (as in classical homogenization) and in infinite strips (to take into account the phenomena near the boundary/interface). We establish well posedness for the approximate model and error estimates which justify that this new model is more accurate. From a numerical point of view, the only difficulty comes from the problems set in infinite strips. The method has been implemented using Xlife++.

This approach has been extended to the long time homogenisation of the wave equation. It is well known that the classical effective homogenized wave equation does not capture the long time dispersive effects of the waves in the periodic media. Since the works of Santosa and Symes in the 90's, several effective equations (involving differential operators of order at least 4) that capture these dispersive effects have been proposed, but only in infinite media. In presence of boundaries or interfaces, the question of boundary/transmission conditions for these effective equations was never treated. We have first results in that direction.

7.4.2. Transmission conditions between homogeneous medium and periodic cavities

Participant: Jean-François Mercier.

In collaboration with A. Maurel (Langevin Institute), J. J. Marigo (LMS) and K. Pham (Imsia).

We have developed a model for resonant arrays of Helmholtz cavities, thanks to a two scale asymptotic analysis. The model combines volumic homogenization to replace the cavity region by a homogeneous anisotropic slab and interface homogenization to replace the region of the necks by transmission conditions. The coefficients entering in the effective wave equation are simply related to the fraction of air in the periodic cell of the array. Those involved in the jump conditions encapsulate the effects of the neck geometry.

In parallel, this effective model has been exploited to study the resonance of the Helmholtz resonators with a focus on the influence of the neck shape. The homogenization makes a parameter B to appear which determines unambiguously the resonance frequency of any neck. As expected, this parameter depends on the length and on the minimum opening of the neck, and it is shown to depend also on the surface of air inside the neck. Once these three geometrical parameters are known, B has an additional but weak dependence on the neck shape, with explicit bounds.

7.4.3. Mathematical analysis of wave propagation in fractal trees

Participants: Patrick Joly, Maryna Kachanovska.

We have continued our work (in collaboration with A. Semin (TU Darmstadt)) on wave propagation in fractal trees which model human lungs. One of the major results of this year is a complete analysis of such models. In particular, provided Sobolev spaces H^1_μ, L^2_μ (which generalize weighted Sobolev spaces on an interval to the case of fractal trees) we clarified the following questions for a range of parameters of the trees not covered by the previous theory: existence of traces of H^1_μ-functions on fractal trees; approximation of H^1_μ-functions by compactly supported functions; compact embedding of H^1_μ into L^2_μ.

7.4.4. Hyperbolic Metamaterials in Frequency Domain: Free Space

Participants: Patrick Ciarlet, Maryna Kachanovska.

In this project we consider the wave propagation in 2D hyperbolic metamaterials [Poddubny et al., Nature Photonics, 2013], which are modelled by Maxwell equations with a diagonal frequency-dependent tensor of dielectric permittivity ε and scalar frequency-independent magnetic permeability. In the time domain, the corresponding models are well-posed and stable. Surprisingly, in some regimes in the frequency domain, when the signs of the diagonal entries of ε do not coincide, the problem becomes hyperbolic (and hence the name). The main goal of this project is to justify the well-posedness of such models in the frequency domain, first of all starting with the case of the free space. We have obtained partial results in this direction: radiation condition, which ensures the well-posedness of the problem, mapping properties of the resolvent (with refined estimates on the propagation of singularities in these models). We are currently working on the limiting absorption and limiting amplitude principles.

7.5. Spectral theory and modal approaches for waveguides

7.5.1. Scattering solutions in an unbounded strip governed by a plate model

Participants: Laurent Bourgeois, Sonia Fliss.

Together with Lucas Chesnel (EPI DEFI), we have initiated a new work on a particular waveguide which consists of a thin strip governed by a Kirchhoff-Love bilaplacian model. The aim is to build some radiation conditions and prove well-posedness of scattering problems for that simple model and for two kinds of boundary conditions: the strip is either simply supported or clamped. In the first case, we have shown that using a Dirichlet-to-Neumann operator enables us to prove fredholmness. Such approach is not possible in the second case, for which a completely different angle of attack is chosen: a Kondratiev approach involving weighted Sobolev spaces and detached asymptotics.

7.5.2. Modal analysis of electromagnetic dispersive media

Participants: Christophe Hazard, Sandrine Paolantoni.

We investigate the spectral effects of an interface between vacuum and a negative material (NM), that is, a dispersive material whose electric permittivity and/or magnetic permeability become negative in some frequency range. Our first work in this context concerns an elementary situation, namely, a two-dimensional scalar model (derived from the complete Maxwell's equations) which involves the simplest existing model of NM, referred to as the non-dissipative Drude model (for which negativity occurs at low frequencies). By considering a polygonal cavity, we have shown that the presence of the Drude material gives rise to various components of an essential spectrum corresponding to various unusual resonance phenomena: first, a low frequency bulk resonance (accumulation at the zero frequency of positive eigenvalues whose associated eigenvectors are confined in the Drude material); then, a surface resonance for one particular critical frequency (at which the so-called surface plasmons occurs, that is, localized highly oscillating vibrations at the interface between the Drude material and the vacuum); finally, corner resonances in a critical frequency interval (here, localized highly oscillating vibrations occur near any corner of the interface, interpreted as a "black hole" phenomenon). An article which presents these results has been submitted. Most recent works were devoted to the numerical simulation of these resonance phenomena in the context of the code XLiFE++ developped in the lab.

7.5.3. Formulation of invisibility in waveguides as an eigenvalue problem

Participant: Anne-Sophie Bonnet-Ben Dhia.

This work is done in collaboration with Lucas Chesnel from EPI DEFI and Vincent Pagneux from Laboratoire d'Acoustique de l'Université du Maine.

We consider an infinite acoustic waveguide (with a bounded cross-section) which is locally perturbed. At some exceptional frequencies and for particular incident waves, it may occur that all the energy of the incident wave is transmitted, the only effect in reflection being a superposition of evanescent modes in the vicinity of the perturbation. We have proposed an approach for which these reflection-less frequencies appear directly as eigenvalues of a new problem. This problem is very similar to the formulation of the scattering problem using Perfectly Matched Layers, except a slight modification in the PML. Precisely, we use two conjugated dilation parameters, α in the outlet and $\overline{\alpha}$ in the inlet, in order to select outgoing waves in the outlet and ingoing waves in the inlet. In fact, we show that the real eigenfrequencies that are obtained correspond either to trapped modes or to reflection-less modes. In addition to this real spectrum, we find intrinsic complex frequencies, which also contain information about the quality of the transmission through the waveguide. Mathematically, the non-selfadjoint eigenvalue problem with conjugated PMLs has strange properties: the discreteness of the point spectrum is not stable by compact perturbations and pathological examples can be exhibited.

7.6. Inverse problems

7.6.1. Linear Sampling Method with realistic data in waveguides

Participants: Laurent Bourgeois, Arnaud Recoquillay.

Our activities in the field of inverse scattering in waveguides with the help of sampling methods has now a quite long history. Very recently, we have focused on elastodynamics and realistic data, that is surface data in the time domain. This has been the subject of the PhD of Arnaud Recoquillay. It was motivated by Non Destructive Testing activities for tubular structures and was the object of a partnership with CEA List (Vahan Baronian).

Our strategy consists in transforming the time domain problem into a multi-frequency problem by the Fourier transform. This allows us to take full advantage of the established efficiency of modal frequency-domain sampling methods. In particular, we have shown how to optimize the number of sources/receivers and the distance between them in order to obtain the best possible imaging results.

Our main achievement is an experimental validation of such approach in the presence of real data: the measurements were carried at CEA on steel plates with the help of piezoelectric sensors. The identification results are encouraging and pave the way of a future integration of sampling methods in real NDT activities.

7.6.2. The "exterior approach" to solve inverse obstacle problems

Participants: Laurent Bourgeois, Arnaud Recoquillay, Dmitry Ponomarev.

This work is done in collaboration with Jérémi Dardé (IMT Toulouse).

We consider some inverse obstacle problems in acoustics by using a single incident wave, either in the frequency or in the time domain. When so few data are available, a Linear Sampling type method cannot be applied. In order to solve those kinds of problem, we propose an "exterior approach", coupling a mixed formulation of quasi-reversibility and a simple level set method. In such iterative approach, for a given defect D, we update the solution u with the help of a mixed formulation of quasi-reversibility while for a given solution u, we update the defect D with the help of a level set method based on a Poisson problem. We have studied two cases. The first case concerns the waveguide geometry in the frequency domain. The second case concerns a bounded spatial set in the time domain when data are given in a finite time interval. This last case is challenging because it raises the (open) question of the minimal final time which is required to ensure uniqueness of the obstacle from the lateral Cauchy data.

7.6.3. Inverse acoustic scattering using high-order small-inclusion expansion of misfit function

Participant: Marc Bonnet.

This work concerns an extension of the topological derivative concept for 3D inverse acoustic scattering problems involving the identification of penetrable obstacles, whereby the featured data-misfit cost function J is expanded in powers of the characteristic radius a of a single small inhomogeneity. The $O(a^6)$ approximation of J is derived and justified for a single obstacle of given location, shape and material properties embedded in a 3D acoustic medium of arbitrary shape, and the generalization to multiple small obstacles is outlined. Simpler and more explicit expressions are obtained when the scatterer is centrally-symmetric or spherical. An approximate and computationally light global search procedure, where the location and size of the unknown object are estimated by minimizing the $O(a^6)$ approximation over a search grid, is proposed and demonstrated on numerical experiments, where the identification from known acoustic pressure on the surface of a penetrable scatterer embedded in a acoustic semi-infinite medium, and whose shape may differ from that of the trial obstacle assumed in the expansion of J, is considered. measurements configuration situated far enough from the probing region.

7.6.4. Microstructural topological sensitivities of the second-order macroscopic model for waves in periodic media

Participant: Marc Bonnet.

This work is done in collaboration with Bojan Guzina (University of Minnesota, USA) and Rémi Cornaggia (IRMAR, Rennes).

We consider scalar waves in periodic media through the lens of a second-order effective i.e. macroscopic description, and we aim to compute the sensitivities of the relevant effective parameters due to topological perturbations of a microscopic unit cell. Specifically, our analysis focuses on the tensorial coefficients in the governing mean-field equation – including both the leading order (i.e. quasi-static) terms, and their second-order counterparts. The results demonstrate that the sought sensitivities are computable in terms of (i) three unit-cell solutions used to formulate the unperturbed macroscopic model; (ii) two adoint-field solutions driven by the mass density variation inside the unperturbed unit cell; and (iii) the usual polarization tensor, appearing in the related studies of non-periodic media, that synthesizes the geometric and constitutive features of a point-like perturbation. The proposed developments may be useful toward (a) the design of periodic media to manipulate macroscopic waves via the microstructure-generated effects of dispersion and anisotropy, and (b) sub-wavelength sensing of periodic defects or perturbations.

7.6.5. Analysis of topological derivative as a tool for qualitative identification

Participant: Marc Bonnet.

This work is a collaboration with Fioralba Cakoni (Rutgers University, USA).

The concept of topological derivative 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 topological derivative, 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. Our paper extends the analysis there to the case of anisotropic scatterers and background with near field data. Topological derivative-based imaging functional is analyzed using a suitable factorization of the near fields, which became achievable thanks to a new volume integral formulation recently obtained in Bonnet (J. Integral Equ. Appl. 29:271-295, 2017). Our results include justification of sign heuristics for the topological derivative 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.

7.6.6. Elasticity imaging by error in constitutive equation functionals

Participant: Marc Bonnet.

This work is done in collaboration with Wilkins Aquino (Duke University, USA).

We formulate the identification of heterogeneous linear elastic moduli in the context of time-harmonic elastodynamics as the minimization of the modified error in constitutive equation (MECE) functional. Our main goal is to develop theoretical foundations, in a continuous setting, allowing to explain and justify some known beneficial properties of this treatment. A specific feature of MECE formulations is that forward and adjoint solutions are governed by a fully coupled system, whose mathematical properties play a fundamental role in the qualitative and computational aspects of MECE minimization. We prove that this system has a unique and stable solution at any frequency, provided data is abundant enough (in a sense made precise), even though the relevant forward problem is not *a priori* clearly defined. This result has practical implications such as applicability of MECE to partial interior data (with important practical applications including ultrasound elastography), convergence of finite element discretizations and differentiability of the reduced MECE functional. In addition, we establish that usual least squares and pure ECE formulations are limiting cases of MECE formulations for small and large values of the weight of the data misfit component of the functional, respectively. For the latter case, we furthermore show that the reduced MECE Hessian is asymptotically positive for any parameter perturbation supported on the measurement region, thereby corroborating existing computational evidence on convexity improvement brought by MECE functionals. Finally, numerical studies including parameter reconstruction examples using interior data support our findings.

7.6.7. A continuation method for building large invisible obstacles in waveguides

Participants: Antoine Bera, Anne-Sophie Bonnet-Ben Dhia.

This work is done on collaboration with Lucas Chesnel (EPI DEFI).

We are interested in building invisible obstacles in waveguides, at a given frequency. The invisibility is characterized by the nullity of the scattering coefficients associated to propagating modes. In previous papers, a method has been proposed to prove the existence of invisible obstacles and to build them. But its main drawback was its limitation to small obstacles. In order to get larger invisible obstacles, we have developed a new approach which combines the previous idea with a continuation method: we are building a sequence of invisible obstacles, each of them being a small perturbation of the previous one. This algorithm is based, at each step, on the ontoness of an application and on the fixed-point theorem. We have implemented the method in the finite element library XLiFE++, in the case of penetrable obstacles of a two-dimensional acoustic waveguide, in multi-modal regime. A remarkable result is that the ontoness condition can be ensured in many cases, so that the algorithm can be iterated as long as required. Another interesting feature of our approach is that it allows to prescribe some properties of the obstacle (shape of the obstacle, piecewise constant index, ...), but a drawback is that the algorithm can produce non-realistic negative indices. This is a question that we are currently working on. Finally, let us emphasize that the formalism of the method is very general and flexible. In particular, it can be directly extended to 3D waveguides, or to the scattering in free space.

7.7. Acoustics and aeroacoustics

7.7.1. High-order absorbing boundary conditions with corner treatment for high-frequency acoustic scattering

Participant: Axel Modave.

This work is done in collaboration with C. Geuzaine (University of Liège) and X. Antoine (IECL & EPI SPHINX)

We address the design and validation of accurate local absorbing boundary conditions set on convex polygonal computational domains for the finite element solution of high-frequency acoustic scattering problems. While high-order absorbing boundary conditions (HABCs) are accurate for smooth fictitious boundaries, the precision of the solution drops in the presence of corners if no specific treatment is applied. We analyze two strategies to preserve the accuracy of Padé-type HABCs at corners: first by using compatibility relations (derived for right angle corners) and second by regularizing the boundary at the corner. We show that the former strategy is well-adapted to right corners and efficient for nearly-right corners, while the later is better for very obtuse corners. Numerical results are proposed to analyze and compare the approaches for two-and three-dimensional problems.

7.7.2. Time-harmonic acoustic scattering in a vortical flow

Participants: Antoine Bensalah, Patrick Joly, Jean-François Mercier.

We study the time-harmonic acoustic radiation in a fluid in flow. To go beyond the convected Helmholtz equation, only adapted to potential flows, we use Goldstein's equations, coupling exactly the acoustic waves to the hydrodynamic field. We have studied the hydrodynamic part of Goldstein equations, corresponding to a generalized time-harmonic transport equation and we have investigated its well-posedness. The result has been established under the assumption of a domain-filling flow, which in 2D is simply equivalent to a flow that does not vanish. The approach relies on the method of characteristics, which leads to the resolution of the transport equation along the streamlines and on general results of functional analysis. The theoretical results have been illustrated with numerical results obtained with a SUPG Finite Element scheme.

In complement we have developed a new model for Goldstein's equations in which the description of the hydrodynamic phenomena is simplified. The model, initially developed for a carrier flow of low Mach number M, is proved theoretically to remain accurate for moderate Mach numbers, associated to a low error bounded by M^2. Numerical experiments confirm the M^2 law and the good quality of the model for flows of non-small Mach numbers.

7.8. Numerical analysis for PDEs

7.8.1. A family of Crouzeix-Raviart Finite Elements in 3D

Participant: Patrick Ciarlet.

This work is done in collaboration with C. Dunkl (University of Virginia) and S. Sauter (Universität Zürich).

We develop a family of non-conforming "Crouzeix–Raviart" type finite elements in three dimensions. They consist of local polynomials of maximal degree p on simplicial finite element meshes while certain jump conditions are imposed across adjacent simplices. We will prove optimal a priori estimates for these finite elements. The characterization of this space via jump conditions is implicit and the derivation of a local basis requires some deeper theoretical tools from orthogonal polynomials on triangles and their representation. We will derive these tools for this purpose. These results allow us to give explicit representations of the local basis functions. Finally, we will analyze the linear independence of these sets of functions and discuss the question whether they span the whole non-conforming space.

7.8.2. Numerical analysis of the mixed finite element method for the neutron diffusion eigenproblem with heterogeneous coefficients

Participants: Patrick Ciarlet, Léandre Giret, Félix Kpadonou.

This work is done in collaboration with E. Jamelot (CEA).

We study first the convergence of the finite element approximation of the mixed diffusion equations with a source term, in the case where the solution is of low regularity. Such a situation commonly arises in the presence of three or more intersecting material components with different characteristics. Then we focus on the approximation of the associated eigenvalue problem. We prove spectral correctness for this problem in the mixed setting. These studies are carried out without, and then with a domain decomposition method. The domain decomposition method can be non-matching in the sense that the traces of the finite element spaces may not fit at the interface between subdomains. Finally, numerical experiments illustrate the accuracy of the method.

7.8.3. Localization of global norms and robust a posteriori error control for transmission problems with sign-changing coefficients

Participant: Patrick Ciarlet.

This work is done in collaboration with M. Vohralik (EPI SERENA).

We present a posteriori error analysis of diffusion problems where the diffusion tensor is not necessarily symmetric and positive definite and can in particular change its sign. We first identify the correct intrinsic error norm for such problems, covering both conforming and nonconforming approximations. It combines a dual (residual) norm together with the distance to the correct functional space. Importantly, we show the equivalence of both these quantities defined globally over the entire computational domain with the Hilbertian sums of their localizations over patches of elements. In this framework, we then design a posteriori estimators which deliver simultaneously guaranteed error upper bound, global and local error lower bounds, and robustness with respect to the (sign-changing) diffusion tensor. Robustness with respect to the approximation polynomial degree is achieved as well. The estimators are given in a unified setting covering at once conforming, nonconforming, mixed, and discontinuous Galerkin finite element discretizations in two or three space dimensions. Numerical results illustrate the theoretical developments.

7.8.4. On the convergence in H^1-norm for the fractional Laplacian

Participant: Patrick Ciarlet.

This work is done in collaboration with J.P. Borthagaray (University of Maryland).

We consider the numerical solution of the fractional Laplacian of index $s \in (1/2, 1)$ in a bounded domain Ω with homogeneous boundary conditions. Its solution a priori belongs to the fractional order Sobolev space $\widetilde{H}^s(\Omega)$. For the Dirichlet problem and under suitable assumptions on the data, it can be shown that 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 $H^1(\Omega)$. A natural question is then whether one can obtain error estimates in $H^1(\Omega)$-norm, in addition to the classical ones that can be derived in the $\widetilde{H}^s(\Omega)$ energy norm. We address this issue, and in particular we derive error estimates for the Lagrange finite element solutions on both quasi-uniform and graded meshes.

AVIZ Project-Team

6. New Results

6.1. Declarative Rendering Model for Multiclass Density Maps

Participants: Jaemin Jo [Dept. of Computer Science and Engineering, Seoul National University, South Korea], Pierre Dragicevic, Jean-Daniel Fekete [correspondent].

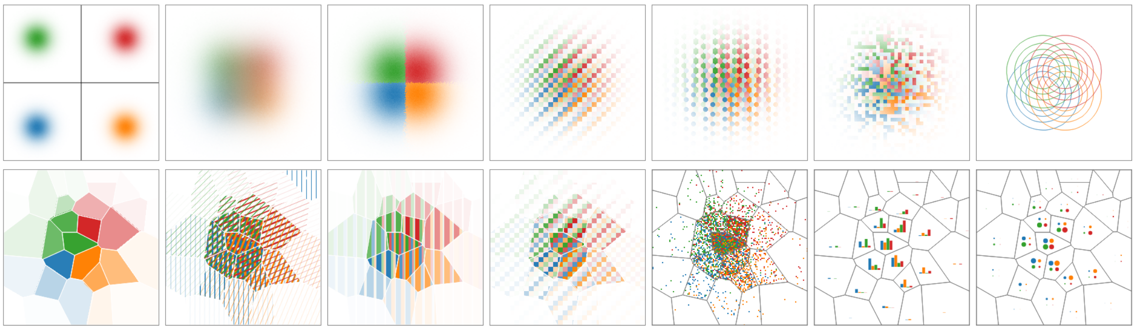


Figure 3. Design alternatives for a four-class density map.

Multiclass maps are scatterplots, multidimensional projections, or thematic geographic maps where data points have a categorical attribute in addition to two quantitative attributes. This categorical attribute is often rendered using shape or color, which does not scale when overplotting occurs. When the number of data points increases, multiclass maps must resort to data aggregation to remain readable. We use a novel model called *multiclass density maps*: multiple 2D histograms computed for each of the category values. Multiclass density maps are meant as a building block to improve the expressiveness and scalability of multiclass map visualization. This library implements our declarative model: a simple yet expressive JSON grammar associated with visual semantics, that specifies a wide design space of visualizations for multiclass density maps. Our declarative model is expressive and can be efficiently implemented in visualization front-ends such as modern web browsers. Furthermore, it can be reconfigured dynamically to support data exploration tasks without recomputing the raw data. Finally, we demonstrate how our model can be used to reproduce examples from the past and support exploring data at scale.

More on the project page: Multiclass Density Maps.

6.2. Reducing Affective Responses to Surgical Images through Color Manipulation and Stylization

Participants: Lonni Besançon [Linköping University Norrköping, Sweden], Amir Semmo [Hasso Plattner Institute, University of Potsdam, Germany], David Biau [Assistance Publique – Hôpitaux de Paris, France], Bruno Frachet [Assistance Publique – Hôpitaux de Paris, France], Virginie Pineau [Institut Curie, France], El Hadi Sariali [Assistance Publique – Hôpitaux de Paris, France], Rabah Taouachi [Institut Curie, France], Tobias Isenberg, Pierre Dragicevic [correspondant].

Figure 4. One of the surgery filters used in our study.

We presented the first empirical study on using color manipulation and stylization to make surgery images more palatable [38]. While aversion to such images is natural, it limits many people's ability to satisfy their curiosity, educate themselves, and make informed decisions. We selected a diverse set of image processing techniques, and tested them both on surgeons and lay people. While many artistic methods were found unusable by surgeons, edge-preserving image smoothing gave good results both in terms of preserving information (as judged by surgeons) and reducing repulsiveness (as judged by lay people). Color manipulation turned out to be not as effective.

This study is an initial investigation but opens up exciting avenues for future research. These include supporting surgery videos, other types of medical images than open surgery (e.g., skin diseases), as well as disturbing imagery outside the medical domain, such as offensive user-generated content that can psychologically impact professionals who monitor it.

All supplemental material is on the OSF page: osf.io/4pfes/.

6.3. Conceptual and Methodological Issues in Evaluating Multidimensional Visualizations for Decision Support

Participants: Evanthia Dimara [ISIR, Sorbonne Université, France], Anastasia Bezerianos [ISIR, Sorbonne Université, France], Pierre Dragicevic [correspondant].

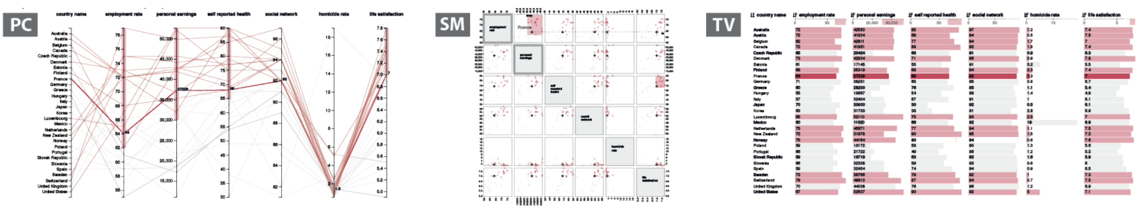


Figure 5. The three visualization techniques tested in our study.

We explored how to rigorously evaluate multidimensional visualizations for their ability to support decision making [22]. We first defined multi-attribute choice tasks, a type of decision task commonly performed with such visualizations. We then identified which of the existing multidimensional visualizations are compatible with such tasks, and evaluated three elementary visualizations: parallel coordinates, scatterplot matrices and tabular visualizations. Our method consisted in first giving participants low-level analytic tasks, in order to ensure that they properly understood the visualizations and their interactions. Participants were then given multi-attribute choice tasks consisting of choosing holiday packages. We assessed decision support through multiple objective and subjective metrics, including a decision accuracy metric based on the consistency between the choice made and self-reported preferences for attributes. We found the three visualizations to be comparable on most metrics, with a slight advantage for tabular visualizations. In particular, tabular visualizations allowed participants to reach decisions faster. Thus, although decision time is typically not central in assessing decision support, it can be used as a tie-breaker when visualizations achieve similar decision accuracy. Our results also suggest that indirect methods for assessing choice confidence may allow to better distinguish between visualizations than direct ones.

All supplemental material is on the project web page: aviz.fr/dm.

6.4. Blinded with Science or Informed by Charts? A Replication Study

Participants: Pierre Dragicevic [correspondant], Yvonne Jansen [ISIR, Sorbonne Université, France].

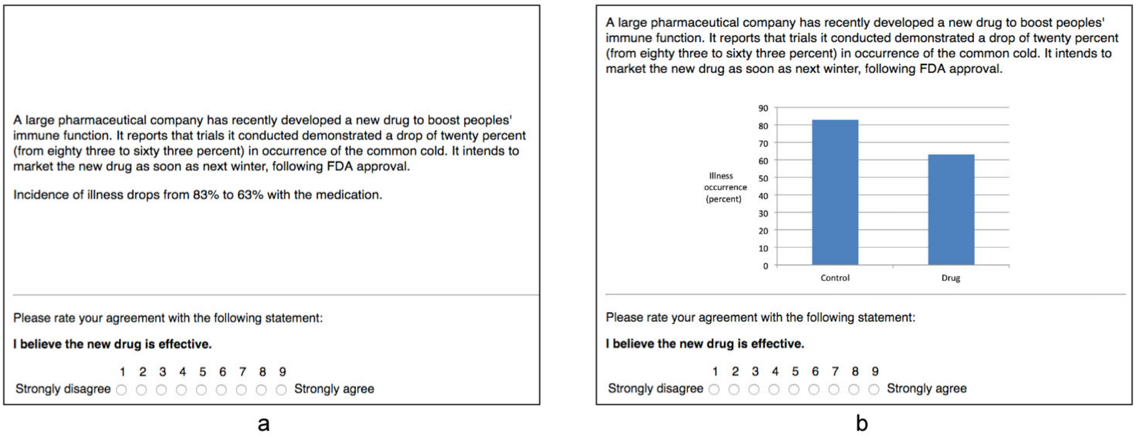


Figure 6. a) text without chart, b) text with "trivial" chart.

We provided a reappraisal of Tal and Wansink's study "Blinded with Science", where seemingly trivial charts were shown to increase belief in drug efficacy, presumably because charts are associated with science. Through a series of four replications conducted on two crowdsourcing platforms, we investigated an alternative explanation, namely, that the charts allowed participants to better assess the drug's efficacy [24]. Considered together, our experiments suggested that the chart seems to have indeed promoted understanding, although the effect is likely very small. Meanwhile, we were unable to replicate the original study's findings, as text with chart appeared to be no more persuasive – and sometimes less persuasive – than text alone. This suggests that the effect may not be as robust as claimed and may need specific conditions to be reproduced. Regardless, within our experimental settings and considering our study as a whole (N = 623), the chart's contribution to understanding was clearly larger than its contribution to persuasion.

The main lesson from our study is that with charts, the peripheral route of persuasion cannot be studied independently from the central route: in order to establish that a chart biases judgment, it is necessary to also rigorously establish that it does not aid comprehension. Our replication also opens many relevant questions for infovis. Are charts really associated with science? More generally, what associations do charts or visualizations trigger depending on their visual design? When exactly is a chart trivial?

All supplemental material is on the project web page: aviz.fr/blinded.

6.5. A Model of Spatial Directness in Interactive Visualization

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

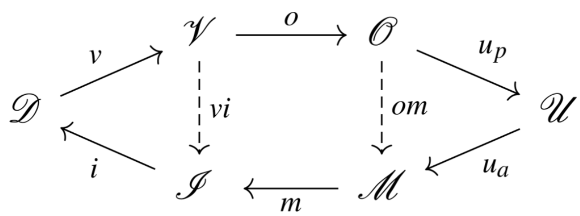


Figure 7. Illustration of the model of spatial directness.

We discussed the concept of directness in the context of spatial interaction with visualization. In particular, we proposeed a model (see Figure 7) 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 distinguished between different types of directness. 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 showed how to apply it to several real-world interaction scenarios in visualization, and thus discussed the resulting types of spatial directness, without recommending either more direct or more indirect interaction techniques. In particular, we demonstrated descriptive and evaluative usage of the proposed model, and also briefly discussed its generative usage.

More on the project Web page: https://tobias.isenberg.cc/VideosAndDemos/Bruckner2018MSD.

6.6. Multiscale Visualization and Scale-Adaptive Modification of DNA Nanostructures

Participants: Haichao Miao [TU Wien, Austria, and Austrian Institute of Technology, Vienna, Austria], Elisa de Llano [Austrian Institute of Technology, Vienna, Austria], Johannes Sorger [Complexity Science Hub Vienna, Austria], Yasaman Ahmadi [Austrian Institute of Technology, Vienna, Austria], Tadija Kekic [Austrian Institute of Technology, Vienna, Austria], Tobias Isenberg [correspondant], M. Eduard Gröller [TU Wien, Austria], Ivan Barišic [Austrian Institute of Technology, Vienna, Austria], Ivan Viola [TU Wien, Austria and KAUST, Kingdom of Saudi Arabia].

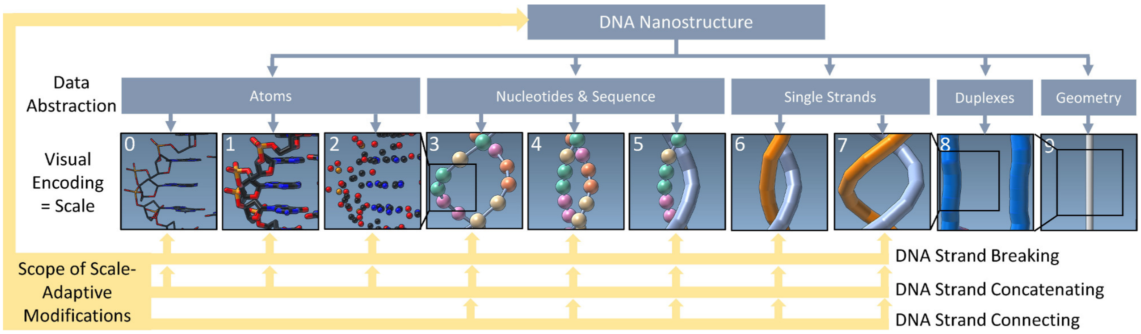


Figure 8. Illustration of the abstraction space.

We presented an approach to represent DNA nanostructures in varying forms of semantic abstraction, describe ways to smoothly transition between them, and thus create a continuous multiscale visualization and interaction space for applications in DNA nanotechnology. This new way of observing, interacting with, and creating DNA nanostructures enables domain experts to approach their work in any of the semantic abstraction levels, supporting both low-level manipulations and high-level visualization and modifications. Our approach allows them to deal with the increasingly complex DNA objects that they are designing, to improve their features, and to add novel functions in a way that no existing single-scale approach offers today. For this purpose we collaborated with DNA nanotechnology experts to design a set of ten semantic scales (see Figure 8). These scales take the DNA's chemical and structural behavior into account and depict it from atoms to the targeted architecture with increasing levels of abstraction. To create coherence between the discrete scales, we seamlessly transition between them in a well-defined manner. We used special encodings to allow experts to estimate the nanoscale object's stability. We also added scale-adaptive interactions that facilitate the intuitive modification of complex structures at multiple scales. We demonstrate the applicability of our approach on an experimental use case. Moreover, feedback from our collaborating domain experts confirmed an increased time efficiency and certainty for analysis and modification tasks on complex DNA structures. Our method thus offers exciting new opportunities with promising applications in medicine and biotechnology.

More on the project Web page: https://tobias.isenberg.cc/VideosAndDemos/Miao2018MVS.

6.7. DimSUM: Dimension and Scale Unifying Maps for Visual Abstraction of DNA Origami Structures

Participants: Haichao Miao [TU Wien, Austria, and Austrian Institute of Technology, Vienna, Austria], Elisa de Llano [Austrian Institute of Technology, Vienna, Austria], Tobias Isenberg [correspondant], M. Eduard Gröller [TU Wien, Austria], Ivan Barišic [Austrian Institute of Technology, Vienna, Austria], Ivan Viola [TU Wien, Austria and KAUST, Kingdom of Saudi Arabia].

We presented a novel visualization concept for DNA origami structures that integrates a multitude of representations into a DimSUM. This novel abstraction map (see Figure 9) provides means to analyze, smoothly transition between, and interact with many visual representations of the DNA origami structures in an effective way that was not possible before. DNA origami structures are nanoscale objects, which are challenging to model in silico. In our holistic approach we seamlessly combined three-dimensional realistic shape models, two-dimensional diagrammatic representations, and ordered alignments in one-dimensional arrangements, with semantic transitions across many scales. To navigate through this large, two-dimensional abstraction map we highlighted locations that users frequently visit for certain tasks and datasets. Particularly interesting viewpoints can be explicitly saved to optimize the workflow. We have developed DimSUM together

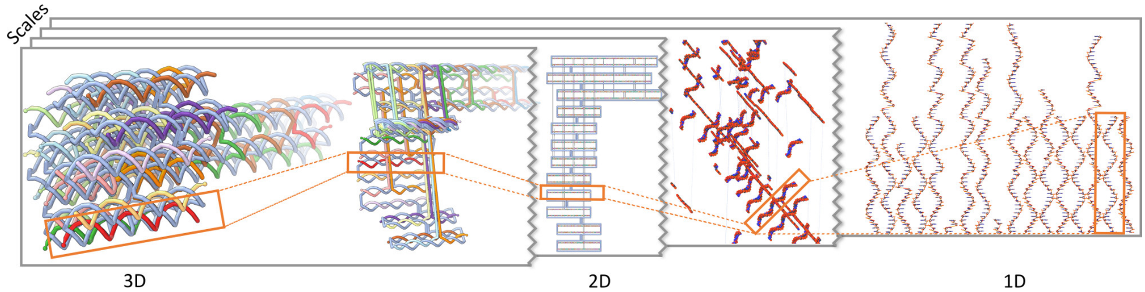


Figure 9. Illustration of the DimSUM space.

with domain scientists specialized in DNA nanotechnology. In the paper we discussed our design decisions for both the visualization and the interaction techniques. We demonstrateed two practical use cases in which our approach increases the specialists' understanding and improves their effectiveness in the analysis. Finally, we discussed the implications of our concept for the use of controlled abstraction in visualization in general.

More on the project Web page: https://tobias.isenberg.cc/VideosAndDemos/Miao2018DDS.

6.8. Pondering the Concept of Abstraction in (Illustrative) Visualization

Participants: Ivan Viola [TU Wien, Austria and KAUST, Kingdom of Saudi Arabia], Tobias Isenberg [correspondant].

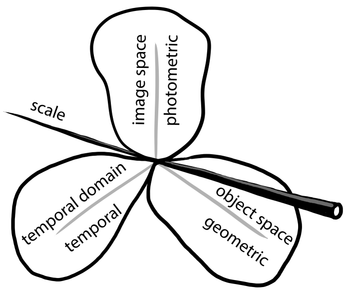


Figure 10. Illustration of the abstraction concept.

We discussed the concept of directness in the context of spatial interaction with visualization (Figure 10). In particular, we proposed a model (autoreffig:directness) 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 distinguished between different types of directness. 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 showed how to apply it to several real-world interaction scenarios in visualization, and thus discussed the resulting types of spatial directness, without recommending either more direct or more indirect interaction techniques. In particular, we demonstrated descriptive and evaluative usage of the proposed model, and also briefly discussed its generative usage.

More on the project Web page: https://tobias.isenberg.cc/VideosAndDemos/Bruckner2018MSD.

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

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

Those of us who study large effects may believe ourselves to be unaffected by the reproducibility problems that plague other areas. 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.

6.10. Visualizing Ranges over Time on Mobile Phones: A Task-Based Crowdsourced Evaluation

Participants: Matthew Brehmer [Microsoft Research, USA], Bongshin Lee [Microsoft Research, USA], Petra Isenberg [correspondant], Eun Kyoung Choe [University of Maryland, USA].

In the first crowdsourced visualization experiment conducted exclusively on mobile phones, we experimentally compare approaches to visualizing ranges over time on small displays. People routinely consume such data via a mobile phone, from temperatures in weather forecasting apps to sleep and blood pressure readings in personal health apps. However, we lack guidance on how to effectively visualize ranges on small displays in the context of different value retrieval and comparison tasks, or with respect to different data characteristics such as periodicity, seasonality, or the cardinality of ranges. Central to our experiment is a comparison between two ways to lay out ranges: a more conventional linear layout strikes a balance between quantitative and chronological scale resolution, while a less conventional radial layout emphasizes the cyclicality of time and may prioritize discrimination between values at its periphery. With results from 87 crowd workers, we found that while participants completed tasks more quickly with linear layouts than with radial ones, there were few differences in terms of error rate between layout conditions. We also found that participants performed similarly with both layouts in tasks that involved comparing superimposed observed and average ranges.

More on the project Web page.

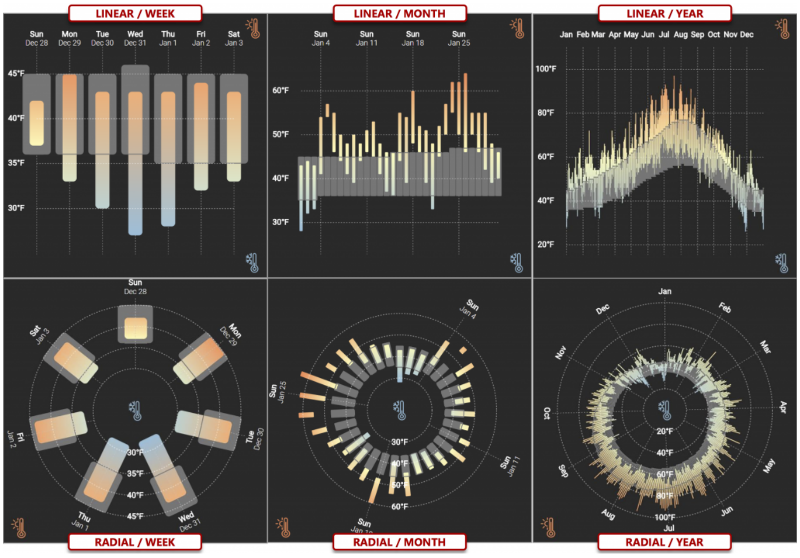


Figure 11. Linear and Radial temperature range charts designed for mobile phone displays, representative of the stimuli used in our crowdsourced experiment. The gradient bars encode observed temperature ranges and are superimposed on gray bars encoding average temperature ranges. Corresponding Week, Month, and Year charts display the same data.

CEDAR Project-Team

7. New Results

7.1. Interactive Data Exploration at Scale

Building upon our prior work in active learning-based interactive database exploration system, we improved this system in terms of efficiency and effectiveness. First, we formally defined the class of user interest queries to which our proposed Dual Space Model (DSM) can bring significant improvement in accuracy. Second, we generalized the DSM to arbitrary queries by forcing our system to fall back to the traditional active learning-based techniques if the requested query properties are not satisfied. Third, we launched a user study to collect real-world datasets and user interest patterns for comparison experiments. The evaluation results showed that our new system outperformed the start-of-the-art active learning techniques and data exploration systems. Fourth, to show the robustness of our system, we added some label noise into the experiments. It turned out that our system maintained a good performance and significantly outperformed traditional active learning-based system. These results have appeared in the prestigious PVLDB journal [10]. In addition, we have been working on integrating DSM with version space algorithms and designing more advanced methods to deal with label noise. In the near feature, a new software based on our proposed techniques will be put into use for interactive database exploration.

7.2. A learning-based approach to optimizing large-scale data analytics

As part of my PhD thesis of K. Zaouk, we have proposed two neural network architectures to support in-situ modeling of user objectives in large-scale data analytics. Although conceptually these architectures can work with any big data system, the modeling of user-objectives on analytics run was applied on Spark Streaming. In our problem settings where only few traces are run whenever a new workload is submitted to the cloud, we have proposed new optimizations to improve the accuracy and efficiency of the auto-encoder based architecture. Thus, we have developed a prototype that included these neural network architectures and optimizations. This prototype was then used to evaluate a benchmark of stream analytics that we developed and instrumented on top of two clusters that collect Spark Streaming workloads' traces.

We analyzed the performance of the proposed techniques and demonstrated their performance benefits over state of the art performance modeling techniques based on machine learning (such as Ottertune used in tuning traditional RDBMS). Our latest results show that we outperform Ottertune in robustness and in our problem settings. These results consolidated in a paper "Boosting Big Data Analytics with Deep Learning Models and Optimization Methods" submitted for publication, alongside with other scientific results in multi-objective optimization contributed by the co-author Fei Song. Work on this topic continues.

7.3. Event stream analysis

As enterprise information systems are collecting event streams from various sources, the ability of a system to automatically detect anomalous events and further provide human readable explanations is of paramount importance. In a position paper [19], we argue for the need of a new type of data stream analytics that can address anomaly detection and explanation discovery in a single, integrated system, which not only offers increased business intelligence, but also opens up opportunities for improved solutions. In particular, we propose a two-pass approach to building such a system, highlight the challenges, and offer initial directions for solutions.

7.4. Quotient summarization of RDF graphs

We have continued our work on efficiently computing informative summaries of large, heterogeneous RDF graphs.

First, we have noticed that type information, when available, can be used to group RDF nodes in interesting, pertinent equivalence classes. However, the integration of type in our quotient summarization framework (presented in ISWC 2017) is not straightforward, since an RDF node may have zero, one, or more than one types. In [15], we have identified a sufficient, flexible condition under which we are able to propose a form of quotient summarization based on types, even if a node has multiple types, and even if they are not organized in a tree-shape classification, but instead in a directed acyclic graph (DAG).

In parallel, we have finalized a comprehensive survey of RDF graph summarization techniques which appeared in the VLDB Journal [8]. We have also completely re-developed our RDF graph summarization platform, in order to ensure correctness, to factorize common elements across all the summarization methods, and to implement new, incremental summarization algorithms [21]. This work has attracted significant visibility through an invited keynote at the ESWC conference [25], and through an ISWC "Resource" publication where our summaries are integrated in a LOD visual exploration portal developed by the ILDA team of Inria [17].

7.5. Semantic integration of heterogeneous data

A large amount of data sources are publicly available in *heterogeneous formats* such as relational, RDF and JSON. These data sources can share information about common entities, which the users may want to query as a single dataset, possibly exploiting also a set of semantic constraints which serve as a common integration perspective. We proposed a new approach to query such *integration* of datasources in a *global RDF graph* using an *RDFS ontology* and user-specified entailment rules. Previous approaches to query answering in the presence of knowledge involve either the materialization of inferred data, or reformulation of the query; both approches have well-known drawbacks. We introduce a new way of query answering as a reduction to view-based answering in [11]. This approach avoids both materialization in the data and query reformulation.

We have also developed an RDF Schema *reformulation algorithm* taking into account the reasoning on the ontology. This algorithm reduces query answering on data in the presence of an ontology, to query evaluation (solely on the data). In particular, this reformulation algorithm can be used to speed up query answering in the integration system mentioned above.

7.6. Fact-checking: a content management perspective

Throughout the year, we have worked within the ANR ContentCheck project to analyze and systematize computational fact-checking as a discipline of computer science; we have analyzed and classified existing works in this area, proposed a generic architecture for computational fact-checking, and highlighted perspectives in a Web Conference (formerly known as WWW) article [18] and two tutorials, presented respectively at the Web conference [16] and the PVLDB conference [7]. This work has also been featured in an invited keynote at the BDA 2018 conference [24].

7.7. Novel fact-checking architectures and algorithms

Still part of our work in ContentCheck, we have worked to devise new algorithms and architectures for data journalism and journalistic fact checking.

First, we have considered the problem of making it easy to check the accuracy of a statistic claim, in the statistic database published by INSEE, the leading french statistic institute. In prior work, we had shown how the INSEE data can be converted into a collection of open data adherent to the best practices of the W3C (RDF graphs). Following up on that work, we have proposed a novel algorithm which allows to search these RDF datasets by means of user-friendly keyword queries. Our algorithm returns ranked answers at the granularity of the RDF dataset (corresponding to a spreadsheet in a statistic dataset published by INSEE) or, when possible, at the granularity of individual cells, or line/column in a spreadsheet that best matches the user query [13], [12].

Second, we have devised a new architecture for keyword search in a polystore systems, where users ask a set of keywords, and receive results showing how occurrences of these keywords across the set of data sources can be connected. This allows identifying possibly unforeseen connections across heterogeneous data sources. We have implemented this architecture in the ConnectionLens prototype, which we demonstrated in VLDB [9] and also informally at BDA [14].

EX-SITU Project-Team

7. New Results

7.1. Fundamentals of Interaction

Participants: Michel Beaudouin-Lafon [correspondant], Wendy Mackay, Cédric Fleury, Theophanis Tsandilas, Dimitrios Christaras Papageorgiou, Han Han, Germán Leiva, Nolwenn Maudet, Yujiro Okuya, Miguel Renom, Philip Tchernavskij, Andrew Webb.

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.

Continuing our long-standing exploration of Fitts' law, we demonstrated the dangers of confounding factors in Fitts'-like experimental designs and recommended how to avoid them [20]. Confounds come from the fact that traditional Fitts'-like experiments use geometric progressions of the two main factors (target distance D and amplitude W) and aggregate data points per $ID = log(1 + D/W)$. This typically leads to a strong confound between D and ID, whereby an effect attributed to ID may in fact be due solely to D. We showed evidence of published results where this confound led to the misinterpretation of experimental results, and proposed stochastic sampling of D and W as a technique to avoid such problems.

We also reviewed statistical methods for the analysis of user-elicited gestural vocabularies [16] and argued that current statistics for assessing agreement across participants are problematic. First, we showed that raw agreement rates disregard agreement that occurs by chance and do not reliably capture how participants distinguish among referents. Second, we explained why current recommendations on how to interpret agreement scores rely on incorrect assumptions. Third, we demonstrated that significance tests for comparing agreement rates, either within or between participants, yield large Type I error rates ($> 40\%$ for $\alpha = .05$). As alternatives, we presented agreement indices that are routinely used in inter-rater reliability studies. We discussed how to apply them to gesture elicitation studies. We also demonstrated how to use common resampling techniques to support statistical inference with interval estimates. We applied these methods to reanalyze and reinterpret the findings of four gesture elicitation studies. We also participated in an invited formal debate at ACM/CHI 2018 to discuss the issue of replicability in HCI experiments, specifically whether or not the community should adopt the TOP (Transparency and Openness) guidelines for data and code transparency, citation, experiment preregistration and replication of experiments.

In order to explore novel forms of interaction based on the concepts of *interaction instruments* and *interactive substrates*, we conducted several studies and developed prototypes in three main areas:

First, we challenged the notion of application as the main organizing principle of digital environments. Most of our current interactions with the digital world are mediated by applications that impose artificial limits on collaboration among users and distribution across devices, and the constantly changing procedures that disrupt everyday use. These limitations are due partly to the engineering principles of encapsulation and program-data separation, which highlight the needs for appropriate conceptual models of interaction [18]. We proposed new architectural principles [28], [17] that address these issues by considering interactions as first-class objects that can be dynamically created, added to and removed from an interactive system.

Second, we addressed the needs of designers and developers of interactive systems through a series of studies and prototypes. Current prototyping tools do not adequately support the early stages of design, nor the necessary communication between designers and developers. We created and evaluated VideoClipper and Montage [21], two tools that facilitate video prototyping for the early sketching of ideas. VideoClipper facilitates the planning and capturing of video brainstorming ideas and video prototypes, while Montage (fig. 2) uses chroma-keying to create more advanced video prototypes and facilitating their reuse in different

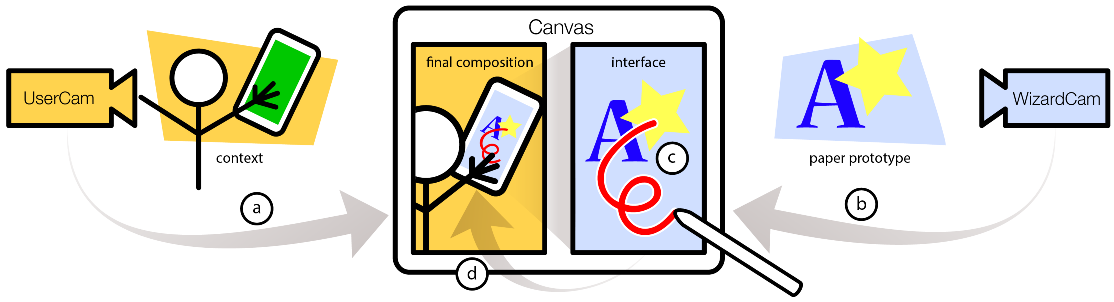


Figure 2. Montage: the UserCam captures the context (a) and the WizardCam captures the paper prototype (b); Both live-stream video to the Canvas, where the designer can add digital sketches (c). Montage replaces the green screen with the interface to create the final composition (d).

contexts. We also created Enact (under submission), a prototyping tool that lets designers and developers work in the same environment to create novel touch-based interaction techniques. Germán Leiva, supervised by Michel Beaudouin-Lafon, successfully defended his Ph.D. thesis *Interactive Prototyping of Interactions: From Throwaway Prototypes to Takeaway Prototyping* [34] on this topic.

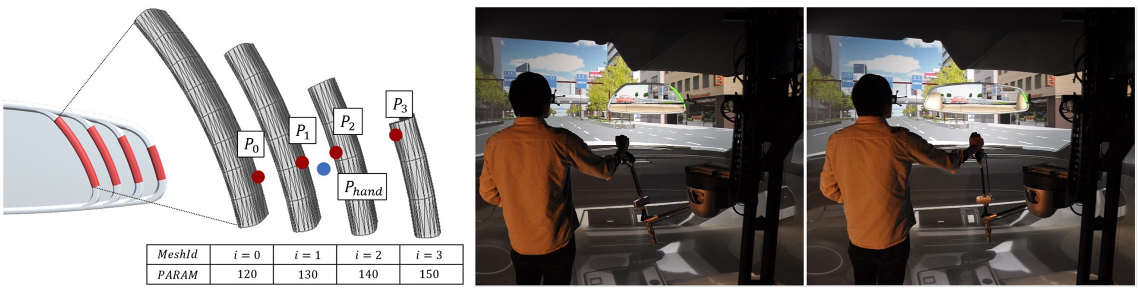


Figure 3. Pre-computed meshes of a rear-view mirror while modifying the right part: the user's hand position (P_{hand}) determines the selected shape (left). A virtual car cockpit where the user modifies the rear-view mirror shape in real time, using haptic force feedback (right).

Third, in the context of Computer Aided Design (CAD), we explored solutions for modifying parametric CAD objects in an immersive virtual reality system. In particular, we developed *ShapeGuide* [14], a technique that lets users modify parameter values by directly pushing or pulling the surface of a CAD object (Figure 3). Including force feedback increases the precision of the users' hand motions in the 3D space. In a controlled experiment, we compared *ShapeGuide* to a standard one-dimensional scroll technique to measure its added value for parametric CAD data modification on a simple industrial object. We also evaluated the effect of force feedback assistance on both techniques. We demonstrated that *ShapeGuide* is significantly faster and more efficient than the scroll technique. In addition, we showed that force feedback assistance enhances the precision of both techniques.

7.2. Human-Computer Partnerships

Participants: Wendy Mackay [correspondant], Baptiste Caramiaux, Téo Sanchez, Marianela Ciolfi Felice, Carla Griggio, Shu Yuan Hsueh, Wanyu Liu, John Maccallum, Nolwenn Maudet, Joanna Mcgrenere, Midas Nouwens, Andrew Webb.

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.

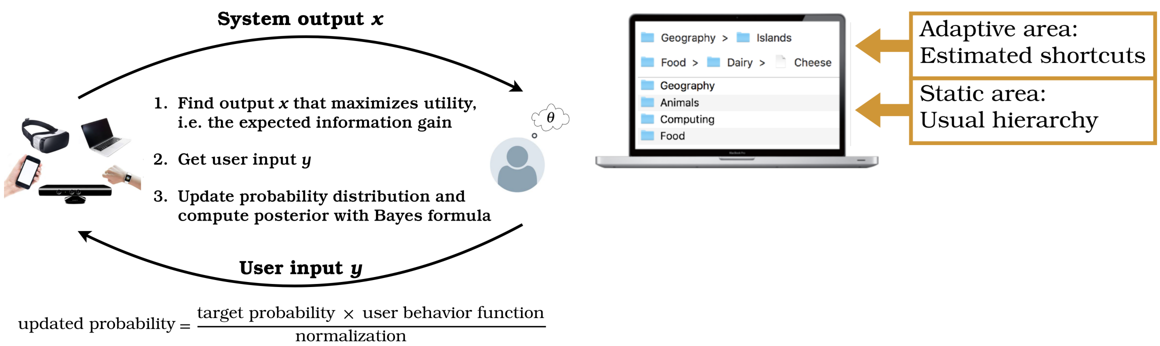


Figure 4. The BIG framework (left) and its application to the BIGFile split-adaptive interface for file navigation (right).

The *Bayesian Information Gain* (BIG) project uses Bayesian Experimental Design, where the criterion is to maximize the information-theoretic concept of mutual information, also known as information gain (fig. 4 -left). The resulting interactive system "runs experiments" on the user in order to maximize the information gain from the user's next input and get to the user's goal more efficiently. *BIGnav* applies BIG to multiscale navigation [7]. Rather than simply executing the navigation commands issued by the user, *BIGnav* interprets them to update its knowledge about the user's intended target, and then computes a new view that maximizes the expected information gain provided by the user's next input. This view is located such that, from the system's perspective, the possible navigation commands are uniformly probable, to the extent possible. *BIGFile* [22] (ACM CHI Honorable Mention award) uses a similar approach for file navigation, with a split interface (fig. 4 -right) that combines a classical area where users can navigate the file system as usual and an adaptive area with a set of shortcuts calculated with BIG. *BIGnav* and *BIGFile* create a novel form of human-computer partnership, where the computer challenges the user in order to extract more information from the user's input, making interaction more efficient. We showed that both techniques are significantly faster (40% and more) than conventional navigation techniques. Wanyu Liu, supervised by Michel Beaudouin-Lafon, successfully defended her Ph.D. thesis *Information theory as a unified tool for understanding and designing human-computer interaction* [35] on this topic.

In the area of visualization, we studied the common challenge faced by domain experts when identifying and comparing patterns in time series data. While automatic measures exist to compute time series similarity, human intervention is often required to visually inspect these automatically generated results. In collaboration with the ILDA Inria team and Univ. Paris-Descartes, we studied how different visualization techniques affect similarity perception in EEG signals [12], [31]. Our goal was to understand if the time series results returned from automatic similarity measures are perceived in a similar manner, irrespective of the visualization technique; and if what people perceive as similar with each visualization aligns with different automatic measures and their similarity constraints. Overall, our work indicates that the choice of visualization affects which temporal patterns we consider to be similar, i.e., the notion of similarity in a time series is not visualization independent. This demonstrates the need for effective human-computer partnerships in which the computer complements, rather than replaces, human skills and expertise.

We began to explore *human-centred machine learning*, which takes advantage of *active machine learning* to facilitate personalization of an interactive system. We developed a gesture-based recognition system where the user iteratively provides instances and also answers the system's queries. Our results demonstrated the phenomenon of co-adaptation between the human user and the system, which challenges the state of the art in conventional active learning. We further explored interactive reinforcement learning as a way to explore high-dimensional parametric space efficiently [24].

7.3. Creativity

Participants: Sarah Fdili Alaoui [correspondant], Marianela Ciolfi Felice, Carla Griggio, Shu Yuan Hsueh, Germán Leiva, John Maccallum, Wendy Mackay, Baptiste Caramiaux, Nolwenn Maudet, Joanna Mcgrenere, Midas Nouwens, Jean-Philippe Rivière, Nicolas Taffin, Philip Tchernavskij, Theophanis Tsandilas, Andrew Webb, Michael Wessely.

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 identified diverse strategies for recording choreographic fragments and, influenced by the concept of *information substrates*, designed *Knotation* [19], a mobile pen-based tool where choreographers sketch representations of their choreographic ideas and make them interactive (Figure 5). Subsequent studies showed that *Knotation* supports both dance-then-record and record-then-dance strategies. Marianela Ciolfi Felice, supervised by Wendy Mackay and Sarah Fdili Alaoui, successfully defended her Ph.D. thesis *Supporting Expert Creative Practice* on this topic [32].

Figure 5. A choreographer uses Knotation to specify and interact with the spatial and temporal layout of a piece.

We are also developing a *Choreographer's Workbench*, a full-body interactive system that helps choreographers explore dance movements by linking previously recorded movement ideas and revealing their underlying relationships. The system emphasizes discoverability and appropriation of movement ideas, using feedforward to visualize movement characteristics. We studied how dancers learn complex expressive movements [23], and studied how variability during practice affects learning motor and timing skills [11]. We contributed to soma-based design, i.e. movement-based designs and design practices specifically engaging with aesthetics [13]. We also collaborated with Ircam on a tool that uses reinforcement learning to explore high-dimensional sound spaces [24]. Users enter likes and dislikes to guide navigation within the sound space, shifting from a parameter-based to a reward-based exploration strategy.

We also are interested in how makers transition between physical and digital designs. Makers often create both physical and digital prototypes to explore a design, taking advantage of the subtle feel of physical materials and the precision and power of digital models. We developed *ShapeMe* [25], a novel smart material that captures its own geometry as it is physically cut by an artist or designer. *ShapeMe* includes a software toolkit that lets its users generate customized, embeddable sensors that can accommodate various object shapes. As the designer works on a physical prototype, the toolkit streams the artist's physical changes to its digital counterpart in a 3D CAD environment (Figure 6). We used a rapid, inexpensive and simple-to-manufacture inkjet printing technique to create embedded sensors. We successfully created a linear predictive model of the sensors' lengths, and our empirical tests of *ShapeMe* showed an average accuracy of 2 to 3 mm. We further presented an application scenario for modeling multi-object constructions, such as architectural models, and 3D models consisting of multiple layers stacked one on top of each other.

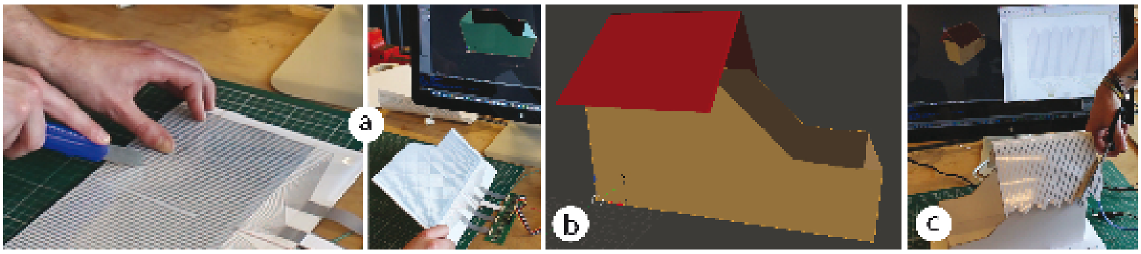


Figure 6. ShapeMe is a novel sensing technology that enables physical modeling with shape-aware material: (a) The maker cuts a foamcore piece to reshape the walls of a house model. The updated shape is captured by a grid of length-aware sensors and is communicated to 3D modeling software. (b) The makers digitally creates the pieces of the roof and then produces its physical model. (c) The maker explores variations of the roof by cutting its side with scissors, while its shape is continuously captured.

We also presented *Interactive Tangrami* [29], a method for prototyping interactive physical interfaces from functional paper-folded building blocks (Tangramis). *Interactive Tangrami* can contain various sensor input and visual output capabilities. Our digital design tool lets makers design the shape and interactive behavior of custom user interfaces. The software manages the communication with the paper-folded blocks and streams the interaction data via the Open Sound protocol (OSC) to an application prototyping environment, such as MaxMSP. The building blocks are fabricated digitally with a rapid and inexpensive ink-jet printing method. Our systems allows to prototype physical user interfaces within minutes and without knowledge of the underlying technologies. Finally, we continued our work with Saarland University, TU Berlin and MIT on digitally fabricated *directional screens* [15]. Michael Wessely, supervised by Theophanis Tsandilas and Wendy Mackay, successfully defended his Ph.D. thesis *Fabricating Malleable Interaction-Aware Material* [36] on these topics.

7.4. Collaboration

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

ExSitu is interested in exploring new ways of supporting collaborative interaction and remote communication. We investigated how large interactive spaces such as wall-sized displays or immersive virtual reality systems can foster collaboration in both co-located and remote situations in the context of Digiscope (http://digiscope.fr/). We also conducted in-depth studies to better understand communication through social networks.

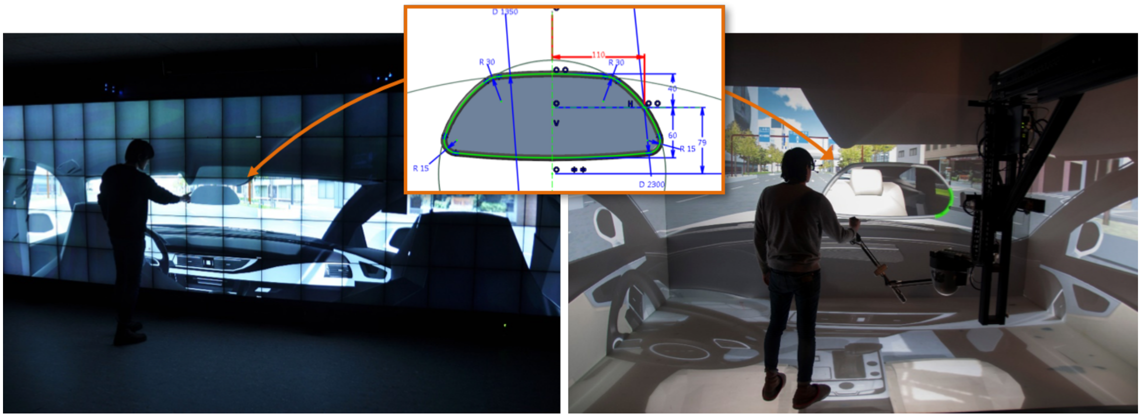


Figure 7. Collaborative CAD data modification between a wall-sized display (left) and a CAVE system (right).

Remote users can have significantly different display and interaction capabilities, such as a wall-size display v.s. an immersive CAVE. We started to explore how such asymmetric interaction capabilities provide interesting opportunities for new collaboration strategies. In particular, we developed a distributed architecture allowing the collaborative modifications of CAD data across heterogeneous platforms [27] and tested it between the EVE and WILDER platforms of Digiscope (CAVE vs. wall-sized touch display – Figure 7).

Remote collaboration across large interactive spaces also requires telepresence systems which support audio-video communication among users as they move in front of the display or inside of the immersive virtual reality system. We have added 3D audio to improve spatial awareness of remote users [26]: 3D audio lets us position a sound source for each remote participant at the virtual position occupied by this participant in the local space. When using video as well as audio, this lets us position the audio feed so that it is congruent with the position of the video feed.

Finally, we conducted an in-depth study of how users communicate via multiple social network apps that offer almost identical functionality. We studied how and why users distribute their contacts within their app ecosystem. We found that users appropriate the features and technical constraints of their apps to create idiosyncratic “communication places”, each with its own recursively defined membership rules, perceived purposes, and emotional connotations. Users also shift the boundaries of their communication places to accommodate changes in their contacts’ behavior, the dynamics of their relationships, and the restrictions of the technology. We argue that communication apps should support creating multiple “communication places” within the same app, relocating conversations across apps, and accessing functionality from other apps. Carla Griggio, supervised by Wendy Mackay, successfully defended her Ph.D. thesis *Designing for Ecosystems of Communication Apps* [33] on this topic.

ILDA Project-Team

6. New Results

6.1. Gestures and Tangibles

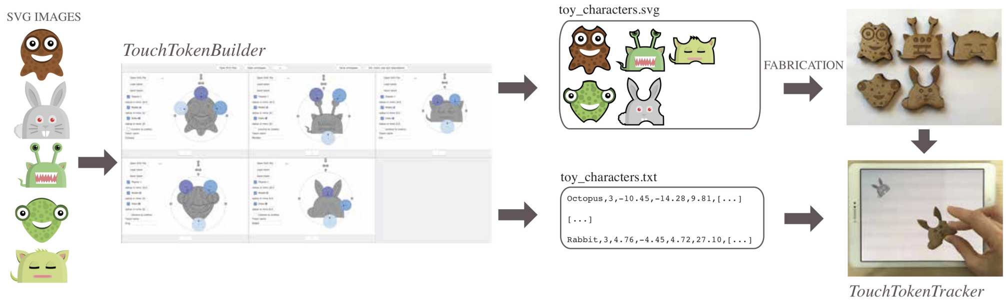


Figure 4. TouchToken-Builder (left) assists users in placing grasping notches on arbitrarily-shaped tokens, warning them about spatial configurations that could generate recognition conflicts or that might be uncomfortable to manipulate. It outputs both a vector and a numerical description of the tokens' geometry (middle). Those are used respectively to build the tokens (top-right), and to track them on any touchscreen using TouchToklen-Tracker (bottom-right).

6.1.1. Custom-made Tangible Interfaces with TouchTokens

One of our main results in this area is the design, development and evaluation of TouchTokens, a new way of prototyping and implementing low-cost tangible interfaces [6]. The approach requires only passive tokens and a regular multi-touch surface. The tokens constrain users' grasp, and thus, the relative spatial configuration of fingers on the surface, theoretically making it possible to design algorithms that can recognize the resulting touch patterns. Our latest project on TouchTokens [17] has been about tailoring tokens, going beyond the limited set of geometrical shapes studied in [6], as illustrated in Figure 4 .

6.1.2. Designing Coherent Gesture Sets for Multi-scale Navigation on Tabletops

We designed a framework for the study of multi-scale navigation (Figure 5) and conducted a controlled experiment of multi-scale navigation on tabletops [25]. We first conducted a guessability study in which we elicited user-defined gestures for triggering a coherent set of navigation actions, and then proposed two interface designs that combine the now-ubiquitous slide, pinch and turn gestures with either two-hand variations on these gestures, or with widgets. In a comparative study, we observed that users can easily learn both designs, and that the gesture-based, visually-minimalist design is a viable option, that saves display space for other controls.

6.1.3. Command Memorization, Gestures and other Triggering Methods

In collaboration with Telecom ParisTech, we studied the impact of semantic aids on command memorization when using either on-body interaction or directional gestures [21]. Previous studies had shown that spatial memory and semantic aids can help users learn and remember gestural commands. Using the body as a support to combine both dimensions had therefore been proposed, but no formal evaluations had been reported. We compared, with or without semantic aids, a new on-body interaction technique (BodyLoci) to mid-air Marking menus in a virtual reality context, considering three levels of semantic aids: no aid, story-making, and story-making with background images.

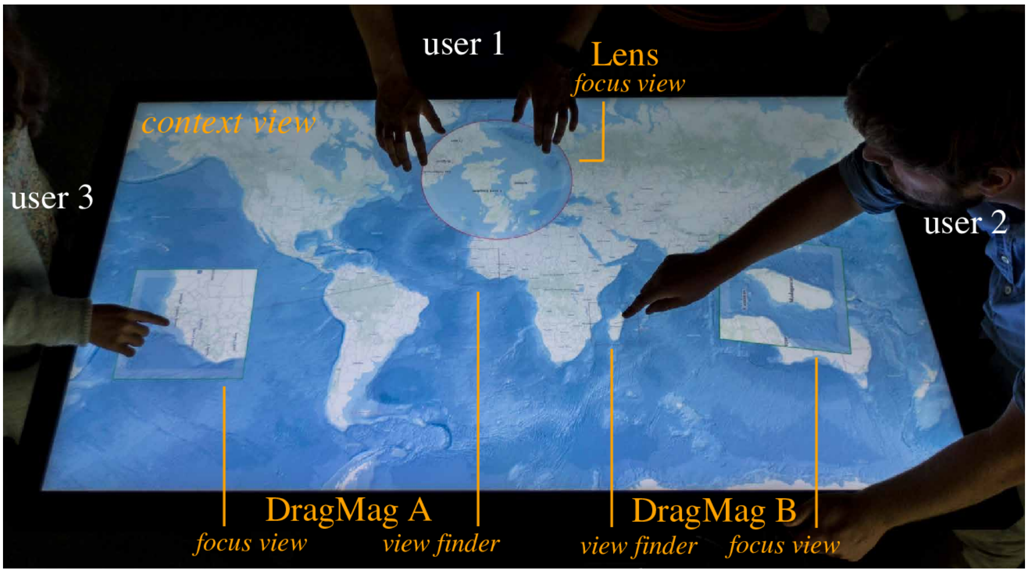


Figure 5. Our framework for the study of multi-scale navigation on tabletops enables users to both pan & zoom the context view and to create independent focus views, either DragMags or lenses.

As part of the same collaboration, we also studied how memorizing positions or directions affects gesture learning for command selection. Many selection techniques either rely on directional gestures (e.g. Marking menus) or pointing gestures using a spatially-stable arrangement of items (e.g. FastTap). Both types of techniques are known to leverage memorization, but not necessarily for the same reasons. We investigated whether using directions or positions affects gesture learning [20].

6.2. Interacting with the Semantic Web of Linked Data

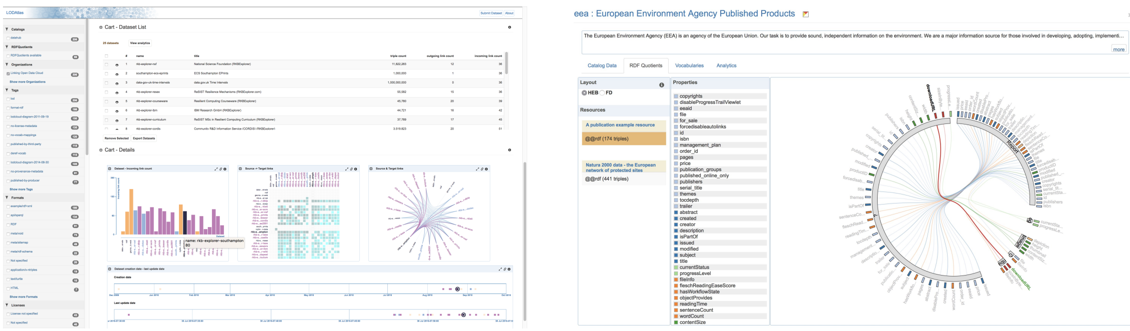


Figure 6. Browsing Linked Data Catalogs with LODAtlas [22]. Left: Visualization of the characteristics of, and links between, datasets selected by the user. Right: RDFQuotients-derived visual summary of a dataset. The summary shows how properties relate instances of the different classes.

The Web of Data is growing fast, as exemplified by the evolution of the Linked Open Data (LOD) cloud over the last ten years. One of the consequences of this growth is that it is becoming increasingly difficult for application developers and end-users to find the datasets that would be relevant to them. Semantic Web search engines, open data catalogs, datasets and frameworks such as LODStats and LOD Laundromat, are all useful but only give partial, even if complementary, views on what datasets are available on the Web. We started working on a platform called LODAtlas in 2016. LODAtlas [22] is a portal that enables users to find datasets of interest (see Figure 6) . Users can make different types of queries about both the datasets' metadata and contents, aggregated from multiple sources. They can then quickly evaluate the matching datasets' relevance, thanks to summary visualizations of their general metadata, connections and contents. The latter has been developed in collaboration with project-team CEDAR, based on their recent work on RDF Quotients.

Linked Data is structured as a directed labeled graph, or more precisely as a multitude of such graphs, that can be interlinked and distributed over the World Wide Web. Graph structures play an essential role at different scales in the Web of Data, and while it is now clear that basic approaches based on node-link diagram representations are only useful for small datasets, such visualizations remain meaningful for the representation of subsets of these multi-variate data. As part of a larger effort that started in the summer of 2016 to investigate novel interactive visual exploration techniques for multi-variate graphs, we introduced a design space and Web-based framework for generating what we call *animated edge textures*. Network edge data attributes are usually encoded using color, opacity, stroke thickness and stroke pattern, or some combination thereof. But in addition to these static variables, it is also possible to animate dynamic particles flowing along the edges. These can be seen as animated edge textures, that offer additional visual encodings that have potential not only in terms of visual mapping capacity but also playfulness and aesthetics. While such particle-based visual encodings have been featured in several commercial and design-oriented visualizations, this has to our knowledge almost always been done in a relatively ad hoc manner. Beyond the design space and Web framework, we also conducted an initial evaluation of particle properties – particle speed, pattern and frequency – in terms of visual perception. This work [24] was performed in collaboration with Nathalie Henry-Riche from Microsoft Research and Benjamin Bach from Edimburgh University.

6.3. Visualization

A significant part of our activity in this axis has been dedicated to geovisualization for various surfaces, including desktop workstations, tabletops and wall displays, in the context of ANR project MapMuxing. We investigated the representation of time in geovisualizations, more particularly how to convey changes in satellite images. Before-and-after images show how entities in a given region have evolved over a specific period of time. These images are used both for data analysis and to illustrate the resulting findings to diverse audiences. We introduced Baia [4], a framework to create advanced animated transitions, called animation plans, between before-and-after images. Baia relies on a pixel-based transition model that gives authors much expressive power, while keeping animations for common types of changes easy to create thanks to predefined animation primitives (Figures 7 and 2).

Still in the area of geovisualization, in the context of ADT project Seawall, conducted in collaboration with project-team Lemon at Inria SAM / Montpellier and with Inria Chile, we have participated to the 2018 SciVis contest, which this year was about the visualization of data related to tsunamis generated by the impact of asteroids in deep water [31]. We used the WILDER ultra-high-resolution wall display to make it easier for analysts to visually compare and contrast different simulations from a deep water asteroid impact ensemble dataset. See Section 5.7.1 and Figure 3 .

In the area of scientific data analysis, we have been collaborating with neuroscientists that explore large quantities of EEG data at different temporal scales. As a first step, we explored if automated algorithmic processes, that aid in the search for similar patterns in large datasets, actually match human intuition. We studied if we perceive as similar the results of these automatic measures, using three time-series visualizations: line charts, horizon graphs and colorfields. Our findings [15], [30] indicate that the notion of similarity is visualization-dependent, and that the best visual encoding varies depending on the automatic similarity measure considered.

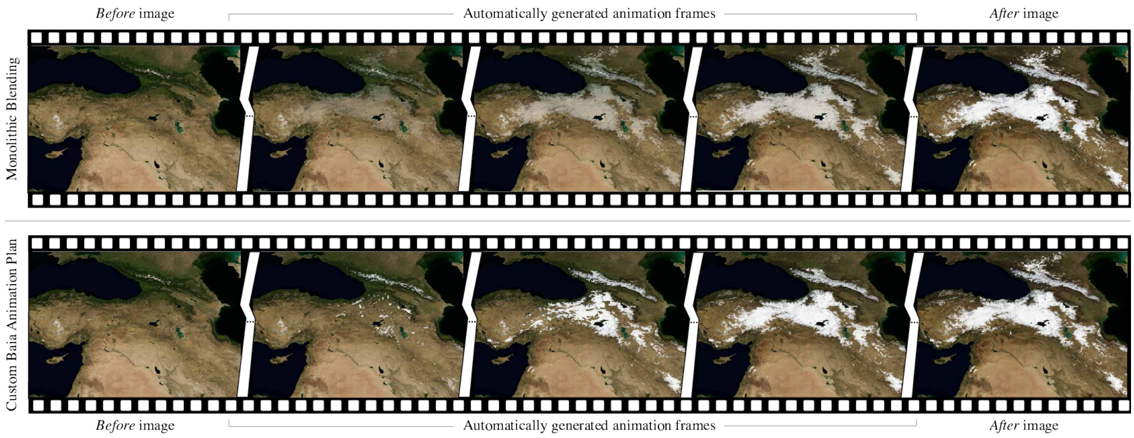


Figure 7. Animated transitions [4] based on one single before-and-after image pair showing seasonal snow cover over northern Middle East. The top row shows keyframes generated using basic monolithic blending. Snow fades in gradually but uniformly, regardless of altitude. The bottom row shows keyframes generated using a Baia animation plan derived from a Digital Elevation Model. Snow fades in gradually, but this time spreading from high-altitude to low-altitude areas.

Anstasia Bezerianos co-advised the PhD work of Evanthia Dimara in project-team Aviz together with P. Dragicevic. Last year, they had already confirmed that the cognitive bias known as the *attraction effect* does exist in visualizations [49]. This was followed-up this year by an exploration of different ways to mitigate this bias [12] (in collaboration with Northwestern University and Sorbonne Université). It was observed that the approach that consists of deleting all unwanted alternatives interactively removed the bias, a result that previous research has shown to be extremely hard to achieve. They also explored how different interactive visualizations of multidimensional datasets can affect decision making [13], and created a task-based taxonomy of cognitive biases for information visualization [14].

Our collaboration with INRA researchers has focused on mixed-initiative systems that combine human learning, machine learning and evolution. Results in this area for this year include an interactive evolutionary algorithm to learn from user interactions and steer the exploration of multidimensional datasets towards two-dimensional projections that are interesting to the analyst, and guidelines on how to evaluate such mixed initiative systems [29].

6.4. Collaboration, Multi-display environments, Large and Small Displays

We studied awareness techniques to aid transitions between personal and shared workspaces in multi-display environments, that include large shared displays and desktops (Figure 8). In such contexts, including crisis management and control rooms, users can engage in both close collaboration and parallel or personal work. Transitioning between different displays can be challenging. To provide workspace awareness and to facilitate these transitions, we designed and implemented three interactions techniques that display users' activities. We explored how and where to display this activity: briefly on the shared display, or more persistently on a peripheral floor display. In a user study motivated by the context of a crisis room where multiple operators with different roles need to cooperate, we tested the usability of the techniques and provided insights on such transitions in systems running on MDEs [23]. We also contributed on a book chapter discussing how to best support collaboration in immersive environments that can range from MDE to mixed reality ones [28].

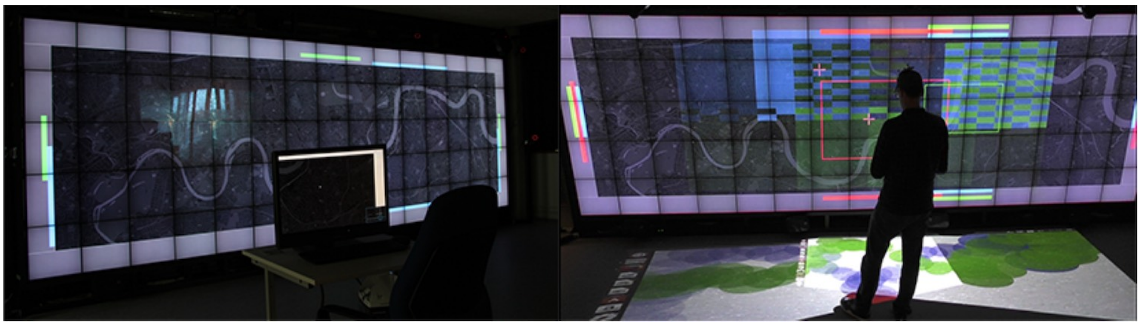


Figure 8. (left) Multi-Display Environment composed of a wall display and two workstations (one visible in the photo). (right) Three workspace awareness techniques: Awareness Bars at the edges of the wall, Focus Map on the wall display, and Step Map projected on the ground.

We collaborated with members from Inria project-team Aviz on the topic of small-scale visualization. This year, new results include a study about the perception of visualizations on smartwatches, performed together with Microsoft Research [11], [26]. The study was designed to assess how quickly people can perform a simple data comparison task for small-scale visualizations on a smartwatch. The goal was to extend our understanding of design constraints for smartwatch visualizations. We tested three chart types common on smartwatches: bar charts, donut charts, and radial bar charts with three different data sizes: 7, 12, and 24 data values. Results show that bar and donut charts should be preferred on smartwatch displays when quick data comparisons are necessary.

PETRUS Project-Team

7. New Results

7.1. Extensive and Secure PDMS Architecture (Axis 1)

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

The Personal Cloud paradigm is emerging through a myriad of solutions offered to users to let them gather and manage their whole digital life. This paradigm shift towards user empowerment raises fundamental questions with regards to the appropriateness of the data management functionalities and protection techniques which are offered by existing solutions to laymen users. This year, we reviewed, compared and analyzed personal cloud alternatives in terms of the functionalities they provide and the threat models they target. From this analysis, we derived a general set of security requirements that any Personal Data Management System (PDMS) should consider. We then identified the challenges of implementing such a PDMS and proposed a preliminary design for an extensive and secure PDMS reference architecture satisfying the considered requirements. Finally, we discussed several important research challenges remaining to be addressed to achieve a mature PDMS ecosystem. A first paper making the functionality and security standpoint in PDMS solutions, proposing five security goals and a preliminary architecture to fulfill these goal based on Trusted Execution Environments was published at IS'19 [12], and preliminary results on the case of a crowdsensing architecture was presented at Middleware'18 [15] and BDA'18 [18].

7.2. Data sharing model for the Personal Cloud (Axis 2)

Participants: Nicolas Anciaux [correspondent], Philippe Pucheral, Guillaume Scerri, Paul Tran Van, Baptiste Crepin.

In the PDMS context, new sharing models are needed to help end-users controlling the sharing policies under use. We proposed an architecture to produce authorizations satisfying users' sharing desires without having to trust the underlying producing these authorizations in the PhD thesis of Paul Tran-Van [11] and we demonstrated the solution at EDBT'18 [14]. We currently investigate the case of a data sharing system producing what we call 'zero-knowledge permissions', i.e., a set of authorizations produced by an untrusted sharing model which is supposed to reveal no information at all about a given subset of documents in the user space.

7.3. SEP2P: Secure and Efficient P2P Personal Data Processing (Axis 3)

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? We studied the feasibility of such a pure P2P personal data management system and provide efficient and scalable mechanisms to reduce the data leakage to its minimum with covert adversaries. In particular, we showed that data processing tasks can be assigned to nodes in a verifiable random way, which cannot be influenced by malicious colluding nodes. We proposed a generic solution which largely minimizes the verification cost. Our experimental evaluation shows that the proposed protocols lead to minimal private information leakage, while the cost of the security mechanisms remains very low even with a large number of colluding corrupted nodes. We illustrated our generic protocol proposal on three data-oriented use-cases, namely, participatory sensing, targeted data diffusion and more general distributed aggregate queries. The full protocol was simulated and evaluated. A first paper focusing on imposed randomness was published at EDBT'19 [13].

7.4. Mobile Participatory Sensing with Strong Privacy Guarantees (Axis 3)

Participant: Iulian Sandu Popa [correspondent].

Mobile participatory sensing could be used in many applications such as vehicular traffic monitoring, pollution tracking, or even health surveying. However, its 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 mobile participatory sensing. 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, we propose an enhanced version of the protocol, named PAMPAS$^+$, to make the system robust even against advanced hardware attacks on the SPs. Hence, the user location privacy leakage remains very low even for an attacker controlling the SSI and a few corrupted SPs. The leakage is proportional with the number of corrupted SPs and thus requires a massive SP corruption to break the system, which is extremely unlikely in practice. This work has been accomplished in collaboration with NJIT (see Section 9.2.1.1) and has been recently submitted as a journal paper.

7.5. Trustworthy Distributed Queries on Personal Data using TEEs (Axis 3)

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

The decentralized way of managing personal data in a PDMS provides a de facto protection against massive attacks usually performed on central servers. But this raises the question of how to preserve individuals' trust on their PDMS when performing global computations crossing data from multiple individuals? And how to guarantee the integrity of the final result when it has been computed by a myriad of collaborative but independent PDMSs? We study a secure decentralized computing framework where each participant gains the assurance that his data is only used for the purpose he consents to and that only the final result is disclosed. Conversely, the goal is to provides the querier with the guarantee that this result has been honesty computed, by the expected code on the expected data. A preliminary solution which capitalizes on the use of Trusted Execution Environments (TEE) at the edge of the network was presented at BDA'18 [19] and APVP'18 [20].

7.6. Performance of large scale data-oriented operations under TEE constraints (Axis 3)

Participants: Robin Carpentier [correspondent], Nicolas Anciaux, Iulian Sandu Popa, Guillaume Scerri.

The rise of Trusted Execution Environments like Intel SGX, and their more and more widespread use for data processing raises the question of their impact on performance, specifically for data oriented operations. While some works aim at embedding either the entirety of part of a database engine within a TEE, the direct impact of processing data with TEEs as opposed to more classical environment has not been studied yet. In particular, the cryptographic overhead of accessing persistent data outside the TEE enclave, the limited RAM amount of each TEE enclave, the cost of external function calls and memory access overheads, may slow the computing by orders of magnitude compared to a regular environment, and have to be taken into account. Preliminary results presenting both a benchmark of data operations within Intel SGX, together with optimisation of search algorithm dealing with the specific way of accessing external memory from inside SGX have been presented at BDA'18 [16].