



RESEARCH CENTER
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FIELD

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Section Scientific Foundations

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3. Scientific Foundations

3.1. Research method

We are inspired by formal methods and logic to construct new tools for software analysis, transformation and generation. We try and proof the correctness of new algorithms using any means necessary.

Nevertheless we mainly focus on the study of existing (large) software artifacts to validate the effectiveness of new tools. We apply the scientific method. To (in)validate our hypothesis we often use detailed manual source code analysis, or we use software metrics, and we have started to use more human subjects (programmers).

Note that we maintain ties with the CWI spinoff “Software Improvement Group” which services most of the Dutch software industry and government and many European companies as well. This provides access to software systems and information about software systems that is valuable in our research.

3.2. Software analysis

This research focuses on source code; to analyze it and to transform it. Each analysis or transformation begins with fact extraction. After the we may analyze specific software systems or large bodies of software systems. Our goal is to improve software systems by learning to understand the causes of complexity.

The mother and father of fact extraction techniques are probably Lex, a scanner generator, and AWK, a language intended for fact extraction from textual records and report generation. Lex is intended to read a file character-by-character and produce output when certain regular expressions (for identifiers, floating point constants, keywords) are recognized. AWK reads its input line-by-line and regular expression matches are applied to each line to extract facts. User-defined actions (in particular print statements) can be associated with each successful match. This approach based on regular expressions is in wide use for solving many problems such as data collection, data mining, fact extraction, consistency checking, and system administration. This same approach is used in languages like Perl, Python, and Ruby. Murphy and Notkin have specialized the AWK-approach for the domain of fact extraction from source code. The key idea is to extend the expressivity of regular expressions by adding context information, in such a way that, for instance, the begin and end of a procedure declaration can be recognized. This approach has, for instance, been used for call graph extraction but becomes cumbersome when more complex context information has to be taken into account such as scope information, variable qualification, or nested language constructs. This suggests using grammar-based approaches as will be pursued in the proposed project. Another line of research is the explicit instrumentation of existing compilers with fact extraction capabilities. Examples are: the GNU C compiler GCC, the CPPX C++ compiler, and the Columbus C/C++ analysis framework. The Rigi system provides several fixed fact extractors for a number of languages. The extracted facts are represented as tuples (see below). The CodeSurfer source code analysis tool extracts a standard collection of facts that can be further analyzed with built-in tools or user-defined programs written in Scheme. In all these cases the programming language as well as the set of extracted facts are fixed thus limiting the range of problems that can be solved.

The approach we want to explore is the use of syntax-related program patterns for fact extraction. An early proposal for such a pattern-based approach is described in: a fixed base language (either C or PL/1 variant) is extended with pattern matching primitives. In our own previous work on RScript we have already proposed a query algebra to express direct queries on the syntax tree. It also allows the querying of information that is attached to the syntax tree via annotations. A unifying view is to consider the syntax tree itself as “facts” and to represent it as a relation. This idea is already quite old. For instance, Linton proposes to represent all syntactic as well as semantic aspects of a program as relations and to use SQL to query them. Due to the lack of expressiveness of SQL (notably the lack of transitive closures) and the performance problems encountered, this approach has not seen wider use.

Another approach is proposed by de Moor and colleagues and uses path expressions on the syntax tree to extract program facts and formulate queries on them. This approach builds on the work of Paige and attempts to solve a classic problem: how to incrementally update extracted program facts (relations) after the application of a program transformation.

Parsing is a fundamental tool for fact extraction for source code. Our group has longstanding contributions in the field of Generalized LR parsing and Scannerless parsing. Such generalized parsing techniques enable generation of parsers for a wide range of real (legacy) programming languages, which is highly relevant for experimental research and validation.

3.2.1. Goals

The main goal is to replace labour-intensive manual programming of fact extractors by automatic generation from annotated grammars or other concise and formal notation. There is a wide open scientific challenge here: to create a uniform and generic framework for fact extraction that is superior to current more ad-hoc approaches. We expect to develop new ideas and techniques for generic (language-parametric) fact extraction from source code and other software artifacts.

Given the advances made in fact extraction we are starting to apply our techniques to observe source code and analyze it in detail.

3.3. Relational paradigm

For any source code analysis or transformation, after fact extraction comes elaboration, aggregation or other further analyses of these facts. For fact analysis, we base our entire research on the simple formal concept of a “relation”.

There are at least three lines of research that have explored the use of relations. First, in SQL, n -ary relations are used as basic data type and queries can be formulated to operate on them. SQL is widely used in database applications and a vast literature on query optimization is available. There are, however, some problems with SQL in the applications we envisage: (a) Representing facts about programs requires storing program fragments (e.g., tree-structured data) and that is not easy given the limited built-in datatypes of SQL; (b) SQL does not provide transitive closures, which are essential for computing many forms of derived information; (c) More generally, SQL does not provide fixed-point computations that help to solve sets of equations. Second, in Prolog, Horn clauses can be used to represent relational facts and inference rules for deriving new facts. Although the basic paradigm of Prolog is purely declarative, actual Prolog implementations add imperative features that increase the efficiency of Prolog programs but hide the declarative nature of the language. Extensions of Prolog with recursion have resulted in Datalog in many variations [AHV95]. In F(p)-L a Prolog database and a special-purpose language are used to represent and query program facts.

Third, in SETL, the basic data type was the set. Since relations can easily be represented as sets of tuples, relation-based computations can, in principle, be expressed in SETL. However, SETL as a language was very complicated and has not survived. However, work on programming with sets, bags and lists has continued well into the 90's and has found a renewed interest with the revival of Lisp dialects in 2008 and 2009.

We have already mentioned the relational program representation by Linton. In Rigi, a tuple format (RSF) is introduced to represent untyped relations and a language (RCL) to manipulate them. Relational algebra is used in GROK, Crocopat and Relation Partition Algebra (RPA) to represent basic facts about software systems and to query them. In GUPRO graphs are used to represent programs and to query them. Relations have also been proposed for software manufacture, software knowledge management, and program slicing. Sometimes, set constraints are used for program analysis and type inference. More recently, we have carried out promising experiments in which the relational approach is applied to problems in software analysis and feature analysis. Typed relations can be used to decouple extraction, analysis and visualization of source code artifacts. These experiments confirm the relevance and viability of the relational approach to software analysis, and also indicate a certain urgency of the research direction of this team.

3.3.1. Goals

- New ideas and techniques for the efficient implementation of a relation-based specification formalism.
- Design and prototype implementation of a relation-based specification language that supports the use of extracted facts (Rascal).
- We target at uniform reformulations of existing techniques and algorithms for software analysis as well as the development of new techniques using the relational paradigm.
- We apply the above in the reformulation of refactorings for Java and domain specific languages.

3.4. Refactoring and Transformation

The final goal, to be able to safely refactor or transform source code can be realized in strong collaboration with extraction and analysis.

Software refactoring is usually understood as changing software with the purpose of increasing its readability and maintainability rather than changing its external behavior. Refactoring is an essential tool in all agile software engineering methodologies. Refactoring is usually supported by an interactive refactoring tool and consists of the following steps:

- Select a code fragment to refactor.
- Select a refactoring to apply to it.
- Optionally, provide extra parameter needed by the refactoring (e.g., a new name in a renaming).

The refactoring tool will now test whether the preconditions for the refactoring are satisfied. Note that this requires fact extraction from the source code. If this fails the user is informed. The refactoring tool shows the effects of the refactoring before effectuating them. This gives the user the opportunity to disable the refactoring in specific cases. The refactoring tool applies the refactoring for all enabled cases. Note that this implies a transformation of the source code. Some refactorings can be applied to any programming language (e.g., rename) and others are language specific (e.g., Pull Up Method). At <http://www.refactoring.com> an extensive list of refactorings can be found.

There is hardly any general and pragmatic theory for refactoring, since each refactoring requires different static analysis techniques to be able to check the preconditions. Full blown semantic specification of programming languages have turned out to be infeasible, let alone easily adaptable to small changes in language semantics. On the other hand, each refactoring is an instance of the extract, analyze and transform paradigm. Software transformation regards more general changes such as adding functionality and improving non-functional properties like performance and reliability. It also includes transformation from/to the same language (source-to-source translation) and transformation between different languages (conversion, translation). The underlying techniques for refactoring and transformation are mostly the same. We base our source code transformation techniques on the classical concept of term rewriting, or aspects thereof. It offers simple but powerful pattern matching and pattern construction features (list matching, AC Matching), and type-safe heterogeneous data-structure traversal methods that are certainly applicable for source code transformation.

3.4.1. Goals

Our goal is to integrate the techniques from program transformation completely with relational queries. Refactoring and transformation form the Achilles Heel of any effort to change and improve software. Our innovation is in the strict language-parametric approach that may yield a library of generic analyses and transformations that can be reused across a wide range of programming and application languages. The challenge is to make this approach scale to large bodies of source code and rapid response times for precondition checking.

3.5. The Rascal Meta-programming language

The Rascal Domain Specific Language for Source code analysis and Transformation is developed by ATeams. It is a language specifically designed for any kind of meta programming.

Meta programming is a large and diverse area both conceptually and technologically. There are plentiful libraries, tools and languages available but integrated facilities that combine both source code analysis and source code transformation are scarce. Both domains depend on a wide range of concepts such as grammars and parsing, abstract syntax trees, pattern matching, generalized tree traversal, constraint solving, type inference, high fidelity transformations, slicing, abstract interpretation, model checking, and abstract state machines. Examples of tools that implement some of these concepts are ANTLR, ASF+SDF, CodeSurfer, Crocopat, DMS, Grok, Stratego, TOM and TXL. These tools either specialize in analysis or in transformation, but not in both. As a result, combinations of analysis and transformation tools are used to get the job done. For instance, ASF+SDF relies on RScript for querying and TXL interfaces with databases or query tools. In other approaches, analysis and transformation are implemented from scratch, as done in the Eclipse JDT. The TOM tool adds transformation primitives to Java, such that libraries for analysis can be used directly. In either approach, the job of integrating analysis with transformation has to be done over and over again for each application and this requires a significant investment.

We propose a more radical solution by completely merging the set of concepts for analysis and transformation of source code into a single language called Rascal. This language covers the range of applications from pure analyses to pure transformations and everything in between. Our contribution does not consist of new concepts or language features *per se*, but rather the careful collaboration, integration and cross-fertilization of existing concepts and language features.

3.5.1. Goals

The goals of Rascal are: (a) to remove the cognitive and computational overhead of integrating analysis and transformation tools, (b) to provide a safe and interactive environment for constructing and experimenting with large and complicated source code analyses and transformations such as, for instance, needed for refactorings, and (c) to be easily understandable by a large group of computer programming experts. Rascal is not limited to one particular object programming language, but is generically applicable. Reusable, language specific, functionality is realized as libraries.

DART Project-Team

3. Scientific Foundations

3.1. Introduction

The main research topic of the DaRT team-project concerns the hardware/software codesign of embedded systems with high performance processing units like DSP or SIMD processors. A special focus is put on multi processor architectures on a single chip (System-on-Chip). The contribution of DaRT is organized around the following items:

Co-modeling for High Performance SoC design: We define our own metamodels to specify application, architecture, and (software hardware) association. These metamodels present new characteristics as high level data parallel constructions, iterative dependency expression, data flow and control flow mixing, hierarchical and repetitive application and architecture models. All these metamodels are implemented with respect to the MARTE standard profile of the OMG group, which is dedicated to the modeling of embedded and real-time systems.

Model-based optimization and compilation techniques: We develop automatic transformations of data parallel constructions. They are used to map and to schedule an application on a particular architecture. This architecture is by nature heterogeneous and appropriate techniques used in the high performance community can be adapted. We developed new heuristics to minimize the power consumption. This new objective implies to specify multi criteria optimization techniques to achieve the mapping and the scheduling.

SoC simulation, verification and synthesis: We develop a SystemC based simulation environment at different abstraction levels for accurate performance estimation and for fast simulation. To address an architecture and the applications mapped on it, we simulate in SystemC at different abstraction levels the result of the SoC design. This simulation allows us to verify the adequacy of the mapping and the schedule, e.g., communication delay, load balancing, memory allocation. We also support IP (Intellectual Property) integration with different levels of specification. On the other hand, we use formal verification techniques in order to ensure the correctness of designed systems by particularly considering the synchronous approach. Finally, we transform MARTE models of data intensive algorithms in VHDL, in order to synthesize a hardware implementation.

3.2. Co-modeling for HP-SoC design

Modeling, UML, Marte, MDE, Transformation, Model, Metamodel

The main research objective is to build a set of metamodels (application, hardware architecture, association, deployment and platform specific metamodels) to support a design flow for SoC design. We use a MDE (Model Driven Engineering) based approach.

3.2.1. Foundations

3.2.1.1. System-on-Chip Design

SoC (System-on-Chip) can be considered as a particular case of embedded systems. SoC design covers a lot of different viewpoints including the application modeling by the aggregation of functional components, the assembly of existing physical components, the verification and the simulation of the modeled system, and the synthesis of a complete end-product integrated into a single chip.

The model driven engineering is appropriate to deal with the multiple abstraction levels. Indeed, a model allows several viewpoints on information defined only once and the links or transformation rules between the abstraction levels permit the re-use of the concepts for a different purpose.

3.2.1.2. Model-driven engineering

Model Driven Engineering (MDE) [68] is now recognized as a good approach for dealing with System on Chip design issues such as the quick evolution of the architectures or always growing complexity. MDE relies on the model paradigm where a model represents an abstract view of the reality. The abstraction mechanism avoids dealing with details and eases reusability.

A common MDE development process is to start from a high level of abstraction and to go to a targeted model by flowing through intermediate levels of abstraction. Usually, high level models contain only domain specific concepts, while technological concepts are introduced smoothly in the intermediate levels. The targeted levels are used for different purposes: code generation, simulation, verification, or as inputs to produce other models, etc. The clear separation between the high level models and the technological models makes it easy to switch to a new technology while re-using the previous high level designs. Transformations allow to go from one model at a given abstraction level to another model at another level, and to keep the different models synchronized

In an MDE approach, a SoC designer can use the same language to design application and architecture. Indeed, MDE is based on proved standards: UML 2 [38] for modeling, the MOF (Meta Object Facilities [63]) for metamodel expression and QVT [64] for transformation specifications. Some profiles, i.e. UML extensions, have been defined in order to express the specificities of a particular domain. In the context of embedded system, the MARTE profile in which we contribute follows the OMG standardization process.

3.2.1.3. Models of computation

We briefly present our reference models of computation that consist of the Array-OL language and the synchronous model. The former allows us to express the parallelism in applications while the latter favors the formal validation of the design.

Array-OL. The Array-OL language [52], [53], [48], [47] is a mixed graphical-textual specification language dedicated to express multidimensional intensive signal processing applications. It focuses on expressing all the potential parallelism in the applications by providing concepts to express data-parallel access in multidimensional arrays by regular tilings. It is a single assignment first-order functional language whose data structures are multidimensional arrays with potentially cyclic access.

The synchronous model. The synchronous approach [46] proposes formal concepts that favor the trusted design of embedded real-time systems. Its basic assumption is that computation and communication are instantaneous (referred to as “synchrony hypothesis”). The execution of a system is seen through the chronology and simultaneity of observed events. This is a main difference from visions where the system execution is rather considered under its chronometric aspect (i.e., duration has a significant role). There are different synchronous languages with strong mathematical foundations. These languages are associated with tool-sets that have been successfully used in several critical domains, e.g. avionics, nuclear power plants.

In the context of the DaRT project, we consider declarative languages such as Lustre [50] and Signal [61] to model various refinements of Array-OL descriptions in order to deal with the control aspect as well as the temporal aspect present in target applications. The first aspect is typically addressed by using concepts such as mode automata, which are proposed as an extension mechanism in synchronous declarative languages. The second aspect is studied by considering temporal projections of array dimensions in synchronous languages based on clock notion. The resulting synchronous models are analyzable using the formal techniques and tools provided by the synchronous technology.

3.2.2. Past contributions of the team on topics continued in 2012

The new team DaRT has been created in order to finalize the works started in the DaRT EPI, and also to explore new topics. We here remind the past contributions of the team on the topics we continued to work on during 2012.

Our proposal is partially based upon the concepts of the “Y-chart” [57]. The MDE contributes to express the model transformations which correspond to successive refinements between the abstraction levels.

Metamodeling brings a set of tools which enable us to specify our application and hardware architecture models using UML tools, to reuse functional and physical IPs, to ensure refinements between abstraction levels via mapping rules, to initiate interoperability between the different abstraction levels used in a same codesign, and to ensure the opening to other tools, like verification tools, through the use of standards.

The application and the hardware architecture are modeled separately using similar concepts inspired by Array-OL to express the parallelism. The placement and scheduling of the application on the hardware architecture is then expressed in an association model.

All the previously defined models, application, architecture and association, are platform independent and they conform to the MARTE OMG Profil (figure 1). No component is associated with an execution, simulation or synthesis technology. Such an association targets a given technology (OpenMP, OpenCL, SystemC/PA, VHDL, etc.). Once all the components are associated with some IPs of the GasparLib library, the deployment is fully realized. This result can be transformed to further abstraction level models via some model transformations (figure 2).

The simulation results can lead to a refinement of the initial application, hardware architecture, association and deployment models. We propose a methodology to work with all these different models. The design steps are:

1. Separation of application and hardware architecture modeling.
2. Association with semi-automatic mapping and scheduling.
3. Selection of IPs from libraries for each element of application/architecture models, to achieve the deployment.
4. Automatic generation of the various platform specific simulation or execution models.
5. Automatic simulation or execution code generation with calls to the IPs.
6. Refinement at the highest level taking account of the simulation results.

3.2.2.1. High-level modeling in Gaspard2

In Gaspard2, models are described by using the recent OMG standard MARTE profile combined with a few native UML concepts and some extensions.

The new release of Gaspard2 uses different packages of MARTE for UML modeling. The Hardware Resource Model (HRM) concepts of MARTE enable to describe the hardware part of a system. The Repetitive Structure Modeling (RSM) concepts allow one to describe repetitive structures (DaRT team was the main contributor of this MARTE package definition). Finally, the Generic Component Modeling (GCM) concepts are used as the base for component modeling.

The above concepts are expressive enough to permit the modeling of different aspects of an embedded system:

- functionality (or applicative part): the focus is mainly put on the expression of data dependencies between components in order to describe an algorithm. Here, the manipulated data are mainly multidimensional arrays. Furthermore, a form of reactive control can be described in modeled applications via the notion of execution modes. This last aspect is modeled with the help of some native UML notions in addition to MARTE.
- hardware architecture: similar mechanisms are also used here to describe regular architectures in a compact way. Regular parallel computation units are more and more present in embedded systems, especially in SoCs. HRM is fully used to model these concepts. Some extensions are proposed for NoC design and FPGA specifications. The GPU have a particular memory hierarchy. In order to model the memory details, we extend the MARTE metamodel to describe low level characteristics of the memory.
- association of functionality with hardware architecture: the main issues concern the allocation of the applicative part of a system onto the available computation resources, and the scheduling. Here also, the allocation model takes advantage of the repetitive and hierarchical representation offered by MARTE to enable the association at different granularity levels, in a factorized way.

In addition to the above usual design aspects, Gaspard2 also defines a notion of *deployment* specification (see Figure 1) in order to select compatible IPs from libraries, at this time models can produce codes. The corresponding package defines concepts that (i) enable to describe the relation between a MARTE representation of an elementary component (a box with ports) to a text-based code (and Intellectual Property - IP, or a function with arguments), and (ii) allow one to inform the Gaspard2 transformations of specific behaviors of each component (such as average execution time, power consumption...) in order to generate a high abstraction level simulation in adequacy with the real system. Recently this package was extended to design reconfigurable systems using dynamical deployment.

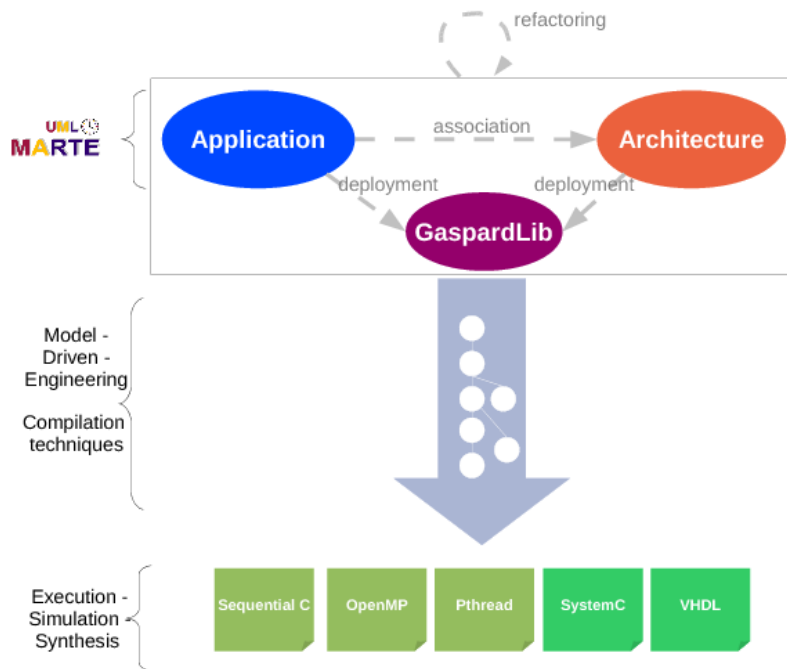


Figure 1. Overview of the design concepts.

3.2.2.2. Intermediate concept modeling and transformations

Gaspard2 targets different technologies for various purposes: formal verification, high-performance computing, simulation and hardware synthesis (Figure 1). This is achieved via model transformations that relate intermediate representations towards the final target representations.

- A metamodel for procedural language with OpenMP (OpenMP in Figure 1). It is inspired by the ANSI C and Fortran grammars and extended by OpenMP statements [41]. The aim of this metamodel is to use the same model to represent Fortran and C code. Thus, from an OpenMP model, it is possible to generate OpenMP/Fortran or OpenMP/C. The generated code includes parallelism directives and control loops to distribute task (IPs code) repetitions over processors [70].
- A VHDL metamodel (VHDL in Figure 1). It gathers the necessary concepts to describe hardware accelerators at the RTL (Register Transfer Level) level, which allows the hardware execution of applications. This metamodel introduces, *e.g.*, the notions of *clock* and *register* in order to manipulate some of the usual hardware design concepts. It is precise enough to enable the generation of synthesizable HDL code [60].

- The two metamodels SystemC and Pthread was redefined to implement both a multi-thread execution model. These are described in the "New results" part.
- Synchronous metamodel (Synchronous Equational). It was used to benefit of the verification tools of synchronous languages. It is not yet maintained in the new release of Gaspard2.

The transformation scheme. In order to target these metamodels, several transformations have been developed (Figure 2). *MartePortInstance* introduces into the MARTE metamodel the concept of *PortInstance* corresponding to an instance of port associated to a part. The *ExplicitAllocation* transformation explicits the association of each application part on the processing units, according to the association of other elements in the application hierarchy. The *LinkTopologyTask* transformation replaces the connectors between a component and an inner repeated part by a task managing the data (*TilerTask*). The scheduling of the application tasks is decomposed into three transformations, *Synchronisation* that associates, to each application component, a local graph of tasks corresponding to its parts; *GlobalSynchronization* that computes a global graph of tasks for the complete application from the local graphs of tasks; and *Scheduling* that schedules the tasks from the global graph. *TilerMapping* maps the *TilerTasks* onto processors. The management of the data in the memory is performed through two transformations. *MemoryMapping* maps the data into memory *i.e.* creates the variables and allocates address spaces. *AddressComputation* computes addresses for each variable. Finally, some transformations are dedicated to targets: *Functional* introduces the concepts relative to procedural languages. *pThread* transforms MARTE elementary tasks into threads and the connectors into buffers. *SystemC* traduces the MARTE architecture into concepts of the SystemC language.

3.2.2.3. MARTE extensions for reconfigurable based systems

Reconfigurable FPGA based Systems-on-Chip (SoC) architectures are increasingly becoming the preferred solution for implementing modern embedded systems. However due to the tremendous amount of hardware resources available in these systems, new design methodologies and tools are required to reduce their design complexity.

In previous work, we provided an initial contribution to the modeling of these systems by extending MARTE profile to incorporate significant design criteria such as power consumption.

In its current version, MARTE lacks dynamic reconfiguration concepts. Even these later are necessary to model and implement rapid prototypes for complex systems.

Our objective is to define all necessary concepts for dynamic reconfiguration issues regarding configuration latency, resources number, etc. Afterwards, these concepts will be integrated to MARTE to obtain an extended and complete profile, which can be called Reconfigurable MARTE (RecoMARTE).

Our current proposals permit us to model fine grain reconfigurable FPGA architectures with an initial extension of the MARTE profile to model Dynamic Reconfiguration at a high-level description.

Since a controller is essential for managing a dynamically reconfigurable region, we modeled a state machine at high abstraction levels using UML state machine diagrams. This state machine is responsible for switching between the available configurations.

As a future work, we will analyze the reconfigurable design flow of Xilinx from the design partitioning to the bitstream generation stage. It is a starting point for understanding how to generate configuration files. Then, we will extract relevant data to define our own design flow.

3.2.2.4. Traceability

We use the transformation mechanism to assist a tester in the mutation analysis process dedicated to model transformations. The mutation analysis aims to qualify a test model set. More precisely, errors are voluntary injected in transformation and the ability of the test models set to highlight these errors is analyzed. If the number of highlighted errors, *i.e.* if the test model set is not enough qualified, new models have to be added in order to raise the set quality [62]. Our approach relies on the hypothesis that it is easier to modify an existing model than to create a new one from scratch. The local trace, coupled to a mutation matrix, helps the tester to identify adequate test models and their relevant parts to modify in order to improve the test data set.

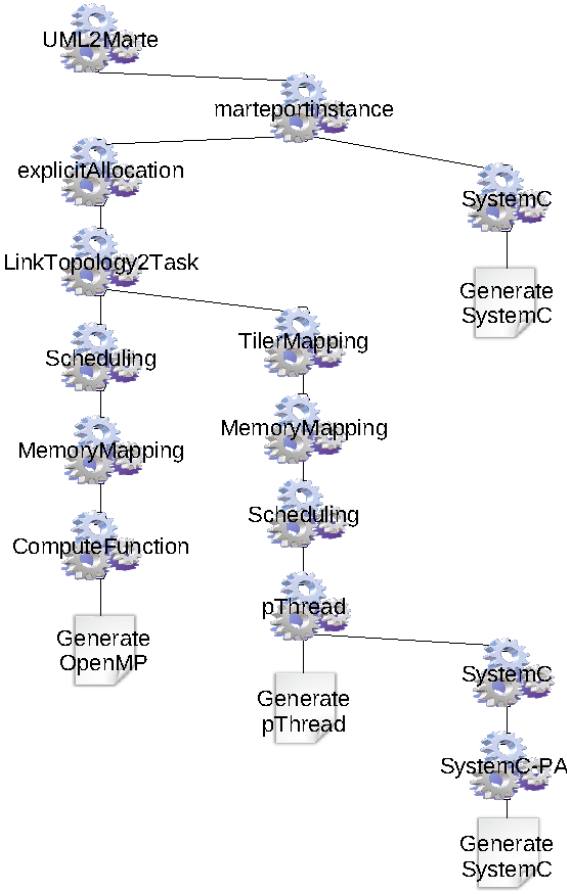


Figure 2. Overview of the transformation chains.

We propose a semi-automation approach that can automatically generate new test model in some cases and efficiently assist the testers in others cases [45].

3.3. Model-based optimization and compilation techniques

Scheduling, Mapping, Compilation, Optimization, Heuristics, Power Consumption, Data-parallelism

3.3.1. Foundations

3.3.1.1. Optimization for parallelism

We study optimization techniques to produce “good” schedules and mappings of a given application onto a hardware SoC architecture. These heuristic techniques aim at fulfilling the requirements of the application, whether they be real time, memory usage or power consumption constraints. These techniques are thus multi-objective and target heterogeneous architectures.

We aim at taking advantage of the parallelism (both data-parallelism and task parallelism) expressed in the application models in order to build efficient heuristics.

Our application model has some good properties that can be exploited by the compiler: it expresses all the potential parallelism of the application, it is an expression of data dependencies –so no dependence analysis is needed–, it is in a single assignment form and unifies the temporal and spatial dimensions of the arrays. This gives to the optimizing compiler all the information it needs and in a readily usable form.

3.3.1.2. Transformation and traceability

Model to model transformations are at the heart of the MDE approach. Anyone wishing to use MDE in its projects is sooner or later facing the question: how to perform the model transformations? The standardization process of Query View Transformation [64] was the opportunity for the development of transformation engine as Viatra, Moflon or Sitra. However, since the standard has been published, only few of investigating tools, such as ATL¹ (a transformation dedicated tool) or Kermeta² (a generalist tool with facilities to manipulate models) are powerful enough to execute large and complex transformations such as in the Gaspard2 framework. None of these engine is fully compliant with the QVT standard. To solve this issue, new engine relying on a subset of the standard recently emerged such as QVTO³ and smartQVT. These engines implement the QVT Operational language.

Traceability may be used for different purposes such as understanding, capturing, tracking and verification on software artifacts during the development life cycle [58]. MDE has as main principle that everything is a model, so trace information is mainly stored as models. Solutions are proposed to keep the trace information in the initials models source or target [71]. The major drawbacks of this solution are that it pollutes the models with additional information and it requires adaptation of the metamodels in order to take into account traceability. Using a separate trace model with a specific semantics has the advantage of keeping trace information independent of initial models [59].

3.3.2. Past contributions of the team on topics continued in 2012

The new team DaRT has been created in order to finalize the works started in the DaRT EPI, and also to explore new topics. We here remind the past contributions of the team on the topics we continued to work on during 2012.

¹<http://www.eclipse.org/m2m/atl>

²<http://www.kermeta.org>

³<http://www.eclipse.org/m2m/qvto/doc>

3.3.2.1. Transformation techniques

In the previous version of Gaspard2, model transformations were complex and monolithic. They were thus hardly evolvable, reusable and maintainable. We thus proposed to decompose complex transformations into smaller ones jointly working in order to build a single output model [56]. These transformations involve different parts of the same input metamodel (e.g. the MARTE metamodel); their application field is localized. The localization of the transformation was ensured by the definition of the intermediary metamodels as delta. The delta metamodel only contains the few concepts involved in the transformation (i.e. modified, or read). The specification of the transformations only uses the concepts of these deltas. We defined the Extend operator to build the complete metamodel from the delta and transposed the corresponding transformations. The complete metamodel corresponds to the merge between the delta and the MARTE metamodel or an intermediary metamodel. The transformation then becomes the chaining of metamodel shifts and the localized transformation. This way to define the model transformations has been used in the Gaspard2 environment. It allowed a better modularity and thus also reusability between the various chains.

3.3.2.2. Traceability

Our traceability solution relies on two models the Local and the Global Trace metamodels. The former is used to capture the traces between the inputs and the outputs of one transformation. The Global Trace metamodel is used to link Local Traces according to the transformation chain. The local trace also proposes an alternative “view” to the common traceability mechanism that does not refer to the execution trace of the transformation engine. It can be used whatever the used transformation language and can easily complete an existing traceability mechanism by providing a more finer grain traceability [43].

Furthermore, based on our trace metamodels, we developed algorithms to ease the model transformation debug. Based on the trace, the localization of an error is eased by reducing the search field to the sequence of the transformation rule calls [44].

3.3.2.3. Modeling for GPU

The model described in UML with Marte profile model is chained in several inout transformations that adds and/or transforms elements in the model. For adding memory allocation concepts to the model, a QVT transformation based on «Memory Allocation Metamodel» provides information to facilitate and optimize the code generation. Then a model to text transformation allows to generate the C code for GPU architecture. Before the standard releases, Acceleo is appropriate to get many aspects from the application and architecture model and transform it in CUDA (.cu, .cpp, .c, .h, Makefile) and OpenCL (.cl, .cpp, .c, .h, Makefile) files. For the code generation, it's required to take into account intrinsic characteristics of the GPUs like data distribution, contiguous memory allocation, kernels and host programs, blocks of threads, barriers and atomic functions.

3.3.2.4. GPGPU code production

The solution of large, sparse systems of linear equations « $Ax=b$ » presents a bottleneck in sequential code executing on CPU. To solve a system bound to Maxwell's equations on Finite Element Method (FEM), a version of conjugate gradient iterative method was implemented in CUDA and OpenCL as well. The aim is to accelerate and verify the parallel code on GPUs. The first results showed a speedup around 6 times against sequential code on CPU. Another approach uses an algorithm that explores the sparse matrix storage format (by rows and by columns). This one did not increase the speedup but it allows to evaluate the impact of the access to the memory.

3.3.2.5. From MARTE to OpenCL.

We have proposed an MDE approach to generate OpenCL code. From an abstract model defined using UML/MARTE, we generate a compilable OpenCL code and then, a functional executable application. As MDE approach, the research results provide, additionally, a tool for project reuse and fast development for not necessarily experts. This approach is an effective operational code generator for the newly released OpenCL standard. Further, although experimental examples use mono device(one GPU) example, this approach provides resources to model applications running on multi devices (homogeneously configured). Moreover, we provide two main contributions for modeling with UML profile to MARTE. On the one hand, an approach to model distributed memory simple aspects, i.e. communication and memory allocations. On the other hand,

an approach for modeling the platform and execution models of OpenCL. During the development of the transformation chain, a hybrid metamodel was proposed for specifying of CPU and GPU programming models. This allows generating other target languages that conform the same memory, platform and execution models of OpenCL, such as CUDA language. Based on other created model to text templates, future works will exploit this multi language aspect. Additionally, intelligent transformations can determine optimization levels in data communication and data access. Several studies show that these optimizations increase remarkably the application performance.

3.3.2.6. *Formal techniques for construction, compilation and analysis of domain-specific languages*

The increasing complexity of software development requires rigorously defined *domain specific modelling languages* (DSML). Model-driven engineering (MDE) allows users to define their language's syntax in terms of *metamodels*. Several approaches for defining operational semantics of DSML have also been proposed [69], [51], [42], [49], [65]. We have also proposed one such approach, based on representing models and metamodels as algebraic specifications, and operational semantics as rewrite rules over those specifications [54], [67]. These approaches allow, in principle, for model execution and for formal analyses of the DSML. However, most of the time, the executions/analyses are performed via transformations to other languages: code generation, resp. translation to the input language of a model checker. The consequence is that the results (e.g., a program crash log, or a counterexample returned by a model checker) may not be straightforward to interpret by the users of a DSML. We have proposed in [66] a formal and operational framework for tracing such results back to the original DSML's syntax and operational semantics, and have illustrated it on SPEM, a language for timed process management.

DOLPHIN Project-Team

3. Scientific Foundations

3.1. Modeling and landscape analysis

The modeling of problems, the analysis of structures (landscapes) of MOPs and the performance assessment of resolution methods are significant topics in the design of optimization methods. The effectiveness of metaheuristics depends on the properties of the problem and its landscape (roughness, convexity, etc). The notion of landscape has been first described in [89] by the way of the study of species evolution. Then, this notion has been used to analyze combinatorial optimization problems.

3.1.1. Modeling of problems

Generally there are several ways of modeling a given problem. First, one has to find the most suitable model for the type of resolution he or she plans to use. The choice can be made after a theoretical analysis of the model, or after computational experiments. The choice of the model depends on the type of method used. For example, a major issue in the design of exact methods is to find tight relaxations for the problem considered.

Let us note that many combinatorial optimization problems of the literature have been studied in their mono-objective form even if a lot of them are naturally of a multi-objective nature.

Therefore, in the DOLPHIN project, we address the modeling of MOPs in two phases. The first one consists in studying the mono-objective version of the problem, where all objectives but one are considered as constraints. In the second phase, we propose methods to adapt the mono-objective models or to create hand-tailored models for the multi-objective case. The models used may come from the first phase, or from the literature.

3.1.2. Analysis of the structure of a problem

The landscape is defined by a neighborhood operator and can be represented by a graph $G = (V, E)$. The vertices represent the solutions of the problem and an edge (e_1, e_2) exists if the solution e_2 can be obtained by an application of the neighborhood operator on the solution e_1 . Then, considering this graph as the ground floor, we elevate each solution to an altitude equals to its cost. We obtain a surface, or landscape, made of peaks, valleys, plateaus, cliffs, etc. The problem lies in the difficulty to have a realistic view of this landscape.

Like others, we believe that the main point of interest in the domain of combinatorial optimization is not the design of the best algorithm for a large number of problems but the search for the most adapted method to an instance or a set of instances of a given problem. Therefore, we are convinced that no ideal metaheuristic, designed as a black-box, may exist.

Indeed, the first studies realized in our research group on the analysis of landscapes of different mono-objective combinatorial optimization problems (traveling salesman problem, quadratic assignment problem) have shown that not only different problems correspond to different structures but also that different instances of the same problem correspond to different structures.

For instance, we have realized a statistical study of the landscapes of the quadratic assignment problem. Some indicators that characterize the landscape of an instance have been proposed and a taxonomy of the instances including three classes has been deduced. Hence it is not enough to adapt the method to the problem under study but it is necessary to specialize it according to the type of the treated instance.

So in its studies of mono-objective problems, the DOLPHIN research group has introduced into the resolution methods some information about the problem to be solved. The landscapes of some combinatorial problems have been studied in order to investigate the intrinsic natures of their instances. The resulting information has been inserted into an optimization strategy and has allowed the design of efficient and robust hybrid methods. The extension of these studies to multi-objective problems is a part of the DOLPHIN project [87], [88].

3.1.3. Performance assessment

The DOLPHIN project is also interested in the performance assessment of multi-objective optimization methods. Nowadays, statistical techniques developed for mono-objective problems can be adapted to the multi-objective case. Nevertheless, specific tools are necessary in many situations: for example, the comparison of two different algorithms is relatively easy in the mono-objective case - we compare the quality of the best solution obtained in a fixed time, or the time needed to obtain a solution of a certain quality. The same idea cannot be immediately transposed to the case where the output of the algorithms is a set of solutions having several quality measures, and not a single solution.

Various indicators have been proposed in the literature for evaluating the performance of multi-objective optimization methods but no indicator seems to outperform the others [90]. The DOLPHIN research group has proposed two indicators: the *contribution* and the *entropy* [82]. The contribution evaluates the supply in term of Pareto-optimal solutions of a front compared to another one. The entropy gives an idea of the diversity of the solutions found. These two metrics are used to compare the different metaheuristics in the research group, for example in the resolution of the bi-objective flow-shop problem, and also to show the contribution of the various mechanisms introduced in these metaheuristics.

3.1.4. Goals

One of the main issues in the DOLPHIN project is the study of the landscape of multi-objective problems and the performance assessment of multi-objective optimization methods to design efficient and robust resolution methods:

- *Landscape study*: The goal here is to extend the study of landscapes of the mono-objective combinatorial optimization problems to multi-objective problems in order to determine the structure of the Pareto frontier and to integrate this knowledge about the problem structure in the design of resolution methods.

This study has been initiated for the bi-objective flow-shop problem. We have studied the convexity of the frontiers obtained in order to show the interest of our Pareto approach compared to an aggregation approach, which only allows one to obtain the Pareto solutions situated on the convex hull of the Pareto front (supported solutions).

Our preliminary study of the landscape of the bi-objective flow-shop problem shows that the supported solutions are very closed to each other. This remark leads us to improve an exact method initially proposed for bi-objective problems. Furthermore, a new exact method able to deal with any number of objectives has been designed.

- *Performance assessment*: The goal here is to extend *GUIMOO* in order to provide efficient visual and metric tools for evaluating the assessment of multi-objective resolution methods.

3.2. Hybrid multi-objective optimization methods

The success of metaheuristics is based on their ability to find efficient solutions in a reasonable time [76]. But with very large problems and/or multi-objective problems, efficiency of metaheuristics may be compromised. Hence, in this context it is necessary to integrate metaheuristics in more general schemes in order to develop even more efficient methods. For instance, this can be done by different strategies such as cooperation and parallelization.

The DOLPHIN project deals with “*a posteriori*” multi-objective optimization where the set of Pareto solutions (solutions of best compromise) have to be generated in order to give the decision maker the opportunity to choose the solution that interests him/her.

Population-based methods, such as evolutionary algorithms, are well fitted for multi-objective problems, as they work with a set of solutions [59], [74]. To be convinced one may refer to the list of references on Evolutionary Multi-objective Optimization maintained by Carlos A. Coello Coello ⁴, which contains more

⁴<http://www.lania.mx/~ccoello/EMOO/EMOObib.html>

than 5500 references. One of the objectives of the project is to propose advanced search mechanisms for intensification and diversification. These mechanisms have been designed in an adaptive manner, since their effectiveness is related to the landscape of the MOP and to the instance solved.

In order to assess the performances of the proposed mechanisms, we always proceed in two steps: first, we carry out experiments on academic problems, for which some best known results exist; second, we use real industrial problems to cope with large and complex MOPs. The lack of references in terms of optimal or best known Pareto set is a major problem. Therefore, the obtained results in this project and the test data sets will be available at the URL <http://dolphin.lille.inria.fr/> at 'benchmark'.

3.2.1. Cooperation of metaheuristics

In order to benefit from the various advantages of the different metaheuristics, an interesting idea is to combine them. Indeed, the hybridization of metaheuristics allows the cooperation of methods having complementary behaviors. The efficiency and the robustness of such methods depend on the balance between the exploration of the whole search space and the exploitation of interesting areas.

Hybrid metaheuristics have received considerable interest these last years in the field of combinatorial optimization. A wide variety of hybrid approaches have been proposed in the literature and give very good results on numerous single objective optimization problems, which are either academic (traveling salesman problem, quadratic assignment problem, scheduling problem, etc) or real-world problems. This efficiency is generally due to the combinations of single-solution based methods (iterative local search, simulated annealing, tabu search, etc) with population-based methods (genetic algorithms, ants search, scatter search, etc). A taxonomy of hybridization mechanisms may be found in [84]. It proposes to decompose these mechanisms into four classes:

- *LRH class - Low-level Relay Hybrid*: This class contains algorithms in which a given metaheuristic is embedded into a single-solution metaheuristic. Few examples from the literature belong to this class.
- *LTH class - Low-level Teamwork Hybrid*: In this class, a metaheuristic is embedded into a population-based metaheuristic in order to exploit strengths of single-solution and population-based metaheuristics.
- *HRH class - High-level Relay Hybrid*: Here, self contained metaheuristics are executed in a sequence. For instance, a population-based metaheuristic is executed to locate interesting regions and then a local search is performed to exploit these regions.
- *HTH class - High-level Teamwork Hybrid*: This scheme involves several self-contained algorithms performing a search in parallel and cooperating. An example will be the island model, based on GAs, where the population is partitioned into small subpopulations and a GA is executed per subpopulation. Some individuals can migrate between subpopulations.

Let us notice, that if hybrid methods have been studied in the mono-criterion case, their application in the multi-objective context is not yet widely spread. The objective of the DOLPHIN project is to integrate specificities of multi-objective optimization into the definition of hybrid models.

3.2.2. Cooperation between metaheuristics and exact methods

Until now only few exact methods have been proposed to solve multi-objective problems. They are based either on a Branch-and-bound approach, on the algorithm A^{\star} , or on dynamic programming. However, these methods are limited to two objectives and, most of the time, cannot be used on a complete large scale problem. Therefore, sub search spaces have to be defined in order to use exact methods. Hence, in the same manner as hybridization of metaheuristics, the cooperation of metaheuristics and exact methods is also a main issue in this project. Indeed, it allows us to use the exploration capacity of metaheuristics, as well as the intensification ability of exact methods, which are able to find optimal solutions in a restricted search space. Sub search spaces have to be defined along the search. Such strategies can be found in the literature, but they are only applied to mono-objective academic problems.

We have extended the previous taxonomy for hybrid metaheuristics to the cooperation between exact methods and metaheuristics. Using this taxonomy, we are investigating cooperative multi-objective methods. In this context, several types of cooperations may be considered, according to the way the metaheuristic and the exact method cooperate. For instance, a metaheuristic can use an exact method for intensification or an exact method can use a metaheuristic to reduce the search space.

Moreover, a part of the DOLPHIN project deals with studying exact methods in the multi-objective context in order: i) to be able to solve small size problems and to validate proposed heuristic approaches; ii) to have more efficient/dedicated exact methods that can be hybridized with metaheuristics. In this context, the use of parallelism will push back limits of exact methods, which will be able to explore larger size search spaces [68].

3.2.3. Goals

Based on the previous works on multi-objective optimization, it appears that to improve metaheuristics, it becomes essential to integrate knowledge about the problem structure. This knowledge can be gained during the search. This would allow us to adapt operators which may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure. Moreover, regarding the hybridization and the cooperation aspects, the objectives of the DOLPHIN project are to deepen these studies as follows:

- *Design of metaheuristics for the multi-objective optimization:* To improve metaheuristics, it becomes essential to integrate knowledge about the problem structure, which we may get during the execution. This would allow us to adapt operators that may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure.
- *Design of cooperative metaheuristics:* Previous studies show the interest of hybridization for a global optimization and the importance of problem structure study for the design of efficient methods. It is now necessary to generalize hybridization of metaheuristics and to propose adaptive hybrid models that may evolve during the search while selecting the appropriate metaheuristic. Multi-objective aspects have to be introduced in order to cope with the specificities of multi-objective optimization.
- *Design of cooperative schemes between exact methods and metaheuristics:* Once the study on possible cooperation schemes is achieved, we will have to test and compare them in the multi-objective context.
- *Design and conception of parallel metaheuristics:* Our previous works on parallel metaheuristics allow us to speed up the resolution of large scale problems. It could be also interesting to study the robustness of the different parallel models (in particular in the multi-objective case) and to propose rules that determine, given a specific problem, which kind of parallelism to use. Of course these goals are not disjointed and it will be interesting to simultaneously use hybrid metaheuristics and exact methods. Moreover, those advanced mechanisms may require the use of parallel and distributed computing in order to easily make cooperating methods evolve simultaneously and to speed up the resolution of large scale problems.
- *Validation:* In order to validate the obtained results we always proceed in two phases: validation on academic problems, for which some best known results exist and use on real problems (industrial) to cope with problem size constraints.

Moreover, those advanced mechanisms are to be used in order to integrate the distributed multi-objective aspects in the ParadisEO platform (see the paragraph on software platform).

3.3. Parallel multi-objective optimization: models and software frameworks

Parallel and distributed computing may be considered as a tool to speedup the search to solve large MOPs and to improve the robustness of a given method. Moreover, the joint use of parallelism and cooperation allows improvements on the quality of the obtained Pareto sets. Following this objective, we will design and implement parallel models for metaheuristics (evolutionary algorithms, tabu search approach) and exact methods (branch-and-bound algorithm, branch-and-cut algorithm) to solve different large MOPs.

One of the goal of the DOLPHIN project is to integrate the developed parallel models into software frameworks. Several frameworks for parallel distributed metaheuristics have been proposed in the literature. Most of them focus only either on evolutionary algorithms or on local search methods. Only few frameworks are dedicated to the design of both families of methods. On the other hand, existing optimization frameworks either do not provide parallelism at all or just supply at most one parallel model. In this project, a new framework for parallel hybrid metaheuristics is proposed, named *Parallel and Distributed Evolving Objects (ParadisEO)* based on EO. The framework provides in a transparent way the hybridization mechanisms presented in the previous section, and the parallel models described in the next section. Concerning the developed parallel exact methods for MOPs, we will integrate them into well-known frameworks such as COIN.

3.3.1. Parallel models

According to the family of addressed metaheuristics, we may distinguish two categories of parallel models: parallel models that manage a single solution, and parallel models that handle a population of solutions. The major single solution-based parallel models are the following: the *parallel neighborhood exploration model* and the *multi-start model*.

- The *parallel neighborhood exploration model* is basically a "low level" model that splits the neighborhood into partitions that are explored and evaluated in parallel. This model is particularly interesting when the evaluation of each solution is costly and/or when the size of the neighborhood is large. It has been successfully applied to the mobile network design problem (see Application section).
- The *multi-start model* consists in executing in parallel several local searches (that may be heterogeneous), without any information exchange. This model raises particularly the following question: is it equivalent to execute k local searches during a time t than executing a single local search during $k \times t$? To answer this question we tested a multi-start Tabu search on the quadratic assignment problem. The experiments have shown that the answer is often landscape-dependent. For example, the multi-start model may be well-suited for landscapes with multiple basins.

Parallel models that handle a population of solutions are mainly: the *island model*, the *central model* and the *distributed evaluation of a single solution*. Let us notice that the last model may also be used with single-solution metaheuristics.

- In the *island model*, the population is split into several sub-populations distributed among different processors. Each processor is responsible of the evolution of one sub-population. It executes all the steps of the metaheuristic from the selection to the replacement. After a given number of generations (synchronous communication), or when a convergence threshold is reached (asynchronous communication), the migration process is activated. Then, exchanges of solutions between sub-populations are realized, and received solutions are integrated into the local sub-population.
- The *central (Master/Worker) model* allows us to keep the sequentiality of the original algorithm. The master centralizes the population and manages the selection and the replacement steps. It sends sub-populations to the workers that execute the recombination and evaluation steps. The latter returns back newly evaluated solutions to the master. This approach is efficient when the generation and evaluation of new solutions is costly.
- The *distributed evaluation model* consists in a parallel evaluation of each solution. This model has to be used when, for example, the evaluation of a solution requires access to very large databases (data mining applications) that may be distributed over several processors. It may also be useful in a multi-objective context, where several objectives have to be computed simultaneously for a single solution.

As these models have now been identified, our objective is to study them in the multi-objective context in order to use them advisedly. Moreover, these models may be merged to combine different levels of parallelism and to obtain more efficient methods [73], [83].

3.3.2. Goals

Our objectives focus on these issues are the following:

- *Design of parallel models for metaheuristics and exact methods for MOPs:* We will develop parallel cooperative metaheuristics (evolutionary algorithms and local search algorithms such as the Tabu search) for solving different large MOPs. Moreover, we are designing a new exact method, named PPM (Parallel Partition Method), based on branch and bound and branch and cut algorithms. Finally, some parallel cooperation schemes between metaheuristics and exact algorithms have to be used to solve MOPs in an efficient manner.
- *Integration of the parallel models into software frameworks:* The parallel models for metaheuristics will be integrated in the ParadisEO software framework. The proposed multi-objective exact methods must be first integrated into standard frameworks for exact methods such as COIN and BOB++. A *coupling* with ParadisEO is then needed to provide hybridization between metaheuristics and exact methods.
- *Efficient deployment of the parallel models on different parallel and distributed architecture including GRIDs:* The designed algorithms and frameworks will be efficiently deployed on non-dedicated networks of workstations, dedicated cluster of workstations and SMP (Symmetric Multi-processors) machines. For GRID computing platforms, peer to peer (P2P) middlewares (XtremWeb-Condor) will be used to implement our frameworks. For this purpose, the different optimization algorithms may be re-visited for their efficient deployment.

MODAL Project-Team

3. Scientific Foundations

3.1. Generative model design

The first objective of MODAL consists in designing, analyzing, estimating and evaluating new generative parametric models for multivariate and/or heterogeneous data. It corresponds typically to continuous and categorical data but it includes also other widespread ones like ordinal, functional, ranks,... Designed models have to take into account potential correlations between variables while being (1) justifiable and realistic, (2) meaningful and parsimoniously parameterized, (3) of low computational complexity. The main purpose is to identify a few theoretical and general principles for model generation, loosely dependent on the variable nature. In this context, we propose two concurrent approaches which could be general enough for dealing with correlation between many types of homogeneous or heterogeneous variables:

- Designs general models by combining two extreme models (full dependent and full independent) which are well-defined for most of variables;
- Uses kernels as a general way for dealing with multivariate and heterogeneous variables.

3.2. Data visualization

The second objective of MODAL is to propose meaningful and quite accurate low dimensional visualizations of data typically in two-dimensional (2D) space, less frequently in one-dimensional (1D) or three-dimensional (3D) spaces, by using the generative models designed in the first objective. We propose also to visualize simultaneously the data and the model. All visualizations will depend on the aim at hand (typically clustering, classification or density estimation). The main originality of this objective lies in the use of models for visualization, strategy from which we expect to have a better control on the subjectivity necessarily induced by any graphical display. In addition, the proposed approach has to be general enough to be independent on the variable nature. Note that the visualization objective is consistent with the dissemination of our methodologies through specific softwares. Indeed, displaying data is an important step in the data analysis process.

NON-A Project-Team

3. Scientific Foundations

3.1. Fast parametric estimation and its applications

Parametric estimation may often be formalized as follows:

$$y = F(x, \Theta) + n, \quad (1)$$

where:

- the measured signal y is a functional F of the "true" signal x , which depends on a set Θ of parameters,
- n is a noise corrupting the observation.

Finding a "good" approximation of the components of Θ has been the subject of a huge literature in various fields of applied mathematics. Most of those researches have been done in a probabilistic setting, which necessitates a good knowledge of the statistical properties of n . Our project is devoted to a new standpoint, which does not require this knowledge and which is based on the following tools, which are of algebraic flavor:

- differential algebra ², which plays with respect to differential equations a similar role that the commutative algebra plays with respect to algebraic equations;
- module theory, i.e. linear algebra over rings, which are not necessarily commutative;
- operational calculus, which is the most classical tool among control and mechanical engineers ³.

3.1.1. Linear identifiability

In the most problems, which appear in linear control as well as in signal processing, the unknown parameters are *linearly identifiable*: standard elimination procedures are yielding the following matrix equation

$$P \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_r \end{pmatrix} = Q, \quad (2)$$

where:

- $\theta_i, 1 \leq i \leq r$ represents unknown parameter,
- P is a $r \times r$ square matrix and Q is a $r \times 1$ column matrix,
- the entries of P and Q are finite linear combinations of terms of the form $t^\nu \frac{d^\mu \xi}{dt^\mu}$, $\mu, \nu \geq 0$, where ξ is an input or output signal,
- the matrix P is *generically* invertible, i.e., $\det(P) \neq 0$.

3.1.2. How to deal with perturbations and noises?

With noisy measurements equation (2) becomes:

²Differential algebra was introduced in nonlinear control theory by one of us almost twenty years ago for understanding some specific questions like input-output inversion. It allowed us to recast the whole of nonlinear control into a more realistic light. The best example is of course the discovery of *flat* systems, which are now quite popular in industry.

³Operational calculus is often formalized *via* the Laplace transform whereas the Fourier transform is today the cornerstone in estimation. Note that the one-sided Laplace transform is causal, but the Fourier transform over \mathbb{R} is not.

$$P \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_r \end{pmatrix} = Q + R, \quad (3)$$

where R is a $r \times 1$ column matrix, whose entries are finite linear combinations of terms of the form $t^\nu \frac{d^\mu \eta}{dt^\mu}$, $\mu, \nu \geq 0$, where η is a perturbation or a noise.

3.1.2.1. Structured perturbations

A perturbation π is said to be *structured* if, and only if, it can be annihilated by a linear differential operator of the form $\sum_{\text{finite}} a_k(t) \frac{d^k}{dt^k}$, where $a_k(t)$ is a rational function of t , i.e. $\left(\sum_{\text{finite}} a_k(t) \frac{d^k}{dt^k} \right) \pi = 0$. Note that many classical perturbations, like a constant bias, are annihilated by such an operator. An *unstructured* noise cannot be annihilated by a non-zero differential operator.

By well-known properties of the non-commutative ring of differential operators, we can multiply both sides of equation (3) by a suitable differential operator Δ such that equation (3) becomes:

$$\Delta P \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_r \end{pmatrix} = \Delta Q + R', \quad (4)$$

where the entries of the $r \times 1$ column matrix R' are unstructured noises.

3.1.2.2. Attenuating unstructured noises

Unstructured noises are usually dealt with stochastic processes like white Gaussian noises. They are considered here as highly fluctuating phenomena, which may therefore be attenuated *via* low pass filters. Note that no precise knowledge of the statistical properties of the noises is required.

3.1.2.3. Comments

Although the previous noise attenuation procedure⁴ may be fully explained *via* formula (4), its theoretical comparison⁵ with today's literature⁶ has yet to be done. It will require a complete resetting of the notions of noises and perturbations. Besides some connections with physics, it might lead to quite new "epistemological" issues [101].

3.1.3. Some hints on the calculations

The time derivatives of the input and output signals appearing in equations (2), (3), (4) can be suppressed in the two following ways which might be combined:

- integrate both sides of the equation a sufficient number of times,
- take the convolution product of both sides by a suitable low pass filter.

The numerical values of the unknown parameters $\Theta = (\theta_1, \dots, \theta_r)$ can be obtained by integrating both sides of the modified equation (4) during a very short time interval.

3.1.4. A first, very simple example

Let us illustrate on a very basic example, the grounding ideas of the algebraic approach. For this purpose consider the first order linear system:

⁴It is reminiscent to that the most practitioners in electronics are doing.

⁵Let us stress again that many computer simulations and several laboratory experiments have been already successfully achieved and can be quite favorably compared with the existing techniques.

⁶Especially in signal processing.

$$\dot{y}(t) = ay(t) + u(t) + \gamma_0, \tag{5}$$

where a is an unknown parameter to be identified and γ_0 is an unknown constant perturbation. With the notations of operational calculus and $y_0 = y(0)$, equation (5) reads:

$$s\hat{y}(s) = a\hat{y}(s) + \hat{u}(s) + y_0 + \frac{\gamma_0}{s} \tag{6}$$

where $\hat{y}(s)$ represents the Laplace transform of $y(t)$.

In order to eliminate the term γ_0 , multiply first the both hand-sides of this equation by s and next take their derivatives with respect to s :

$$\frac{d}{ds} \left[s \left\{ s\hat{y}(s) = a\hat{y}(s) + \hat{u}(s) + y_0 + \frac{\gamma_0}{s} \right\} \right] \tag{7}$$

$$\Rightarrow 2s\hat{y}(s) + s^2\hat{y}'(s) = a(s\hat{y}'(s) + \hat{y}(s)) + s\hat{u}'(s) + \hat{u}(s) + y_0. \tag{8}$$

Recall that $\hat{y}'(s) \triangleq \frac{d\hat{y}(s)}{ds}$ corresponds to $-ty(t)$. Assume $y_0 = 0$ for simplicity of presentation ⁷. Then for any $\nu > 0$,

$$s^{-\nu} [2s\hat{y}(s) + s^2\hat{y}'(s)] = s^{-\nu} [a(s\hat{y}'(s) + \hat{y}(s)) + s\hat{u}'(s) + \hat{u}(s)]. \tag{9}$$

For $\nu = 3$, we obtained the estimated value a :

$$a = \frac{2 \int_0^T d\lambda \int_0^\lambda y(t)dt - \int_0^T ty(t)dt + \int_0^T d\lambda \int_0^\lambda tu(t)dt - \int_0^T d\lambda \int_0^\lambda d\sigma \int_0^\sigma u(t)dt}{\int_0^T d\lambda \int_0^\lambda d\sigma \int_0^\sigma y(t)dt - \int_0^T d\lambda \int_0^\lambda ty(t)dt} \tag{10}$$

Since $T > 0$ can be very small, estimation *via* (10) is very fast.

Note that equation (10) represents an on-line algorithm, which involves only two kinds of operations on u and y : (1) multiplications by t , and (2) integrations over a pre-selected time interval.

If we now consider an additional noise of zero mean in (5), say:

$$\dot{y}(t) = ay(t) + u(t) + \gamma_0 + n(t), \tag{11}$$

it can be considered as a fast fluctuating signal. The order ν in (9) determines the order of iterations in the integrals (3 integrals in (10)). Those iterated integrals are low-pass filters which are attenuating the fluctuations.

This example, even simple, clearly demonstrates how algebraic techniques proceed:

- they are algebraic: operations on s -functions;
- they are non-asymptotic: parameter a is obtained from (10) in a finite time;
- they are deterministic: no knowledge of the statistical properties of the noise n is required.

⁷If $y_0 \neq 0$ one has to take above derivatives of order 2 with respect to s , in order to eliminate the initial condition.

3.1.5. A second simple example, with delay

Consider the first order, linear system with constant input delay ⁸:

$$\dot{y}(t) + ay(t) = y(0)\delta + \gamma_0 H + bu(t - \tau). \quad (12)$$

Here we use a distributional-like notation, where δ denotes the Dirac impulse and H is its integral, i.e. the Heaviside function (unit step) ⁹. Still for simplicity, we suppose that the parameter a is known. The parameter to be identified is now the delay τ . As previously, γ_0 is a constant perturbation, a , b , and τ are constant parameters. Consider also a step input $u = u_0 H$. A first order derivation yields:

$$\ddot{y} + a\dot{y} = \varphi_0 + \gamma_0 \delta + b u_0 \delta_\tau, \quad (13)$$

where δ_τ denotes the delayed Dirac impulse and $\varphi_0 = (\dot{y}(0) + ay(0))\delta + y(0)\delta^{(1)}$, of order 1 and support $\{0\}$, contains the contributions of the initial conditions. According to Schwartz theorem, multiplication by a function α such that $\alpha(0) = \alpha'(0) = 0$, $\alpha(\tau) = 0$ yields interesting simplifications. For instance, choosing $\alpha(t) = t^3 - \tau t^2$ leads to the following equalities (to be understood in the distributional framework):

$$\begin{aligned} t^3 [\ddot{y} + a\dot{y}] &= \tau t^2 [\ddot{y} + a\dot{y}], \\ b u_0 t^3 \delta_\tau &= b u_0 \tau t^2 \delta_\tau. \end{aligned} \quad (14)$$

The delay τ becomes available from $k \geq 1$ successive integrations (represented by the operator H), as follows:

$$\tau = \frac{H^k(w_0 + a w_3)}{H^k(w_1 + a w_2)}, \quad t > \tau, \quad (15)$$

where the w_i are defined using the notation $z_i = t^i y$ by:

$$\begin{aligned} w_0 &= t^3 y^{(2)} = -6 z_1 + 6 z_2^{(1)} - z_3^{(2)}, \\ w_1 &= t^2 y^{(2)} = -2 z_0 + 4 z_1^{(1)} - z_2^{(2)}, \\ w_2 &= t^2 y^{(1)} = 2 z_1 - z_2^{(1)}, \\ w_3 &= t^3 y^{(1)} = 3 z_2 - z_3^{(1)}. \end{aligned}$$

These coefficients show that $k \geq 2$ integrations avoid any derivation in the delay identification.

Figure 1 gives a numerical simulation with $k = 2$ integrations and $a = 2, b = 1, \tau = 0.6, y(0) = 0.3, \gamma_0 = 2, u_0 = 1$. Due to the non identifiability over $(0, \tau)$, the delay τ is set to zero until the numerator or the denominator in the right hand side of (15) reaches a significant nonzero value.

Again, note the realization algorithm (15) involves two kinds of operators: (1) integrations and (2) multiplications by t . It relies on the measurement of y and on the knowledge of a . If a is also unknown, the same approach can be utilized for a simultaneous identification of a and τ . The following relation is derived from (14):

⁸This example is taken from [93]. For further details, we suggest the reader to refer to it.

⁹In this document, for the sake of simplicity, we make an abuse of the language since we merge in a single notation the Heaviside function H and the integration operator. To be rigorous, the iterated integration (k times) corresponds, in the operational domain, to a division by s^k , whereas the convolution with H (k times) corresponds to a division by $s^k / (k - 1)!$. For $k = 0$, there is no difference and $H * y$ realizes the integration of y . More generally, since we will always apply these operations to complete equations (left- and right-hand sides), the factor $(k - 1)!$ makes no difference.

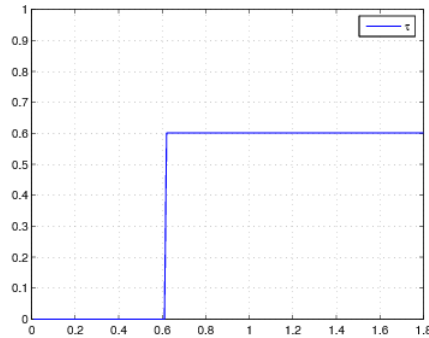


Figure 1. Delay τ identification from algorithm (15)

$$\tau(H^k w_1) + a \tau(H^k w_2) - a(H^k w_3) = H^k w_0, \tag{16}$$

and a linear system with unknown parameters (τ, a, τ, a) is obtained by using different integration orders:

$$\begin{pmatrix} H^2 w_1 & H^2 w_2 & H^2 w_3 \\ H^3 w_1 & H^3 w_2 & H^3 w_3 \\ H^4 w_1 & H^4 w_2 & H^4 w_3 \end{pmatrix} \begin{pmatrix} \hat{\tau} \\ \hat{a}\tau \\ -\hat{a} \end{pmatrix} = \begin{pmatrix} H^2 w_0 \\ H^3 w_0 \\ H^4 w_0 \end{pmatrix}.$$

The resulting numerical simulations are shown in Figure 2. For identifiability reasons, the obtained linear system may be not consistent for $t < \tau$.

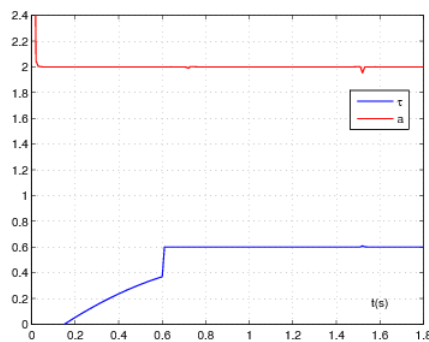


Figure 2. Simultaneous identification of a and τ from algorithm (16)

3.2. Finite time estimation of derivatives

Numerical differentiation, i.e. determining the time derivatives of various orders of a noisy time signal, is an important but difficult ill-posed theoretical problem. This fundamental issue has attracted a lot of attention in many fields of engineering and applied mathematics (see, e.g. in the recent control literature [94], [95], [109], [108], [115], [116], and the references therein).

3.2.1. Model-free techniques for numerical differentiation

A common way of estimating the derivatives of a signal is to resort to a least squares fitting and then take the derivatives of the resulting function. In [119], [117] this problem was revised through our algebraic approach. The approach can be briefly explained as follows:

- The coefficients of a polynomial time function are linearly identifiable. Their estimation can therefore be achieved as above. Indeed, consider a real-valued polynomial function $x_N(t) = \sum_{\nu=0}^N x^{(\nu)}(0) \frac{t^\nu}{\nu!} \in \mathbb{R}[t]$, $t \geq 0$, of degree N . Rewrite it in the well-known notations of operational calculus:

$$X_N(s) = \sum_{\nu=0}^N \frac{x^{(\nu)}(0)}{s^{\nu+1}}.$$

Here we use $\frac{d}{ds}$, which corresponds in the time domain to the multiplication by $-t$. Multiply both sides by $\frac{d^\alpha}{ds^\alpha} s^{N+1}$, $\alpha = 0, 1, \dots, N$. The quantities $x^{(\nu)}(0)$, $\nu = 0, 1, \dots, N$ are given by the triangular system of linear equations:

$$\frac{d^\alpha s^{N+1} X_N}{ds^\alpha} = \frac{d^\alpha}{ds^\alpha} \left(\sum_{\nu=0}^N x^{(\nu)}(0) s^{N-\nu} \right). \quad (17)$$

The time derivatives, i.e. $s^\mu \frac{d^\mu X_N}{ds^\mu}$, $\mu = 1, \dots, N$, $0 \leq \nu \leq N$ are removed by multiplying both sides of Equation (17) by s^{-N} , $N > N$.

- For an arbitrary analytic time function, let us apply the preceding calculations to a suitable truncated Taylor expansion. Consider a real-valued analytic time function defined by the convergent power series $x(t) = \sum_{\nu=0}^{\infty} x^{(\nu)}(0) \frac{t^\nu}{\nu!}$, where $0 \leq t < \rho$. Approximate $x(t)$ in the interval $(0, \varepsilon)$, $0 < \varepsilon \leq \rho$ by its truncated Taylor expansion $x_N(t) = \sum_{\nu=0}^N x^{(\nu)}(0) \frac{t^\nu}{\nu!}$ of order N . Introduce the operational analogue of $x(t)$, i.e. $X(s) = \sum_{\nu \geq 0} \frac{x^{(\nu)}(0)}{s^{\nu+1}}$. Denote by $[x^{(\nu)}(0)]_{e_N}(t)$, $0 \leq \nu \leq N$, the numerical estimate of $x^{(\nu)}(0)$, which is obtained by replacing $X_N(s)$ by $X(s)$ in Eq. (17). It can be shown [104] that a good estimate is obtained in this way.

Thus using elementary differential algebraic operations, we derive an explicit formulae yielding point-wise derivative estimation for each given order. Interesting enough, it turns out that the Jacobi orthogonal polynomials [129] are inherently connected with the developed algebraic numerical differentiators. A least-squares interpretation then naturally follows [118], [119] and this leads to a key result: the algebraic numerical differentiation is as efficient as an appropriately chosen time delay. Though, such a delay may not be tolerable in some real-time applications. Moreover, instability generally occurs when introducing delayed signals in a control loop. Note however that since the delay is known *a priori*, it is always possible to derive a control law, which compensates for its effects (see [127]). A second key feature of the algebraic numerical differentiators is its very low complexity which allows for a real-time implementation. Indeed, the n^{th} order derivative estimate (that can be directly managed for $n \geq 2$, without using n cascaded estimators) is expressed as the output of the linear time-invariant filter, with finite support impulse response $h_{\kappa, \mu, n, r}(\cdot)$. Implementing such a stable and causal filter is easy and simple. This is achieved either in continuous-time or in discrete-time when only discrete-time samples of the observation are available. In the latter case, we obtain a tapped delay line digital filter by considering any numerical integration method with equally-spaced abscissas.

3.2.2. Model-based estimation of derivatives

If we assume that the derivatives to be estimated are unmeasured states of a process that generates the signal, then the differentiation techniques can be considered as left invertibility algorithms. In this sense, the previous algebraic estimation achieves a “model-free” left inversion. Now, when such a model is available, the *finite-time observers* relying on higher order sliding modes [123] and homogeneity properties [124], [120] also represent possible non-asymptotic algorithms for differentiation¹⁰. Using such model-based techniques appears to be complementary¹¹. The left-inversion results have been already obtained for several classes of models: linear systems [106], nonlinear systems [92], delay systems [2] and hybrid systems [114].

¹⁰Usually, observer design yields asymptotic convergence of the estimation error dynamics. The main advantages of such a technique in the case of linear systems are simplicity of design, estimation with a filtering action and global stability property. Nevertheless, the filtering property is not ensured for nonlinear systems and the stability property is generally obtained only locally. For these reasons, in the case of nonlinear systems, finite-time observers and estimators have been proposed in the literature [116], [124], [125], [105]...

¹¹The choice between the two approaches will be done after comparison with respect to the indicators 1–3, and taking into account the application (for instance, the system bandwidth, system dimension), the kind of discontinuity, the observer in the control loop or not...

SEQUEL Project-Team

3. Scientific Foundations

3.1. Introduction

SEQUEL is primarily grounded on two domains:

- the problem of decision under uncertainty,
- statistical analysis and statistical learning, which provide the general concepts and tools to solve this problem.

To help the reader who is unfamiliar with these questions, we briefly present key ideas below.

3.2. Decision-making Under Uncertainty

The phrase “Decision under uncertainty” refers to the problem of taking decisions when we do not have a full knowledge neither of the situation, nor of the consequences of the decisions, as well as when the consequences of decision are non deterministic.

We introduce two specific sub-domains, namely the Markov decision processes which models sequential decision problems, and bandit problems.

3.2.1. Reinforcement Learning

Sequential decision processes occupy the heart of the SEQUEL project; a detailed presentation of this problem may be found in Puterman’s book [70].

A Markov Decision Process (MDP) is defined as the tuple $(\mathcal{X}, \mathcal{A}, P, r)$ where \mathcal{X} is the state space, \mathcal{A} is the action space, P is the probabilistic transition kernel, and $r : \mathcal{X} \times \mathcal{A} \times \mathcal{X} \rightarrow \mathbb{R}$ is the reward function. For the sake of simplicity, we assume in this introduction that the state and action spaces are finite. If the current state (at time t) is $x \in \mathcal{X}$ and the chosen action is $a \in \mathcal{A}$, then the Markov assumption means that the transition probability to a new state $x' \in \mathcal{X}$ (at time $t + 1$) only depends on (x, a) . We write $p(x'|x, a)$ the corresponding transition probability. During a transition $(x, a) \rightarrow x'$, a reward $r(x, a, x')$ is incurred.

In the MDP $(\mathcal{X}, \mathcal{A}, P, r)$, each initial state x_0 and action sequence a_0, a_1, \dots gives rise to a sequence of states x_1, x_2, \dots , satisfying $\mathbb{P}(x_{t+1} = x' | x_t = x, a_t = a) = p(x'|x, a)$, and rewards r_1, r_2, \dots defined by $r_t = r(x_t, a_t, x_{t+1})$.

The history of the process up to time t is defined to be $H_t = (x_0, a_0, \dots, x_{t-1}, a_{t-1}, x_t)$. A policy π is a sequence of functions π_0, π_1, \dots , where π_t maps the space of possible histories at time t to the space of probability distributions over the space of actions \mathcal{A} . To follow a policy means that, in each time step, we assume that the process history up to time t is x_0, a_0, \dots, x_t and the probability of selecting an action a is equal to $\pi_t(x_0, a_0, \dots, x_t)(a)$. A policy is called stationary (or Markovian) if π_t depends only on the last visited state. In other words, a policy $\pi = (\pi_0, \pi_1, \dots)$ is called stationary if $\pi_t(x_0, a_0, \dots, x_t) = \pi_0(x_t)$ holds for all $t \geq 0$. A policy is called deterministic if the probability distribution prescribed by the policy for any history is concentrated on a single action. Otherwise it is called a stochastic policy.

We move from an MD process to an MD problem by formulating the goal of the agent, that is what the sought policy π has to optimize? It is very often formulated as maximizing (or minimizing), in expectation, some functional of the sequence of future rewards. For example, an usual functional is the infinite-time horizon sum of discounted rewards. For a given (stationary) policy π , we define the value function $V^\pi(x)$ of that policy π at a state $x \in \mathcal{X}$ as the expected sum of discounted future rewards given that we state from the initial state x and follow the policy π :

¹Note that for simplicity, we considered the case of a deterministic reward function, but in many applications, the reward r_t itself is a random variable.

$$V^\pi(x) = \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r_t | x_0 = x, \pi \right], \quad (18)$$

where \mathbb{E} is the expectation operator and $\gamma \in (0, 1)$ is the discount factor. This value function V^π gives an evaluation of the performance of a given policy π . Other functionals of the sequence of future rewards may be considered, such as the undiscounted reward (see the stochastic shortest path problems [66]) and average reward settings. Note also that, here, we considered the problem of maximizing a reward functional, but a formulation in terms of minimizing some cost or risk functional would be equivalent.

In order to maximize a given functional in a sequential framework, one usually applies Dynamic Programming (DP) [64], which introduces the optimal value function $V^*(x)$, defined as the optimal expected sum of rewards when the agent starts from a state x . We have $V^*(x) = \sup_{\pi} V^\pi(x)$. Now, let us give two definitions about policies:

- We say that a policy π is optimal, if it attains the optimal values $V^*(x)$ for any state $x \in \mathcal{X}$, i.e., if $V^\pi(x) = V^*(x)$ for all $x \in \mathcal{X}$. Under mild conditions, deterministic stationary optimal policies exist [65]. Such an optimal policy is written π^* .
- We say that a (deterministic stationary) policy π is greedy with respect to (w.r.t.) some function V (defined on \mathcal{X}) if, for all $x \in \mathcal{X}$,

$$\pi(x) \in \arg \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x, a) [r(x, a, x') + \gamma V(x')].$$

where $\arg \max_{a \in \mathcal{A}} f(a)$ is the set of $a \in \mathcal{A}$ that maximizes $f(a)$. For any function V , such a greedy policy always exists because \mathcal{A} is finite.

The goal of Reinforcement Learning (RL), as well as that of dynamic programming, is to design an optimal policy (or a good approximation of it).

The well-known Dynamic Programming equation (also called the Bellman equation) provides a relation between the optimal value function at a state x and the optimal value function at the successors states x' when choosing an optimal action: for all $x \in \mathcal{X}$,

$$V^*(x) = \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x, a) [r(x, a, x') + \gamma V^*(x')]. \quad (19)$$

The benefit of introducing this concept of optimal value function relies on the property that, from the optimal value function V^* , it is easy to derive an optimal behavior by choosing the actions according to a policy greedy w.r.t. V^* . Indeed, we have the property that a policy greedy w.r.t. the optimal value function is an optimal policy:

$$\pi^*(x) \in \arg \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x, a) [r(x, a, x') + \gamma V^*(x')]. \quad (20)$$

In short, we would like to mention that most of the reinforcement learning methods developed so far are built on one (or both) of the two following approaches ([76]):

- Bellman's dynamic programming approach, based on the introduction of the value function. It consists in learning a "good" approximation of the optimal value function, and then using it to derive a greedy policy w.r.t. this approximation. The hope (well justified in several cases) is that the performance V^π of the policy π greedy w.r.t. an approximation V of V^* will be close to optimality. This approximation issue of the optimal value function is one of the major challenge inherent to the reinforcement learning problem. **Approximate dynamic programming** addresses

the problem of estimating performance bounds (e.g. the loss in performance $\|V^* - V^\pi\|$ resulting from using a policy π -greedy w.r.t. some approximation V - instead of an optimal policy) in terms of the approximation error $\|V^* - V\|$ of the optimal value function V^* by V . Approximation theory and Statistical Learning theory provide us with bounds in terms of the number of sample data used to represent the functions, and the capacity and approximation power of the considered function spaces.

- Pontryagin’s maximum principle approach, based on sensitivity analysis of the performance measure w.r.t. some control parameters. This approach, also called **direct policy search** in the Reinforcement Learning community aims at directly finding a good feedback control law in a parameterized policy space without trying to approximate the value function. The method consists in estimating the so-called **policy gradient**, i.e. the sensitivity of the performance measure (the value function) w.r.t. some parameters of the current policy. The idea being that an optimal control problem is replaced by a parametric optimization problem in the space of parameterized policies. As such, deriving a policy gradient estimate would lead to performing a stochastic gradient method in order to search for a local optimal parametric policy.

Finally, many extensions of the Markov decision processes exist, among which the Partially Observable MDPs (POMDPs) is the case where the current state does not contain all the necessary information required to decide for sure of the best action.

3.2.2. Multi-arm Bandit Theory

Bandit problems illustrate the fundamental difficulty of decision making in the face of uncertainty: A decision maker must choose between what seems to be the best choice (“exploit”), or to test (“explore”) some alternative, hoping to discover a choice that beats the current best choice.

The classical example of a bandit problem is deciding what treatment to give each patient in a clinical trial when the effectiveness of the treatments are initially unknown and the patients arrive sequentially. These bandit problems became popular with the seminal paper [71], after which they have found applications in diverse fields, such as control, economics, statistics, or learning theory.

Formally, a K -armed bandit problem ($K \geq 2$) is specified by K real-valued distributions. In each time step a decision maker can select one of the distributions to obtain a sample from it. The samples obtained are considered as rewards. The distributions are initially unknown to the decision maker, whose goal is to maximize the sum of the rewards received, or equivalently, to minimize the regret which is defined as the loss compared to the total payoff that can be achieved given full knowledge of the problem, i.e., when the arm giving the highest expected reward is pulled all the time.

The name “bandit” comes from imagining a gambler playing with K slot machines. The gambler can pull the arm of any of the machines, which produces a random payoff as a result: When arm k is pulled, the random payoff is drawn from the distribution associated to k . Since the payoff distributions are initially unknown, the gambler must use exploratory actions to learn the utility of the individual arms. However, exploration has to be carefully controlled since excessive exploration may lead to unnecessary losses. Hence, to play well, the gambler must carefully balance exploration and exploitation. Auer *et al.* [63] introduced the algorithm UCB (Upper Confidence Bounds) that follows what is now called the “optimism in the face of uncertainty principle”. Their algorithm works by computing upper confidence bounds for all the arms and then choosing the arm with the highest such bound. They proved that the expected regret of their algorithm increases at most at a logarithmic rate with the number of trials, and that the algorithm achieves the smallest possible regret up to some sub-logarithmic factor (for the considered family of distributions).

3.3. Statistical analysis of time series

Many of the problems of machine learning can be seen as extensions of classical problems of mathematical statistics to their (extremely) non-parametric and model-free cases. Other machine learning problems are founded on such statistical problems. Statistical problems of sequential learning are mainly those that are concerned with the analysis of time series. These problems are as follows.

3.3.1. Prediction of Sequences of Structured and Unstructured Data

Given a series of observations x_1, \dots, x_n it is required to give forecasts concerning the distribution of the distribution of the future observations x_{n+1}, x_{n+2}, \dots ; in the simplest case, that of the next outcome x_{n+1} . Then x_{n+1} is revealed and the process continues. Different goals can be formulated in this setting. One can either make some assumptions on the probability measure that generates the sequence x_1, \dots, x_n, \dots , such as that the outcomes are independent and identically distributed (i.i.d.), or that the sequence is a Markov chain, that it is a stationary process, etc. More generally, one can assume that the data is generated by a probability measure that belongs to a certain set \mathcal{C} . In these cases the goal is to have the discrepancy between the predicted and the “true” probabilities to go to zero, if possible, with guarantees on the speed of convergence.

Alternatively, rather than making some assumptions on the data, one can change the goal: the predicted probabilities should be asymptotically as good as those given by the best reference predictor from a certain pre-defined set.

Another dimension of complexity in this problem concerns the nature of observations x_i . In the simplest case, they come from a finite space, but already basic applications often require real-valued observations. Moreover, function or even graph-valued observations often arise in practice, in particular in applications concerning Web data. In these settings estimating even simple characteristics of probability distributions of the future outcomes becomes non-trivial, and new learning algorithms for solving these problems are in order.

3.3.2. Hypothesis testing

Given a series of observations of x_1, \dots, x_n, \dots generated by some unknown probability measure μ , the problem is to test a certain given hypothesis H_0 about μ , versus a given alternative hypothesis H_1 . There are many different examples of this problem. Perhaps the simplest one is testing a simple hypothesis “ μ is Bernoulli i.i.d. measure with probability of 0 equals $1/2$ ” versus “ μ is Bernoulli i.i.d. with the parameter different from $1/2$ ”. More interesting cases include the problems of model verification: for example, testing that μ is a Markov chain, versus that it is a stationary ergodic process but not a Markov chain. In the case when we have not one but several series of observations, we may wish to test the hypothesis that they are independent, or that they are generated by the same distribution. Applications of these problems to a more general class of machine learning tasks include the problem of feature selection, the problem of testing that a certain behaviour (such as pulling a certain arm of a bandit, or using a certain policy) is better (in terms of achieving some goal, or collecting some rewards) than another behaviour, or than a class of other behaviours.

The problem of hypothesis testing can also be studied in its general formulations: given two (abstract) hypothesis H_0 and H_1 about the unknown measure that generates the data, find out whether it is possible to test H_0 against H_1 (with confidence), and if yes then how can one do it.

3.3.3. Change Point Analysis

A stochastic process is generating the data. At some point, the process distribution changes. In the “offline” situation, the statistician observes the resulting sequence of outcomes and has to estimate the point or the points at which the change(s) occurred. In online setting, the goal is to detect the change as quickly as possible.

These are the classical problems in mathematical statistics, and probably among the last remaining statistical problems not adequately addressed by machine learning methods. The reason for the latter is perhaps in that the problem is rather challenging. Thus, most methods available so far are parametric methods concerning piecewise constant distributions, and the change in distribution is associated with the change in the mean. However, many applications, including DNA analysis, the analysis of (user) behaviour data, etc., fail to comply with this kind of assumptions. Thus, our goal here is to provide completely non-parametric methods allowing for any kind of changes in the time-series distribution.

3.3.4. Clustering Time Series, Online and Offline

The problem of clustering, while being a classical problem of mathematical statistics, belongs to the realm of unsupervised learning. For time series, this problem can be formulated as follows: given several samples $x^1 = (x_1^1, \dots, x_{n_1}^1), \dots, x^N = (x_1^N, \dots, x_{n_N}^N)$, we wish to group similar objects together. While this is of

course not a precise formulation, it can be made precise if we assume that the samples were generated by k different distributions.

The online version of the problem allows for the number of observed time series to grow with time, in general, in an arbitrary manner.

3.3.5. *Online Semi-Supervised Learning*

Semi-supervised learning (SSL) is a field of machine learning that studies learning from both labeled and unlabeled examples. This learning paradigm is extremely useful for solving real-world problems, where data is often abundant but the resources to label them are limited.

Furthermore, *online* SSL is suitable for adaptive machine learning systems. In the classification case, learning is viewed as a repeated game against a potentially adversarial nature. At each step t of this game, we observe an example \mathbf{x}_t , and then predict its label \hat{y}_t .

The challenge of the game is that we only exceptionally observe the true label y_t . In the extreme case, which we also study, only a handful of labeled examples are provided in advance and set the initial bias of the system while unlabeled examples are gathered online and update the bias continuously. Thus, if we want to adapt to changes in the environment, we have to rely on indirect forms of feedback, such as the structure of data.

3.4. Statistical Learning and Bayesian Analysis

Before detailing some issues in these fields, let us remind the definition of a few terms.

Machine learning refers to a system capable of the autonomous acquisition and integration of knowledge. This capacity to learn from experience, analytical observation, and other means, results in a system that can continuously self-improve and thereby offer increased efficiency and effectiveness.

Statistical learning is an approach to machine intelligence that is based on statistical modeling of data. With a statistical model in hand, one applies probability theory and decision theory to get an algorithm. This is opposed to using training data merely to select among different algorithms or using heuristics/“common sense” to design an algorithm.

Bayesian Analysis applies to data that could be seen as observations in the more general meaning of the term. These data may not only come from classical sensors but also from any *device* recording information. From an operational point of view, like for statistical learning, uncertainty about the data is modeled by a probability measure thus defining the so-called likelihood functions. This last one depend upon parameters defining the state of the world we focus on for decision purposes. Within the Bayesian framework the uncertainty about these parameters is also modeled by probability measures, the priors that are subjective probabilities. Using probability theory and decision theory, one then defines new algorithms to estimate the parameters of interest and/or associated decisions. According to the International Society for Bayesian Analysis (source: <http://bayesian.org>), and from a more general point of view, this overall process could be summarize as follows: one assesses the current state of knowledge regarding the issue of interest, gather new data to address remaining questions, and then update and refine their understanding to incorporate both new and old data. Bayesian inference provides a logical, quantitative framework for this process based on probability theory.

Kernel method. Generally speaking, a kernel function is a function that maps a couple of points to a real value. Typically, this value is a measure of dissimilarity between the two points. Assuming a few properties on it, the kernel function implicitly defines a dot product in some function space. This very nice formal property as well as a bunch of others have ensured a strong appeal for these methods in the last 10 years in the field of function approximation. Many classical algorithms have been “kernelized”, that is, restated in a much more general way than their original formulation. Kernels also implicitly induce the representation of data in a certain “suitable” space where the problem to solve (classification, regression, ...) is expected to be simpler (non-linearity turns to linearity).

The fundamental tools used in SEQUEL come from the field of statistical learning [68]. We briefly present the most important for us to date, namely, kernel-based non parametric function approximation, and non parametric Bayesian models.

3.4.1. Non-parametric methods for Function Approximation

In statistics in general, and applied mathematics, the approximation of a multi-dimensional real function given some samples is a well-known problem (known as either regression, or interpolation, or function approximation, ...). Regressing a function from data is a key ingredient of our research, or to the least, a basic component of most of our algorithms. In the context of sequential learning, we have to regress a function while data samples are being obtained one at a time, while keeping the constraint to be able to predict points at any step along the acquisition process. In sequential decision problems, we typically have to learn a value function, or a policy.

Many methods have been proposed for this purpose. We are looking for suitable ones to cope with the problems we wish to solve. In reinforcement learning, the value function may have areas where the gradient is large; these are areas where the approximation is difficult, while these are also the areas where the accuracy of the approximation should be maximal to obtain a good policy (and where, otherwise, a bad choice of action may imply catastrophic consequences).

We particularly favor non parametric methods since they make quite a few assumptions about the function to learn. In particular, we have strong interests in l_1 -regularization, and the (kernelized-)LARS algorithm. l_1 -regularization yields sparse solutions, and the LARS approach produces the whole regularization path very efficiently, which helps solving the regularization parameter tuning problem.

3.4.2. Nonparametric Bayesian Estimation

Numerous problems may be solved efficiently by a Bayesian approach. The use of Monte-Carlo methods allows us to handle non-linear, as well as non-Gaussian, problems. In their standard form, they require the formulation of probability densities in a parametric form. For instance, it is a common usage to use Gaussian likelihood, because it is handy. However, in some applications such as Bayesian filtering, or blind deconvolution, the choice of a parametric form of the density of the noise is often arbitrary. If this choice is wrong, it may also have dramatic consequences on the estimation quality. To overcome this shortcoming, one possible approach is to consider that this density must also be estimated from data. A general Bayesian approach then consists in defining a probabilistic space associated with the possible outcomes of the *object* to be estimated. Applied to density estimation, it means that we need to define a probability measure on the probability density of the noise : such a measure is called a *random measure*. The classical Bayesian inference procedures can then been used. This approach being by nature non parametric, the associated frame is called *Non Parametric Bayesian*.

In particular, mixtures of Dirichlet processes [67] provide a very powerful formalism. Dirichlet Processes are a possible random measure and Mixtures of Dirichlet Processes are an extension of well-known finite mixture models. Given a mixture density $f(x|\theta)$, and $G(d\theta) = \sum_{k=1}^{\infty} \omega_k \delta_{U_k}(d\theta)$, a Dirichlet process, we define a mixture of Dirichlet processes as:

$$F(x) = \int_{\Theta} f(x|\theta)G(d\theta) = \sum_{k=1}^{\infty} \omega_k f(x|U_k) \quad (21)$$

where $F(x)$ is the density to be estimated. The class of densities that may be written as a mixture of Dirichlet processes is very wide, so that they really fit a very large number of applications.

Given a set of observations, the estimation of the parameters of a mixture of Dirichlet processes is performed by way of a Monte Carlo Markov Chain (MCMC) algorithm. Dirichlet Process Mixture are also widely used in clustering problems. Once the parameters of a mixture are estimated, they can be interpreted as the parameters of a specific cluster defining a class as well. Dirichlet processes are well known within the machine learning community and their potential in statistical signal processing still need to be developed.

3.4.3. Random Finite Sets for multisensor multitarget tracking

In the general multi-sensor multi-target Bayesian framework, an unknown (and possibly varying) number of targets whose states x_1, \dots, x_n are observed by several sensors which produce a collection of measurements z_1, \dots, z_m at every time step k . Well-known models to this problem are track-based models, such as the joint probability data association (JPDA), or joint multi-target probabilities, such as the joint multi-target probability density. Common difficulties in multi-target tracking arise from the fact that the system state and the collection of measures from sensors are unordered and their size evolve randomly through time. Vector-based algorithms must therefore account for state coordinates exchanges and missing data within an unknown time interval. Although this approach is very popular and has resulted in many algorithms in the past, it may not be the optimal way to tackle the problem, since the state and the data are in fact *sets* and not vectors.

The random finite set theory provides a powerful framework to deal with these issues. Mahler's work on finite sets statistics (FISST) provides a mathematical framework to build multi-object densities and derive the Bayesian rules for state prediction and state estimation. Randomness on object number and their states are encapsulated into random finite sets (RFS), namely multi-target(state) sets $X = \{x_1, \dots, x_n\}$ and multi-sensor (measurement) set $Zk = \{z_1, \dots, z_m\}$. The objective is then to propagate the multitarget probability density $f_{k|k}(X|Z(k))$ by using the Bayesian set equations at every time step k :

$$\begin{aligned} f_{k+1|k}(X|Z^{(k)}) &= \int f_{k+1|k}(X|W)f_{k|k}(W|Z^{(k)})\delta W \\ f_{k+1|k+1}(X|Z^{(k+1)}) &= \frac{f_{k+1}(Z_{k+1}|X)f_{k+1|k}(X|Z^{(k)})}{\int f_{k+1}(Z_{k+1}|W)f_{k+1|k}(W|Z^{(k)})\delta W} \end{aligned} \quad (22)$$

where:

- $X = \{x_1, \dots, x_n\}$ is a multi-target state, i.e. a finite set of elements x_i defined on the single-target space \mathcal{X} ; ²
- $Z_{k+1} = \{z_1, \dots, z_m\}$ is the current multi-sensor observation, i.e. a collection of measures z_i produced at time $k + 1$ by all the sensors;
- $Z^{(k)} = \bigcup_{t \leq k} Z_t$ is the collection of observations up to time k ;
- $f_{k|k}(W|Z^{(k)})$ is the current multi-target posterior density in state W ;
- $f_{k+1|k}(X|W)$ is the current multi-target Markov transition density, from state W to state X ;
- $f_{k+1}(Z|X)$ is the current multi-sensor/multi-target likelihood function.

Although equations (5) may seem similar to the classical single-sensor/single-target Bayesian equations, they are generally intractable because of the presence of the *set integrals*. For, a RFS Ξ is characterized by the family of its Janossy densities $j_{\Xi,1}(x_1), j_{\Xi,2}(x_1, x_2) \dots$ and not just by one density as it is the case with vectors. Mahler then introduced the PHD, defined on single-target state space. The PHD is the quantity whose integral on any region S is the expected number of targets inside S . Mahler proved that the PHD is the first-moment density of the multi-target probability density. Although defined on single-state space X , the PHD encapsulates information on both target number and states.

²The state x_i of a target is usually composed of its position, its velocity, etc.

SIMPAF Project-Team

3. Scientific Foundations

3.1. General framework

Partial Differential Equations, Kinetic Equations, Conservation Laws, Hyperbolic Systems, Fluid Mechanics, Parabolic Systems, Computational Fluid Dynamics, Plasma Physics, Asymptotic analysis

The scientific activity of the project is concerned with Partial Differential Equations (PDE) arising from the physical description of particles and fluids. It covers various viewpoints:

- At first, the words “particles and fluids” could simply mean that we are interested independently in models for particles, which can either be considered as individuals (which leads to “ N -particle models”, N ranging from 1 to many) or through a statistical description (which leads to kinetic equations) as well as in models for fluids like Euler and Navier-Stokes equations or plasma physics.
- However, many particle systems can also be viewed as a fluid, via a passage from microscopic to macroscopic viewpoint, that is, a hydrodynamic limit.
- Conversely, a fruitful idea to build numerical solvers for hyperbolic conservation laws consists in coming back to a kinetic formulation. This approach has motivated the introduction of the so-called kinetic schemes.

By nature these problems describe multiscale phenomena and one of the major difficulties when studying them lies in the interactions between the various scales: number of particles, size, different time and length scales, coupling...

The originality of the project is to consider a wide spectrum of potential applications. In particular, the word “particles” covers various and very different physical situations and it has evolved with the composition of the team. One may think of:

- charged particles: description of semi-conductor devices or plasmas;
- bacteria, individuals or genes as in models motivated by biology or population dynamics;
- droplets and bubbles, as in Fluid/Particles Interaction models which arise in the description of sprays and aerosols, smoke and dust, combustion phenomena (aeronautics or engine design), industrial process in metallurgy...
- cross-links in polymer chains to describe rubber elasticity;
- oxyde molecules to model corrosion phenomena at the microscopic scale and derive effective macroscopic equations;
- cold atoms...

We aim at focusing on all the aspects of the problem:

- Modelling mathematically complex physics requires a deep discussion of the leading phenomena and the role of the physical parameters. With this respect, the asymptotic analysis is a crucial issue, the goal being to derive reduced models which can be solved with a reduced numerical cost but still provide accurate results in the physical situations that are considered.
- The mathematical analysis of the equations provides important qualitative properties of the solutions: well-posedness, stability, smoothness of the solutions, large time behavior... which in turn can motivate the design of numerical methods.
- Eventually, we aim at developing specific numerical methods and performing numerical simulations for these models, in order to validate the theoretical results and shed some light on the physics.

The team has been composed in order to study these various aspects simultaneously. In particular, we wish to keep a balance between modelling, analysis, development of original codes and simulations.

3.2. Interactions of Micro- and Macroscopic Scales and Simulations

Statistical Physics, Homogenization, Asymptotic Preserving Schemes

3.2.1. Homogenization methods

Homogenization methods aim at replacing a PDE with highly oscillatory coefficients by an effective PDE with smoother coefficients, whose solution captures the averaged behavior of the true oscillatory solution. The effective determination of the homogenized PDE is however not trivial (especially in the nonlinear or/and stochastic cases). Numerical approximations of the solution of the homogenized PDE is the heart of numerical homogenization.

Homogenization methods are used in many application fields. The two applications we are specifically interested in are material sciences (in particular the determination of macroscopic constitutive laws for rubber starting from polymer-chain networks) and nuclear waste storage (in particular the evolution of nuclear wastes in complex storage devices).

The team is interested in qualitative as well as quantitative results, and theoretical as well as numerical results. Challenging questions are mainly related to nonlinear problems (nonlinear elasticity for instance) and stochastic problems (especially regarding quantitative results).

3.2.2. Statistical physics : molecular dynamics

The team is concerned with the numerical simulation of stochastically perturbed Molecular Dynamics. The main goal is to handle in the same simulation the fastest time scales (e.g. the oscillations of molecular bindings), and the slowest time scales (e.g. the so-called reaction coordinates). Recently, M. Rousset co-authored a monograph [64] which summarizes standard and state-of-the-art free energy calculations, that are used to accelerate slow variables in MD simulations.

3.2.3. Statistical physics: dynamical friction, fluctuations and approach to equilibrium

In models of charge transport, say transport of electrons, a phenomenological friction force is generally introduced, which is proportional to the velocity v . The dissipation induced by such a term is essential for the description of phenomena such as Ohm's law and approach to equilibrium. Our idea is to go back to a microscopic framework, with a description of the energy exchanges between the electrons and the surrounding medium which is the ultimate source of the dissipation of energy by the medium and of an effective friction force. We have shown numerically and argued theoretically that the balance between the fluctuations and the dissipation by the medium drives the particle to thermal equilibrium. The goal is now to provide rigorous proof of this statement. As a first step in this program, results will be obtained in an appropriate weak coupling limit. This program requires efforts in modelling, probability and analysis, but the questions are also really challenging for numerics, due, notably, to the large number of degrees of freedom involved in the equation. The subject is at the heart of the PhD work of É. Soret, now in her second year as a PhD student.

3.2.4. Cold Atoms

In the framework of the Labex CEMPI, C. Besse, S. De Bièvre and G. Dujardin are working, in collaboration with J.-C. Garreau and the cold-atom team at PhLAM, on the mathematical analysis and the numerical simulation of kicked rotor systems. Such systems are experimentally realized at PhLAM. A triple goal is being pursued: understand the effect of non-linearities on dynamical localization, understand dynamical localization in systems other than kicked rotors, and exploring the limits of the analogy between kicked systems and the Anderson model.

3.3. Plasma

In the context of the Galileo satellite-positioning system, C. Besse and C. Yang, members of the ANR Iodissee project, developed a hierarchy of plasma models which describe ionospheric scintillations. This hierarchy involves many small parameters, and they introduced an asymptotic preserving scheme which allows one to take small parameters into account without solving the problem on a very fine grid [8]. The next step is to

understand the fading and phase variations when waves propagate in this medium. This is a work in progress with P. Lafitte and S. Minjeaud (CNRS, Université de Nice).

3.4. Finite element and finite volume methods

Conservation Laws, Anti-Diffusive Schemes, Viscous Flows, Control, Turbulence, Finite element methods, Finite volume methods

3.4.1. Control in Fluid Mechanics

Flow control techniques are widely used to improve the performances of planes or vehicles, or to drive some internal flows arising for example in combustion chambers. Indeed, they can sensibly reduce energy consumption, noise disturbances, or prevent the flow from undesirable behaviors.

E. Creusé is involved in the development of open and closed active flow control, with applications to recirculation in engines or blood flows.

3.4.2. Numerical Methods for Viscous Flows

Numerical investigations are very useful to check the behavior of systems of equations modelling very complicate dynamics. In order to simulate the motion of mixtures of immiscible fluids having different densities, a recent contribution of the team was to develop an hybrid Finite Element / Finite Volume scheme for the resolution of the variable density 2D incompressible Navier-Stokes equations. The main points of this work were to ensure the consistency of the new method [56] as well as its stability for high density ratios [54]. In order to answer these questions, we have developed a MATLAB code and a C++ code. In the following of this work, C. Calgaro and E. Creusé now have in mind the following objectives, in collaboration with T. Goudon (team COFFEE, Inria Sophia-Antipolis) :

- Distribute the matlab version of the code (with an accurate documentation and a graphic interface) to promote new collaborations in the domain and compare alternative numerical solution methods (for instance to compare updating LU factorizations, see [55]);
- To generalize the stability results obtained in [54] for the scalar transport equation to the full 2D Euler system, in particular very low density values density (near vacuum);
- Complete the C++ code to treat more general hydrodynamic models (combustion theory, transport of pollutants). We plan to check the behavior of the equations (typically the Kazhikhov-Smagulov model of powder-snow avalanches) in the regime when the current existence theory does not apply, and extend our kinetic asymptotic-based schemes to such problems.

3.4.3. A posteriori error estimators for finite element methods

A posteriori estimates, finite element methods

The team works on a posteriori error estimators for finite element methods, applied to the resolution of several partial differential equations. The objective is to derive useful tools in order to control the global error between the exact solution and the approximated one (reliability of the estimator), and to control the local error leading to adaptive mesh refinement strategies (efficiency of the estimator).

More specifically, E. Creusé works on the derivation of some "reconstruction estimators" based on gradient averaging, for diffusion problems (with S. Nicaise, LAMAV, Valenciennes), the Reissner-Mindlin system (PhD of É. Verhille), and the Maxwell equations (PhD of Z. Tang).

3.5. Numerical analysis of Schrödinger equations

Dispersive equations, Schrödinger equations

3.5.1. Modelling of quantum dot-helium

In collaboration with G. Reinish (Nice Observatory) and V. Guðmundsson (University of Reykjavik), C. Besse and G. Dujardin are working on the numerical computation of the ground state and the first bound states of the non linear Schrödinger-Poisson system with confining quadratic potential in 2 space dimensions. This models quantum dot helium (*i.e.* the behavior of a pair of quantum electrons in a strong confining potential). The goal is to perform after that numerical time stepping methods to simulate the dynamics of the NLSP system and compute accurately some quantities of physical interest as functions of time, in order to be able to compare the competition between the Coulomb (repulsive) interaction and the binding (attractive) forces due to the confinement in this model as well as in other quantum mechanics models.

3.5.2. Dispersive Schrödinger-like equations

In collaboration with M. Taki (PhLAM laboratory, Lille), C. Besse and G. Dujardin are considering dispersive equations modelling the propagation of a laser beam in an optical fiber. They are trying to explain the possible ways of creating rogue waves in the propagation of laser beams. More generally, they are trying to explain which terms in the dispersive Schrödinger-like equations obtained by the physicists allow which physical behaviour of the solutions (e.g. the creation of rogue waves).

BONSAI Project-Team

3. Scientific Foundations

3.1. Combinatorial discrete models and algorithms

Our research is driven by biological questions. At the same time, we have in mind to develop well-founded models and efficient algorithms. Biological macromolecules are naturally modelled by various types of discrete structures: String, trees, and graphs. String algorithms is an established research subject of the team. We have been working on spaced seed techniques for several years [20], [27], [29], [23], [22]. Members of the team have also a strong expertise in text indexing and compressed index data structures [28], [31], [30]. Such methods are widely-used for the analysis of biological sequences because they allow a data set to be stored and queried efficiently. Ordered trees and graphs naturally arise when dealing with structures of molecules, such as RNAs [32], [26], [25], [24], [17] or non-ribosomal peptides [18]. The underlying questions are: how to compare molecules at structural level, how to search for structural patterns ? String, trees and graphs are also useful to study genomic rearrangements: Neighborhoods of genes can be modelled by oriented graphs, genomes as permutations, strings or trees.

3.2. High-performance computing

High-performance computing is another tool that we use to achieve our goals. It covers several paradigms: grids, single-instruction, multiple-data (SIMD) instructions or manycore processors such as graphics cards (GPU). For example, libraries like CUDA and OpenCL also facilitate the use of these manycore processors. These hardware architectures bring promising opportunities for time-consuming bottlenecks arising in bioinformatics.

3.3. Discrete statistics and probability

At a lower level, our work relies on a basic background on discrete statistics and probability. When dealing with large input data sets, it is essential to be able to discriminate between noisy features observed by chance from those that are biologically relevant. The aim here is to introduce a probabilistic model and to use sound statistical methods to assess the significance of some observations about these data. Examples of such observations are the length of a repeated region, the number of occurrences of a motif (DNA or RNA), the free energy of a conserved RNA secondary structure, etc. Probabilistic models are also used to describe genome evolution. In this context, Bayesian models and their MCMC sampling allow to approximate probability distributions over parameters and to describe more biologically relevant models.

SHACRA Project-Team

3. Scientific Foundations

3.1. Biomechanical Modeling

3.1.1. Biomechanical modeling of solid structures

Soft tissue modeling holds a very important place in medical simulation. A large part of the realism of a simulation, in particular for surgery or laparoscopy simulation, relies upon the ability to describe soft tissue response during the simulated intervention. Several approaches have been proposed over the past ten years to model soft-tissue deformation in real-time (mainly for solid organs), usually based on elasticity theory and a finite element approach to solve the equations. We were among the first to propose such an approach [24], [27] using different computational strategies. Although significant improvements were obtained later on (for instance with the use of co-rotational methods to handle geometrical non-linearities) these works remain of limited clinical use as they rely on linearized constitutive laws.

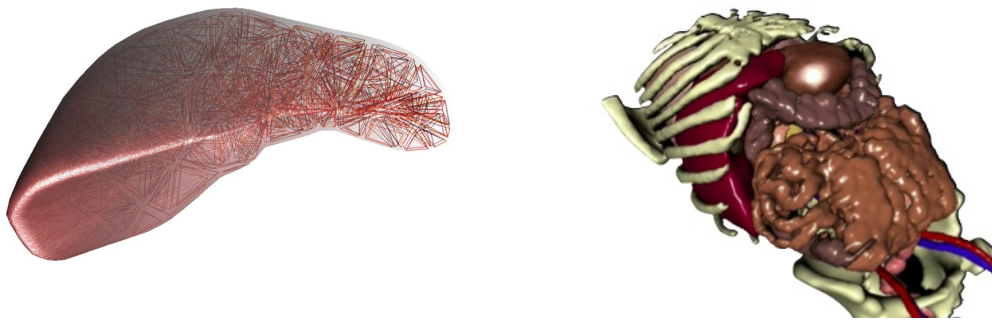


Figure 1. Biomechanical models of organs, based on the Finite Element Method and elasticity theory. Left: a model of the liver based on tetrahedral elements and small strain elasticity. Right: several organ models from a patient dataset combined to create a realistic abdominal anatomy.

An important part of our research is dedicated to the development of new, more accurate models that remain compatible with real-time computation. Such advanced models will not only permit to increase the realism of future training systems, but they will act as a bridge toward the development of patient-specific preoperative planning as well as augmented reality tools for the operating room. Yet, patient-specific planning or preoperative guidance also requires the models to be parametrized with patient-specific biomechanical data. Very little work has been done in this area, in particular when tissue properties need to be measured in vivo non-invasively. New imaging techniques, such as Ultrasound Elastography or Magnetic Resonance Elastography, could be used to this end [23]. We are currently studying the impact of parametrized patient-specific models of the liver in the context of the PASSPORT european project. This will be used to provide information about the deformation, tissue stiffness and tumor location, for various liver pathologies.

3.1.2. Biomechanical modeling of hollow structures

A large number of anatomical structures in the human body are vascularized (brain, liver, heart, kidneys, ...) and recent interventions (such as interventional radiology) rely on the vascular network as a therapeutical pathway. It is therefore essential to model the shape and deformable behavior of blood vessels. This will be

done at two levels. Global deformation of a vascular network: we have demonstrated previously [9] that we could recover the shape of thousands of vessels from medical images by extracting the centerline of each vessel (see Figure 2). The resulting vascular skeleton can be modeled as a deformable (tree) structure which can capture the global aspects of the deformation. More local deformations can then be described by considering now the actual local shape of the vessel. Other structures such as aneurysms, the colon or stomach can also benefit from being modeled as deformable structures. For this we will rely on shell or thin plate theory. We have recently obtained very encouraging results in the context of the Ph.D. thesis of Olivier Comas [26]. Such local and global models of hollow structures will be particularly relevant for planning coil deployment or stent placement, but also in the context of a new laparoscopic technique called NOTES which uses a combination of a flexible endoscope and flexible instruments. Obtaining patient-specific models of vascular structures and associated pathologies remains a challenge from an image processing stand point, and this challenge is even greater once we require these models to be adapted to complex computational strategies. To this extend we will pursue our collaboration with the MAGRIT team at Inria (through a PhD thesis starting in January 2010) and the Massachusetts General Hospital in Boston.

3.1.3. Blood Flow Simulation

Beyond biomechanical modeling of soft tissues, an essential component of a simulation is the modeling of the functional interactions occurring between the different elements of the anatomy. This involves for instance modeling physiological flows (blood flow, air flow within the lungs...). We particularly plan to study the problem of fluid flow in the context of vascular interventions, such as the simulation of three-dimensional turbulent flow around aneurysms to better model coil embolization procedures. Blood flow dynamics is starting to play an increasingly important role in the assessment of vascular pathologies, as well as in the evaluation of pre- and post-operative status. While angiography has been an integral part of interventional radiology procedures for years, it is only recently that detailed analysis of blood flow patterns has been studied as a mean to assess complex procedures, such as coil deployment. A few studies have focused on aneurysm-related hemodynamics before and after endovascular coil embolization. Groden et al. [31] constructed a simple geometrical model to approximate an actual aneurysm, and evaluated the impact of different levels of coil packing on the flow and wall pressure by solving Navier-Stokes equations, while Kakalis et al. [33] relied on patient-specific data to get more realistic flow patterns, and modeled the coiled aneurysm as a porous medium. As these studies aimed at accurate Computational Fluid Dynamics simulation, they rely on commercial software, and the computation times (dozens of hours in general) are incompatible with interactive simulation or even clinical practice. Generally speaking, accuracy and efficiency are two significant pursuits in numerical calculation, but unfortunately very often contradictory.

With the Ph.D. thesis of Yiyi Wei, we have recently started the development of a new technique for accurately computing, in near real-time, the flow of blood within an aneurysm, as well as the interaction between blood and coils. In this approach we rely on the Discrete Exterior Calculus method to obtain an ideal trade-off between accuracy and computational efficiency. Although still at an early stage, these results show that our approach can accurately capture the main characteristics of the complex blood flow patterns in and around an aneurism. The model also takes into account the influence of the coil on the blood flow within the aneurysm. The main difference between our approach and many other work done by internationally renowned teams (such as REO team at Inria or the Computer Vision Laboratory at ETH) comes from the importance we place in the computational efficiency of the method. To some extent our approach is similar to what has been done to obtain real-time finite element methods. We are essentially trying to capture the key characteristics of the behavior for a particular application. This is well illustrated by the work we started on flow modeling, which received an award in September 2009 at the selective conference on Medical Image Computing and Computer Assisted Interventions [10]. We will pursue this direction to accurately model the local flow in a closed domain (blood vessel, aneurysm ventricle, ...) and combine it with some of our previous work describing laminar flow across a large number of vessels [38] in order to define boundary conditions for the three-dimensional model.

3.2. Biomechanical Systems

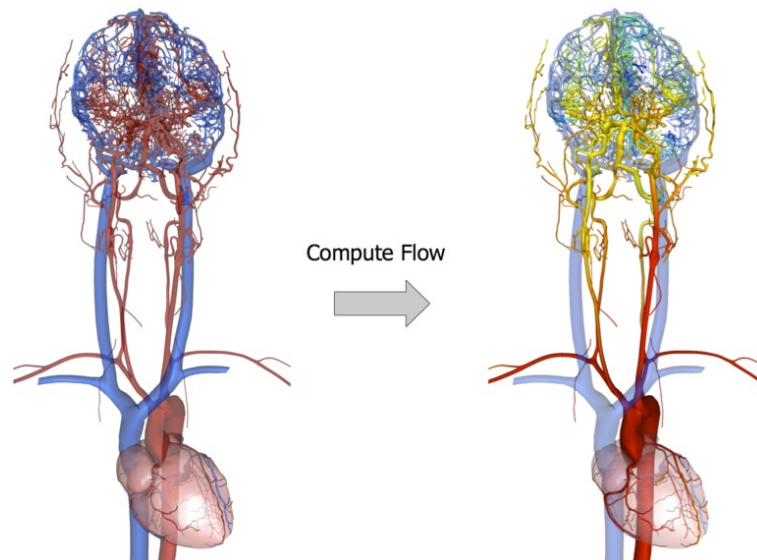


Figure 2. Blood flow and pressure distribution in the cerebrovascular system. The arterial vascular network is composed of more than 3,000 vessels, yet the computation is performed in real-time.

3.2.1. Constraint models and boundary conditions

To accurately model soft tissue deformations, the approach must account for the intrinsic behavior of the target organ, but also for its biomechanical interactions with surrounding tissues or with medical devices. While the biomechanical behavior of important organs (such as the brain or liver) has been well studied, few work exists regarding the mechanical interactions between the anatomical structures. For tissue-tool interactions, most approaches rely on a simple contact models, and rarely account for friction. While this simplification can produce plausible results in the case of an interaction between the end effector of a laparoscopic instrument and the surface of an organ, it is generally an incorrect approximation. As we move towards simulations for planning or rehearsal, accurately modeling contacts will take an increasingly important place. We have recently shown in [28] and [29] that we could compute, in real-time, complex interactions between a coil and an aneurysm, or between a flexible needle and soft-tissues. In laparoscopic surgery, the main challenge lies in the modeling of interactions between anatomical structures rather than between the instruments and the surface of an organ. During the different steps of a procedure organs slides against each other, while respiratory, cardiac and patient motion also generate contacts. Modeling these multiple interactions becomes even more complex when different biomechanical models are used to characterize the various soft tissues of the anatomy. Consequently, our objective is to accurately model resting contacts with friction, in a heterogeneous environment (spring-mass models, finite element models, particle systems, rigid objects, etc.). When different time integration strategies are used, a challenge lies in the computation of contact forces in a way that integrity and stability of the overall simulation are maintained. Our objective is to work on the definition of these various boundary conditions and on new resolution methods for such heterogeneous simulations. In particular we will investigate a simulation process in which each model continues to benefit from its own optimizations while taking into account the mechanical couplings due to interactions between objects.

3.2.2. Vascularized anatomy

From a clinical standpoint, several procedures involve vascularized anatomical structures such as the liver, the kidneys, or the brain. When a therapy needs to be applied on such structures, it is currently possible to perform

a procedure surgically or to use an endovascular approach. This requires to characterize and model the behavior of vessels (arteries and veins) as well as the behavior of soft tissue (in particular the parenchyma). Another challenge of this research will be to model the interactions between the vascular network and the parenchyma where it is embedded. These interactions are key for both laparoscopic surgery and interventional radiology as they allow to describe the motion of the vessels in a vascularized organ during the procedure. This motion is either induced by the surgical manipulation of the parenchymal tissue during surgery or by respiratory, cardiac or patient motion during interventional radiology procedures. From a biomechanical standpoint, capillaries are responsible for the viscoelastic behavior of the vascularized structures, while larger vessels have a direct impact on the overall behavior of the anatomy. In the liver for instance, the apparent stiffness of the organ changes depending on the presence or absence of large vessels. Also, the relatively isotropic nature of the parenchyma is modified around blood vessels. We propose to model the coupling that exists between these two different anatomical structures to account for their respective influence. For this we will initially rely on the work done during the Ph.D. thesis of Christophe Guebert (see ([32] for instance) and we will also investigate coupling strategies based on degrees of freedom reduction to reduce the complexity of the problem (and therefore also computation times). Part of this work is already underway in the context of the PASSPORT european project with IRCAD and soft tissue measurements will be performed in collaboration with the biomechanics laboratory at Strasbourg University.

3.2.3. Parallel Computation

Although the past decade has seen a significant increase in complexity and performance of the algorithms used in medical simulation, major improvements are still required to enable patient-specific simulation and planning. Using parallel architectures to push the complexity of simulated environments further is clearly an approach to consider. However, interactive simulations introduce new constraints and evaluation criteria, such as latencies, multiple update frequencies and dynamic adaptation of precision levels, which require further investigation. New parallel architectures, such as multi-cores CPUs, are now ubiquitous as the performances achieved by sequential units (single core CPUs) stopped to regularly improve. At the same time, graphical processors (GPU) offer a massive computing power that is now accessible to non-graphical tasks thanks to new general-purposes API such as CUDA and OpenCL. GPUs are internally parallel processors, exploiting hundreds of computing units. These architectures can be exploited for more ambitious simulations, as we already have demonstrated in a first step by adding support for CUDA within the SOFA framework. Several preliminary results of GPU-based simulations have been obtained, permitting to reach speedup factors (compared to a single core GPU) ranging from 16x to 55x. Such improvements permit to consider simulations with finer details, or new algorithms modeling biomechanical behaviors more precisely. However, while the fast evolution of parallel architectures is useful to increase the realism of simulations, their varieties (multi-core CPUs, GPUs, clusters, grids) make the design of parallel algorithm challenging. An important effort needs to be made is to minimize the dependency between simulation algorithms and hardware architectures, allowing the reuse of parallelization efforts on all architecture, as well as simultaneously exploiting all available computing resources present in current and future computers. The largest gains could be achieved by combining parallelism and adaptive algorithms. The design and implementation of such a system is a challenging problem, as it is no longer possible to rely on pre-computed repartition of datas and computations. Thus, further research is required in highly adaptive parallel scheduling algorithms, and highly efficient implementation able to handle both large changes in computational loads due to user interactions and multi-level algorithms, and new massively parallel architectures such as GPUs. A direction that we are also investigating is to combine multi-level representations and locally adaptive meshes. Multi-level algorithms are useful not only to speedup computations, but also to describe different characteristics of the deformation at each level. Combined with local change of details of the mesh (possibly using hierarchical structures), the simulation can reach a high level of scalability.

ADAM Project-Team

3. Scientific Foundations

3.1. Introduction

In order to cope with our objective, we will consider software paradigms that will help us in our approach at the various levels of our life-cycle of adaptive systems, but also in the tools themselves for their composition. We will also study these paradigms in the middleware and application design in order to extend them and to have a better understanding. These extensions will be formalized as much as possible.

3.1.1. *Aspect-Oriented Software Development (AOSD)*

In modern software engineering, language constructs are classified according to how they recombine partial solutions for subproblems of a problem decomposition. Some constructs (*e.g.*, methods and classes) recombine partial solutions using classic hierarchical composition. Others recombine the partial solution using what is known as crosscutting (a.k.a. aspectual) composition. With crosscutting composition, two partial solutions (called aspects) are woven into each other in a way that is dictated by so-called pointcut languages. The necessity of crosscutting composition is the main motivation for the AOSD [87], [105] paradigm. The challenge will be first to study new expressive pointcut languages in order to have a better description of composition locations in adaptable software. The second objective will be to extend and to integrate new techniques of weaving at design time, but also at run time in order to compose software safely. The third objective will be to go beyond simple aspects as persistence and logging services. We plan to study complex aspects such as transactions or replication and to control their weaving in order to master the evolution of complex software.

3.1.2. *Component-Based Software Engineering (CBSE)*

In a post-object world [101], software components [110] are, with other artifacts such as aspects, one of the approaches that aims at overcoming the limitations of objects and providing more flexibility and dynamicity to complex applications. For that, software components present many interesting properties, such as modularity, encapsulation, and composability. Yet, many different component models and frameworks exist. A survey of the literature references more than 20 different models (including the most well-known, such as EJB [86] and CCM [85]), but the exact number is certainly closer to 30. Indeed, each new author proposes a model to address her/his own need related to a particular execution environment (from grid computing to embedded systems) or the technical services (from advanced transactions to real-time properties), which must be provided to the application components. These different component models seldom interoperate and their design and implementation are never founded on a common ground. The research challenge that we identify is to define and implement solutions for adaptive software components. These components will be adaptive in the sense that they will be able to accommodate execution environments of various granularities (from grid computing, to Internet-based applications, to mobile applications, to embedded systems) and incorporate on-demand different technical services. This challenge will be conducted by designing a micro-kernel for software components. This micro-kernel will contain a well-defined set of core concepts, which are at the root of all component models. Several concrete software component models will then be derived from this micro-kernel.

3.1.3. *Context-Aware Computing (CAC)*

In adaptive systems, the notion of “*context*” becomes increasingly important. For example, mobile devices sense the environment they are in and react accordingly. This is usually enabled by a set of rules that infer how to react given a certain situation. In the Ambient/Ubiquitous/Pervasive domain ¹, CAC is commonly referred to as the new paradigm that employs this idea of context in order to enmesh computing in our daily lives [113]. Many efforts that exist today focus on human-computer interaction based on context. On

¹These terms are more or less equivalent.

the one hand, computational models, middleware, and programming languages are being developed to take the inherent characteristics of multi-scale environments into account, such as connection volatility, ambient resources, etc. An important challenge is to bridge the gap between the domain level and the computational level. The former is concerned with the expected behavior of the system from a user's viewpoint, such as how and when a system responds to changes in the context, when information can be made public, etc. On the other hand, the computational level deals with the inherent and very stringent hardware phenomena of multi-scale environments. Nevertheless, both levels have to coexist: the computational level needs to be steered by the concepts, behavior and rules which exist at the domain level, whereas the domain needs to adapt to the specificities of the ever changing environment that is monitored and managed by the computational level. In order to address this challenge, we first intend to investigate representations at the domain level of concepts such as user profile, local positioning information and execution context [126]. Furthermore, a mapping has to be devised between these concepts and generic concepts at the computational level, the latter being as independent as possible from concrete platforms or languages. This mapping has to be bidirectional: the computational level needs to be steered by the concepts, behavior and rules that exist at the domain level, whereas the domain needs to adapt to the particulars of the ever-changing environment that is monitored and managed at the computational level. Furthermore, the mapping has to be dynamic since the changes have to be propagated between the levels at run time. An explicit domain level is not only useful for bridging the aforementioned gap, but also for designing and developing open task-specific languages at the domain level, which allow users to dynamically adapt the behavior of the applications in multi-scale environments in well-defined ways.

We will base the design approach of the future implementation prototype on Model Driven Engineering (MDE). The goal of MDE [122] consists of developing, maintaining and evolving complex software systems by raising the level of abstraction from source code to models. The latter is in our case the domain level, which will be connected to the computational level by means of MDE techniques. One added benefit of MDE is that it provides means for managing model inconsistencies.

3.2. Two Research Directions

We propose to follow two research directions to foster software reuse and adaptation. The first direction, that could be coined as the spatial dimension of adaptation, will provide middleware platforms to let applications be adapted to changing execution contexts. The second direction, the so-called temporal dimension of adaptation, will provide concepts and artifacts to let designers specify evolvable applications.

3.2.1. Adaptable Component Frameworks for Middleware

As a cornerstone of next generation software, adaptation is a property which must be present throughout the entire life cycle, from design to execution. We develop then a vision where adaptation is not only a property that is desirable for end-user applications, but also for the middleware platform that executes these applications. Until now, middleware is a rather specialized activity where each new environment forces the development of a corresponding platform, which is specific to the given environment. This has led to a large number of platforms (from Web Services, to EJB, to CORBA, to ad hoc middleware for embedded systems). Although at a high level, solutions for communication interoperability often exist between these platforms, they stay loosely coupled and separated. Furthermore, the concepts which are at the core of these platforms and their architectures are too different to allow, for example, sharing technical services.

The research challenge that we propose here is to define and develop middleware and associated services which could be adapted to a broad range of environments from grid computing, to Internet-based applications, to local networks, to mobile applications on PDA's and smart phones, to embedded systems. The benefits of that are twofold. First, it enables the easier deployment of mobile applications in different environments by taking advantage of the common ground provided by adaptable middleware. Second, middleware is a rapidly changing domain where new technologies appear frequently. Yet, up to now, each new technological shift has imposed a complete re-development of the middleware. Having a common ground on which middleware is built would help in such transitions by fostering reuse. In terms of industrial output, the impact of these

results will also be helpful for software editors and companies to adapt their products more rapidly to new and emerging middleware technologies.

This research challenge has close links with MDE and product line families. We believe that the added value of our proposal is to cover a more integrated solution: we are not only interested in middleware design with MDE technologies, but we also wish to integrate them with software component technologies and advanced programming techniques, such as AOP. We will then cover a broad spectrum of middleware construction, from design (MDE) to implementation (CBSE) to application development (AOP).

3.2.2. *Distributed Application Design for Adaptive Platforms*

Considering adaptation in the first design steps of an application allows for its preparation and follow-up during the entire life-cycle. As mentioned previously, some software paradigms help already in the design and the development of adaptable applications. AOSD proposes separation of concerns and weaving of models in order to increase the mastering and the evolution of software. MDE consists of evolving complex software systems by raising the level of abstraction from source code to models. Several programming approaches, such as AOP or reflective approaches, have gained in popularity to implement flexibility. Other approaches, such as CBSE, propose compositional way for reuse and compose sub-systems in the application building. Finally, context-aware programming for mobile environment proposes solutions in order to consider context evolution. Overall, the objective of these approaches is to assist the development of applications that are generic and that can be adapted with respect to the properties of the domain or the context.

The research challenge that we propose to address here is similar to static points of variation in product line families. We plan to study dynamic points of variation in order to take into account adaptation in the first design steps and to match this variation. The first research challenge is the introduction of elements in the modeling phase that allow the specification of evolution related properties. These properties must make it possible to build safe and dynamic software architectures. We wish to express and validate properties in the entire software life cycle. These properties are functional, non-functional, static, behavioral, or even qualitative properties. We also want to be able to check that all the properties are present, that the obtained behavior is the expected one, and that the quality of service is not degraded after the addition or the withdrawal of functionalities. We will base our approach on the definition of contracts expressed in various formalisms (*e.g.*, first order logic, temporal logic, state automata) and we will propose a composition of these contracts.

The second challenge will be to implement design processes that maintain coherence between the various stages of modeling in a MDE approach of the applications, as well as maintaining coherence between the phases of modeling and implementation. To do so, we will design and implement tools that will enable traceability and coherence checking between models, as well as between models and the application at execution time.

Finally, we will introduce context information in the development process. At the modeling level, we will represent concepts, behavior and rules of adaptive systems to express adaptation abstraction. These models will be dynamic and connected to implementation levels at the computational level and they will consider context knowledge. The goal is to bridge the gap between the computational level and the domain level in adaptive systems by synchronization of models and implementations, but also by representation of such common knowledge.

FUN Team

3. Scientific Foundations

3.1. Introduction

The research area of FUN research group is represented in Figure 1 . FUN research group will address every item of Figure 1 starting from the highest level of the figure, *i.e.* in area of homogeneous FUNs to the lowest one. Going down brings more applications and more issues to solve. Results achieved in the upper levels can be re-used in the lower ones. Current networks encountered nowadays are the ones at the higher level, without any interaction between them. In addition, solutions provided for such networks are rarely directly applicable in realistic networks because of the impact of the wireless medium.

FUN research group intends to fill the scientific gap and extend research performed in the area of wireless sensor and actor networks and RFID systems in two directions that are complementary and should be performed in parallel:

- **From theory to experimentation and reciprocally** On one hand, FUN research group intends to investigate new self-organization techniques for these future networks that take into account realistic parameters, emphasizing experimentation and considering mobility.
- **Towards heterogeneous FUNs** On the other hand, FUN research group intends to investigate techniques to allow heterogeneous FUNs to work together in a transparent way for the user. Indeed, new applications integrating several of these components are very much in demand (*i.e.* smart building) and thus these different technologies need to cooperate.

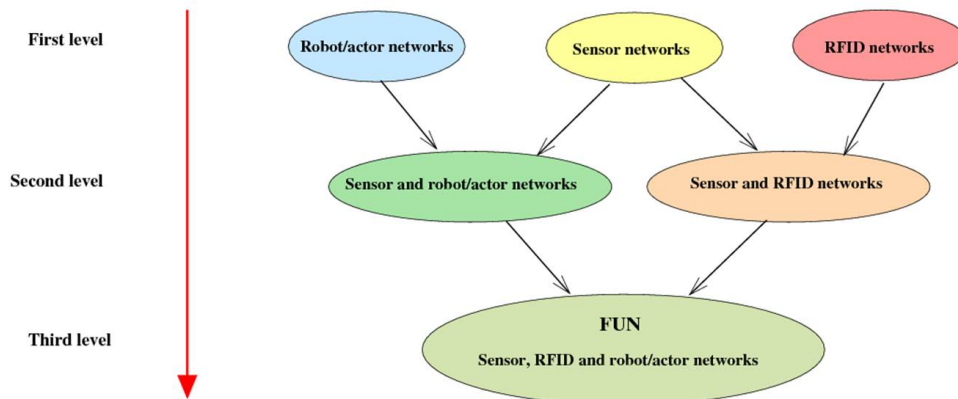


Figure 1. Panorama of FUN.

3.2. From theory to experimentation and reciprocally

Nowadays, even if some powerful and efficient propositions arise in the literature for each of these networks, very few are validated by experimentations. And even when this is the case, no lesson is learnt from it to improve the algorithms. FUN research group needs to study the limits of current assumptions in realistic and mobile environments.

Solutions provided by the FUN research group will mainly be algorithmic. These solutions will first be studied theoretically, principally by using stochastic geometry (like in [47]) or self-stabilization [49] tools in order to derive algorithm behavior in ideal environment. Theory is not an end in itself but only a tool to help in the characterization of the solution in the ideal world. For instance, stochastic geometry will allow quantifying changes in neighborhood or number of hops in a routing path. Self-stabilization will allow measuring stabilization times.

Those same solutions will then be confronted to realistic environments and their 'real' behavior will be analyzed and compared to the expected ones. Comparing theory, simulation and experimentation will allow better measuring the influence of a realistic environment. From this and from the analysis of the information really available for nodes, FUN research group will investigate some means either to counterbalance these effects or to take advantage of them. New solutions provided by the FUN research group will take into consideration the vagaries of a realistic wireless environment and the node mobility. New protocols will take as inputs environmental data (as signal strength or node velocity/position, etc) and node characteristics (the node may have the ability to move in a controlled way) when available. FUN research group will thus adopt a **cross-layered** approach between hardware, physical environment, application requirements, self-organizing and routing techniques. For instance, FUN research group will study how the controlled node mobility can be exploited to enhance the network performance at lowest cost.

Solutions will follow the building process presented by Figure 2 . Propositions will be analyzed not only theoretically and by simulation but also by experimentation to observe the impact of the realistic medium on the behavior of the algorithms. These observations should lead to the derivation of cross-layered models. Experimentation feedbacks will be re-injected in solution design in order to propose algorithms that best fit the environment, and so on till getting satisfactory behavior in both small and large scale environments. All this should be done in such a way that the resulting propositions fit the hardware characteristics (low memory, CPU and energy capacity) and easy to deploy to allow their use by non experts. Since solutions should take into account application requirements as well as hardware characteristics and environment, solutions should be generic enough and then able to self-configure to adapt their environment settings.

In order to achieve this experimental environments, the FUN research group will maintain its strong activity on platform deployment such as SensLAB [52], FIT and Aspire [42]. Next steps will be to experiment not only on testbeds but also on real use cases. These latter will be given through different collaborations.

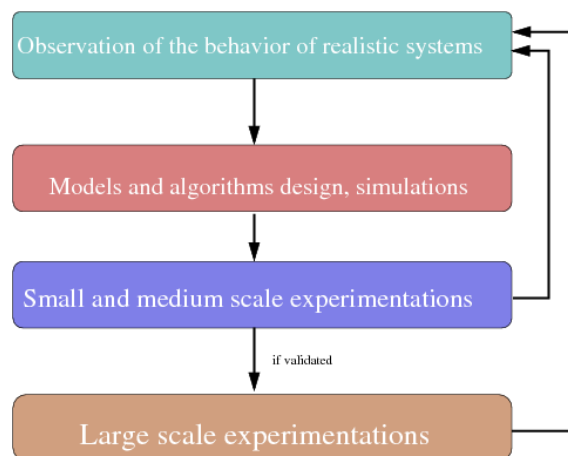


Figure 2. Methodology applied in the FUN research group.

FUN research group will investigate self-organizing techniques for FUNs by providing cross-layered solutions that integrate in their design the adaptability to the realistic environment features. Every solution will be validated with regards to specific application requirements and in realistic environments.

Facing the medium instability. The behavior of wireless propagation is very depending of the surrounding environment (in-door vs outdoor, night vs day, etc) and is very instable. Many experiments in different environment settings should be conducted. Experiment platforms such as SensLAB, FIT, our wifiBot as robots and actuators and our RFID devices will be used offering ways to experiment easily and quickly in different environments but might not be sufficient to experiment every environment.

Adaptability and flexibility. Since from one application to another one, requirements and environments are different, solutions provided by FUN research group should be **generic** enough and **self-adapt** to their environment. Algorithm design and validation should also take into account the targeted applications brought for instance by our industrial partners like Etineo. All solution designs should keep in mind the devices constrained capacities. Solutions should consume low resources in terms of memory, processor and energy to provide better performances and scale. All should be self-adaptive.

FUN research group will try to take advantage of some observed features that could first be seen as drawbacks. For instance, the broadcast nature of wireless networks is first an inconvenient since the use of a link between two nodes inhibits every other communication in the same transmission area. But algorithms should exploit that feature to derive new behaviors and a node blocked by another transmission should overhear it to get more information and maybe to limit the overall information to store in the network or overhead communication.

3.3. Towards unified heterogeneous FUNs

The second main direction to be followed by the FUN research group is to merge networks from the upper layer in Fig. 1 into networks from the lowest level. Indeed, nowadays, these networks are still considered as separated issues. But considering mixed networks bring new opportunities. Indeed, robots can deploy, replace, compensate sensor nodes. They also can collect periodically their data, which avoids some long and multi-hop communications between sensor nodes and thus preserving their resources. Robots can also perform many additional tasks to enhance network performance like positioning themselves on strategic points to ensure area coverage or reduce routing path lengths. Similarly, coupling sensors and RFID tags also brings new opportunities that are more and more in-demand from the industrial side. Indeed, an RFID reader may be a sensor in a wireless sensor network and data hold by RFID tags and collected by readers might need to be reported to a sink. This will allow new applications and possibilities such as the localization of a tagged object in an environment covered by sensors.

When at last all components are gathered, this leads us to a new era in which every object is autonomous. Let's consider for instance a smart home equipped with sensors and RFID reader. An event triggered by a sensor (*i.e.* an increase of the temperature) or a RFID reader (*i.e.* detection of a tag hold by a person) will trigger actions from actuators (*i.e.* lowering of stores, door opening). Possibilities are huge. But with all these new opportunities come new technological issues with other constraints. Every entity is considered as an object possibly mobile which should be dynamically identified and controlled. To support this dynamics, protocols should be localized and distributed. Model derived from experiment observations should be unified to fit all these classes of devices.

FUN research group will investigate new protocols and communication paradigms that allow the transparent merging of technologies. Objects and events might interconnect while respecting on-going standards and building an autonomic and smart network while being compliant with hardware resources and environment.

Technologies such as wireless sensors, wireless robots/actuators and RFID tags/ readers, although presenting many common points are still part of different disciplines that have evolved in parallel ways. Every branch is at different maturity levels and has developed its own standards. Nevertheless, making all these devices part of a single unified network leverages technological issues (partly addressed in the former objective) but also regarding to on-going standards and data formatting. FUN research group will have to study current standards

of every area in order to propose compliant solutions. Such works have been initiated in the POPS research group in the framework of the FP7 ASPIRE project. Members of FUN research group intend to continue and enlarge these works.

Today's EPCGlobal compliant RFID readers must comply to some rules and be configurable through an ALE [45]. While a fixed and connected RFID reader is easily configurable, configuring remotely a mobile RFID reader might be very difficult since it implies to first locate it and then send configuration data through a wireless dynamic network. FUN research group will investigate some tools that make the configuration easy and transparent for the user. This remote configuration of mobile readers through the network should consider application requirements and network and reader characteristics to choose the best trade-off relative to the software part embedded in the reader. The biggest part embedded, the lowest bandwidth overhead (data can be filtered and aggregated in the reader) and the greater mobility (readers are still fully operational even when disconnected) but the more difficult to set up and the more powerful readers. All these aspects will be studied within the FUN research group.

RMOD Project-Team

3. Scientific Foundations

3.1. Software Reengineering

Strong coupling among the parts of an application severely hampers its evolution. Therefore, it is crucial to answer the following questions: How to support the substitution of certain parts while limiting the impact on others? How to identify reusable parts? How to modularize an object-oriented application?

Having good classes does not imply a good application layering, absence of cycles between packages and reuse of well-identified parts. Which notion of cohesion makes sense in presence of late-binding and programming frameworks? Indeed, frameworks define a context that can be extended by subclassing or composition: in this case, packages can have a low cohesion without being a problem for evolution. How to obtain algorithms that can be used on real cases? Which criteria should be selected for a given remodularization?

To help us answer these questions, we work on enriching Moose, our reengineering environment, with a new set of analyses [37], [36]. We decompose our approach in three main and potentially overlapping steps:

1. Tools for understanding applications,
2. Remodularization analyses,
3. Software Quality.

3.1.1. Tools for understanding applications

Context and Problems. We are studying the problems raised by the understanding of applications at a larger level of granularity such as packages or modules. We want develop a set of conceptual tools to support this understanding.

Some approaches based on Formal Concept Analysis (FCA) [65] show that such an analysis can be used to identify modules. However the presented examples are too small and not representative of real code.

Research Agenda.

FCA provides an important approach in software reengineering for software understanding, design anomalies detection and correction, but it suffers from two problems: (i) it produces lattices that must be interpreted by the user according to his/her understanding of the technique and different elements of the graph; and, (ii) the lattice can rapidly become so big that one is overwhelmed by the mass of information and possibilities [23]. We look for solutions to help people putting FCA to real use.

3.1.2. Remodularization analyses

Context and Problems. It is a well-known practice to layer applications with bottom layers being more stable than top layers [53]. Until now, few works have attempted to identify layers in practice: Mudpie [67] is a first cut at identifying cycles between packages as well as package groups potentially representing layers. DSM (dependency structure matrix) [66], [61] seems to be adapted for such a task but there is no serious empirical experience that validates this claim. From the side of remodularization algorithms, many were defined for procedural languages [49]. However, object-oriented programming languages bring some specific problems linked with late-binding and the fact that a package does not have to be systematically cohesive since it can be an extension of another one [68], [40].

As we are designing and evaluating algorithms and analyses to remodularize applications, we also need a way to understand and assess the results we are obtaining.

Research Agenda. We work on the following items:

Layer identification. We propose an approach to identify layers based on a semi-automatic classification of package and class interrelationships that they contain. However, taking into account the wish or knowledge of the designer or maintainer should be supported.

Cohesion Metric Assessment. We are building a validation framework for cohesion/coupling metrics to determine whether they actually measure what they promise to. We are also compiling a number of traditional metrics for cohesion and coupling quality metrics to evaluate their relevance in a software quality setting.

3.1.3. Software Quality

Research Agenda. Since software quality is fuzzy by definition and a lot of parameters should be taken into account we consider that defining precisely a unique notion of software quality is definitively a Grail in the realm of software engineering. The question is still relevant and important. We work on the two following items:

Quality models. We studied existing quality models and the different options to combine indicators — often, software quality models happily combine metrics, but at the price of losing the explicit relationships between the indicator contributions. There is a need to combine the results of one metric over all the software components of a system, and there is also the need to combine different metric results for any software component. Different combination methods are possible that can give very different results. It is therefore important to understand the characteristics of each method.

Bug prevention. Another aspect of software quality is validating or monitoring the source code to avoid the apparition of well known sources of errors and bugs. We work on how to best identify such common errors, by trying to identify earlier markers of possible errors, or by helping identifying common errors that programmers did in the past.

3.2. Language Constructs for Modular Design

While the previous axis focuses on how to help remodularizing existing software, this second research axis aims at providing new language constructs to build more flexible and recomposable software. We will build on our work on traits [63], [38] and classboxes [24] but also start to work on new areas such as isolation in dynamic languages. We will work on the following points: (1) Traits and (2) Modularization as a support for isolation.

3.2.1. Traits-based program reuse

Context and Problems. Inheritance is well-known and accepted as a mechanism for reuse in object-oriented languages. Unfortunately, due to the coarse granularity of inheritance, it may be difficult to decompose an application into an optimal class hierarchy that maximizes software reuse. Existing schemes based on single inheritance, multiple inheritance, or mixins, all pose numerous problems for reuse.

To overcome these problems, we designed a new composition mechanism called Traits [63], [38]. Traits are pure units of behavior that can be composed to form classes or other traits. The trait composition mechanism is an alternative to multiple or mixin inheritance in which the composer has full control over the trait composition. The result enables more reuse than single inheritance without introducing the drawbacks of multiple or mixin inheritance. Several extensions of the model have been proposed [35], [57], [25], [39] and several type systems were defined [41], [64], [58], [51].

Traits are reusable building blocks that can be explicitly composed to share methods across unrelated class hierarchies. In their original form, traits do not contain state and cannot express visibility control for methods. Two extensions, stateful traits and freezable traits, have been proposed to overcome these limitations. However, these extensions are complex both to use for software developers and to implement for language designers.

Research Agenda: Towards a pure trait language. We plan distinct actions: (1) a large application of traits, (2) assessment of the existing trait models and (3) bootstrapping a pure trait language.

- To evaluate the expressiveness of traits, some hierarchies were refactored, showing code reuse [27]. However, such large refactorings, while valuable, may not exhibit all possible composition problems, since the hierarchies were previously expressed using single inheritance and following certain patterns. We want to redesign from scratch the collection library of Smalltalk (or part of it). Such a redesign should on the one hand demonstrate the added value of traits on a real large and redesigned library and on the other hand foster new ideas for the bootstrapping of a pure trait-based language.

In particular we want to reconsider the different models proposed (stateless [38], stateful [26], and freezable [39]) and their operators. We will compare these models by (1) implementing a trait-based collection hierarchy, (2) analyzing several existing applications that exhibit the need for traits. Traits may be flattened [56]. This is a fundamental property that confers to traits their simplicity and expressiveness over Eiffel's multiple inheritance. Keeping these aspects is one of our priority in forthcoming enhancements of traits.

- Alternative trait models. This work revisits the problem of adding state and visibility control to traits. Rather than extending the original trait model with additional operations, we use a fundamentally different approach by allowing traits to be lexically nested within other modules. This enables traits to express (shared) state and visibility control by hiding variables or methods in their lexical scope. Although the traits' "flattening property" no longer holds when they can be lexically nested, the combination of traits with lexical nesting results in a simple and more expressive trait model. We formally specify the operational semantics of this combination. Lexically nested traits are fully implemented in AmbientTalk, where they are used among others in the development of a Morphic-like UI framework.
- We want to evaluate how inheritance can be replaced by traits to form a new object model. For this purpose we will design a minimal reflective kernel, inspired first from ObjVlisp [33] then from Smalltalk [44].

3.2.2. Reconciling Dynamic Languages and Isolation

Context and Problems. More and more applications require dynamic behavior such as modification of their own execution (often implemented using reflective features [48]). For example, F-script allows one to script Cocoa Mac-OS X applications and Lua is used in Adobe Photoshop. Now in addition more and more applications are updated on the fly, potentially loading untrusted or broken code, which may be problematic for the system if the application is not properly isolated. Bytecode checking and static code analysis are used to enable isolation, but such approaches do not really work in presence of dynamic languages and reflective features. Therefore there is a tension between the need for flexibility and isolation.

Research Agenda: Isolation in dynamic and reflective languages. To solve this tension, we will work on *Sure*, a language where isolation is provided by construction: as an example, if the language does not offer field access and its reflective facilities are controlled, then the possibility to access and modify private data is controlled. In this context, layering and modularizing the meta-level [29], as well as controlling the access to reflective features [30], [31] are important challenges. We plan to:

- Study the isolation abstractions available in erights (<http://www.erights.org>) [55], [54], and Java's class loader strategies [50], [45].
- Categorize the different reflective features of languages such as CLOS [47], Python and Smalltalk [59] and identify suitable isolation mechanisms and infrastructure [42].
- Assess different isolation models (access rights, capabilities [60]...) and identify the ones adapted to our context as well as different access and right propagation.
- Define a language based on
 - the decomposition and restructuring of the reflective features [29],

- the use encapsulation policies as a basis to restrict the interfaces of the controlled objects [62],
- the definition of method modifiers to support controlling encapsulation in the context of dynamic languages.

An open question is whether, instead of providing restricted interfaces, we could use traits to grant additional behavior to specific instances: without trait application, the instances would only exhibit default public behavior, but with additional traits applied, the instances would get extra behavior. We will develop *Sure*, a modular extension of the reflective kernel of Smalltalk (since it is one of the languages offering the largest set of reflective features such as pointer swapping, class changing, class definition...) [59].

MINT Project-Team

3. Scientific Foundations

3.1. Human-Computer Interaction

The scientific approach that we follow considers user interfaces as means, not an end: our focus is not on interfaces, but on interaction considered as a phenomenon between a person and a computing system [30]. We *observe* this phenomenon in order to understand it, i.e. *describe* it and possibly *explain* it, and we look for ways to significantly *improve* it. HCI borrows its methods from various disciplines, including Computer Science, Psychology, Ethnography and Design. Participatory design methods can help determine users' problems and needs and generate new ideas, for example [35]. Rapid and iterative prototyping techniques allow to decide between alternative solutions [31]. Controlled studies based on experimental or quasi-experimental designs can then be used to evaluate the chosen solutions [37]. One of the main difficulties of HCI research is the doubly changing nature of the studied phenomenon: people can both adapt to the system and at the same time adapt it for their own specific purposes [34]. As these purposes are usually difficult to anticipate, we regularly *create* new versions of the systems we develop to take into account new theoretical and empirical knowledge. We also seek to *integrate* this knowledge in theoretical frameworks and software tools to disseminate it.

3.2. Numerical and algorithmic real-time gesture analysis

Whatever is the interface, user provides some curves, defined over time, to the application. The curves constitute a gesture (positionnal information, yet may also include pressure). Depending on the hardware input, such a gesture may be either continuous (e.g. data-glove), or not (e.g. multi-touch screens). User gesture can be multi-variate (several fingers captured at the same time, combined into a single gesture, possibly involving two hands, maybe more in the context of co-located collaboration), that we would like, at higher-level, to be structured in time from simple elements in order to create specific command combinations.

One of the scientific foundations of the research project is an algorithmic and numerical study of gesture, which we classify into three points:

- *clustering*, that takes into account intrinsic structure of gesture (multi-finger/multi-hand/multi-user aspects), as a lower-level treatment for further use of gesture by application;
- *recognition*, that identifies some semantic from gesture, that can be further used for application control (as command input). We consider in this topic multi-finger gestures, two-handed gestures, gesture for collaboration, on which very few has been done so far to our knowledge. On the contrary, in the case of single gesture case (i.e. one single point moving over time in a continuous manner), numerous studies have been proposed in the current literature, and interestingly, are of interest in several communities: HMM [38], Dynamic Time Warping [40] are well-known methods for computer-vision community, and hand-writing recognition. In the computer graphics community, statistical classification using geometric descriptors has previously been used [36]; in the Human-Computer interaction community, some simple (and easy to implement) methods have been proposed, that provide a very good compromise between technical complexity and practical efficiency [39].
- *mapping to application*, that studies how to link gesture inputs to application. This ranges from transfer function that is classically involved in pointing tasks [32], to the question to know how to link gesture analysis and recognition to the algorithmic of application content, with specific reference examples.

We ground our activity on the topic of numerical algorithm, expertise that has been previously achieved by team members in the physical simulation community (within which we think that aspects such as elastic deformation energies evaluation, simulation of rigid bodies composed of unstructured particles, constraint-based animation... will bring up interesting and novel insights within HCI community).

3.3. Design and control of haptic devices

Our scientific approach in the design and control of haptic devices is focused on the interaction forces between the user and the device. We search of controlling them, as precisely as possible. This leads to different designs compared to other systems which control the deformation instead. The research is carried out in three steps:

- *identification*: we measure the forces which occur during the exploration of a real object, for example a surface for tactile purposes. We then analyze the record to deduce the key components – *on user's point of view* – of the interaction forces.
- *design*: we propose new designs of haptic devices, based on our knowledge of the key components of the interaction forces. For example, coupling tactile and kinesthetic feedback is a promising design to achieve a good simulation of actual surfaces. Our goal is to find designs which leads to compact systems, and which can stand close to a computer in a desktop environment.
- *control*: we have to supply the device with the good electrical conditions to accurately output the good forces.

MOSTRARE Project-Team

3. Scientific Foundations

3.1. Modeling XML document transformations

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XML document transformations can be defined in W3C standards languages XQuery or XSLT. Programming XML transformations in these languages is often difficult and error prone even if the schemata of input and output documents are known. Advanced programming experience and considerable programming time may be necessary, that are not available in Web services or similar scenarios.

Alternative programming language for defining XML transformations have been proposed by the programming language community, for instance XDuce [46], Xtatic [44], [49], and CDuce [35], [36], [37]. The type systems of these languages simplify the programming tasks considerably. But of course, they don't solve the general difficulty in programming XML transformations manually.

Languages for defining node selection queries arise as sub-language of all XML transformation languages. The W3C standards use XPath for defining monadic queries, while XDuce and CDuce rely on regular queries defined by regular pattern equivalent to tree automata. Indeed, it is natural to look at node selection as a simple form of tree transformation. Monadic node selection queries correspond to deterministic transformations that annotate all selected nodes positively and all others negatively. N-ary node selection queries become non-deterministic transformations, yielding trees annotated by Boolean vectors.

After extensive studies of node selection queries in trees (in XPath and many other languages) the XML community has started more recently to formally investigate XML tree transformations. The expressiveness and complexity of XQuery are studied in [48], [57]. Type preservation is another problem, i.e., whether all trees of the input type get transformed into the output type, or vice versa, whether the inverse image of the output type is contained in the input type [52], [50].

The automata community usually approaches tree transformations by tree transducers [42], i.e., tree automata producing output structure. Macro tree transducers, for instance, have been proposed recently for defining XML transformations [50]. From the view point of logic, tree transducers have been studied for MSO definability [43].

3.2. Machine learning for XML document transformations

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Automatic or semi-automatic tools for inferring tree transformations are needed for information extraction. Annotated examples may support the learning process. The learning target will be models of XML tree transformations specified in some of the languages discussed above.

Grammatical inference is commonly used to learn languages from examples and can be applied to learn transductions. Previous work on grammatical inference for transducers remains limited to the case of strings [38], [53]. For the tree case, so far only very basic tree transducers have been shown to be learnable, by previous work of the Mostrare project. These are node selecting tree transducer (NSTTs) which preserve the structure of trees while relabeling their nodes deterministically.

Statistical inference is most appropriate for dealing with uncertain or noisy data. It is generally useful for information extraction from textual data given that current text understanding tools are still very much limited. XML transformations with noisy input data typically arise in data integration tasks, as for instance when converting PDF into XML.

Stochastic tree transducers have been studied in the context of natural language processing [45], [47]. A set of pairs of input and output trees defines a relation that can be represented by a 2-tape automaton called a *stochastic finite-state transducer* (SFST). A major problem consists in estimating the parameters of such transducer. SFST training algorithms are lacking so far [41].

Probabilistic context free grammars (pCFGs) [51] are used in the context of PDF to XML conversion [39]. In the first step, a labeling procedure of leaves of the input document by labels of the output DTD is learned. In the second step, given a CFG as a generative model of output documents, probabilities are learned. Such two steps approaches are in competition with one step approaches estimating conditional probabilities directly.

A popular non generative model for information extraction is *conditional random fields* (CRF, see a survey [54]). One main advantage of CRF is to take into account long distance dependencies in the observed data. CRF have been defined for general graphs but have mainly been applied to sequences, thus CRF for XML trees should be investigated.

So called *structured output* has recently become a research topic in machine learning [56], [55]. It aims at extending the classical categorization task, which consists to associate one or some labels to each input example, in order to handle structured output labels such as trees. Applicability of structured output learning algorithms remains to be asserted for real tasks such as XML transformations.