



IN PARTNERSHIP WITH:
CNRS

**Institut Polytechnique de
Bordeaux**

Université de Bordeaux

Activity Report 2015

Project-Team HIEPACS

High-End Parallel Algorithms for Challenging
Numerical Simulations

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
**Distributed and High Performance
Computing**

Table of contents

1. Members	1
2. Overall Objectives	2
3. Research Program	4
3.1. Introduction	4
3.2. High-performance computing on next generation architectures	4
3.3. High performance solvers for large linear algebra problems	6
3.3.1. Parallel sparse direct solver	7
3.3.2. Hybrid direct/iterative solvers based on algebraic domain decomposition techniques	7
3.3.3. Linear Krylov solvers	8
3.3.4. Eigensolvers	9
3.3.5. \mathcal{H} -matrix arithmetics to reduce the memory and computation complexity of sparse direct solvers	9
3.4. High performance Fast Multipole Method for N-body problems	9
3.4.1. Improvement of calculation efficiency	10
3.4.2. Non uniform distributions	10
3.4.3. Fast multipole method for dislocation operators	10
3.4.4. Fast multipole method for boundary element methods	10
3.5. Efficient algorithmic for load balancing and code coupling in complex simulations	10
3.5.1. Efficient schemes for multiscale simulations	11
3.5.2. Dynamic load balancing for massively parallel coupled codes	11
3.5.3. Graph partitioning for hybrid solvers	11
4. Application Domains	12
4.1. Material physics	12
4.2. Co-design for scalable numerical algorithms in scientific applications	12
4.2.1. MHD instabilities edge localized modes	13
4.2.2. Turbulence of plasma particules inside a tokamak	13
4.2.3. SN Cartesian solver for nuclear core simulation	13
4.2.4. 3D aerodynamics for unsteady problems with moving bodies	14
5. Highlights of the Year	14
6. New Software and Platforms	14
6.1. Introduction	14
6.2. Chameleon	14
6.3. MaPHyS	15
6.4. PaStiX	15
6.5. HIPS	15
6.6. MetaPart	16
6.7. MPICPL	16
6.8. ScalFMM	16
6.9. ViTE	17
6.10. Other software	17
6.11. Platforms	18
7. New Results	19
7.1. High-performance computing on next generation architectures	19
7.1.1. Soft error sensitivity of PCG and reliability of detection mechanisms	19
7.1.2. Resilience of parallel sparse hybrid solvers	19
7.1.3. Hierarchical DAG scheduling for hybrid distributed systems	20
7.1.3.1. Comparison of Static and Dynamic Resource Allocation Strategies for Matrix Multiplication	20
7.1.3.2. Scheduling Trees of Malleable Tasks for Sparse Linear Algebra	20

7.1.3.3.	Task-based multifrontal QR solver for GPU-accelerated multicore architectures	21
7.1.3.4.	Fast and Accurate Simulation of Multithreaded Sparse Linear Algebra Solvers	21
7.2.	High performance solvers for large linear algebra problems	21
7.2.1.	Divide and conquer symmetric tridiagonal eigensolver for multicore architectures	21
7.2.2.	Blocking strategy optimizations for sparse direct linear solver on heterogeneous architectures	22
7.2.3.	On the use of \mathcal{H} -Matrix Arithmetic in PaStiX: a Preliminary Study	22
7.2.4.	Data sparse techniques for parallel hybrid solvers	22
7.2.5.	Analysis of the rounding error accumulation in Conjugate Gradient to improve the maximal attainable accuracy of pipelined CG	22
7.3.	High performance Fast Multipole Method for N-body problems	23
7.3.1.	Task-based Fast Multipole Method	23
7.3.2.	Time-domain boundary element method	24
7.3.3.	Randomized algorithms for covariance matrices	24
7.3.3.1.	Covariance kernel matrices	24
7.3.3.2.	New applications: Data Assimilation and Taxonomy	24
7.4.	Efficient algorithmic for load balancing and code coupling in complex simulations	25
7.5.	Application Domains	25
7.5.1.	Material physics	25
7.5.1.1.	Molecular Vibrational Spectroscopy	25
7.5.1.2.	Dislocations	26
7.5.1.2.1.	Direct evaluation of the anisotropic elastic force field	26
7.5.1.2.2.	Parallel dislocation dynamics simulation	26
7.5.2.	Co-design for scalable numerical algorithms in scientific applications	26
7.5.2.1.	MHD instabilities edge localized modes	26
7.5.2.2.	Turbulence of plasma particules inside a tokamak	26
7.5.2.3.	SN Cartesian solver for nuclear core simulation	27
7.5.2.4.	3D aerodynamics for unsteady problems with moving bodies	27
7.5.2.5.	Spectral recycling strategies for the solution of nonlinear eigenproblems in thermoacoustics	28
7.5.2.6.	A conservative 2-D advection model towards large-scale parallel calculation	28
8.	Bilateral Contracts and Grants with Industry	28
8.1.	Bilateral Contracts with Industry	28
8.2.	Bilateral Grants with Industry	29
9.	Partnerships and Cooperations	29
9.1.	Regional Initiatives	29
9.2.	National Initiatives	30
9.2.1.	Inria Project Lab	30
9.2.2.	ANR	30
9.2.2.1.	SOLHAR: SOLvers for Heterogeneous Architectures over Runtime systems	30
9.2.2.2.	SONGS: Simulation Of Next Generation Systems	31
9.2.2.3.	ANEMOS: Advanced Numeric for ELMs : Modeling and Optimized Schemes	31
9.2.2.4.	RESCUE: RÉsilience des applications SCientifiqUEs	32
9.2.2.5.	DEDALES: Algebraic and Geometric Domain Decomposition for Subsurface/Groundwater Flows	33
9.2.2.6.	TECSER: Novel high performance numerical solution techniques for RCS computations	33
9.3.	European Initiatives	34
9.3.1.1.	HPC4E	34
9.3.1.2.	EXA2CT	34
9.4.	International Initiatives	35

9.4.1. Inria Associate Teams not involved in an Inria International Labs	35
9.4.1.1. MORSE	35
9.4.1.2. FASTLA	36
9.4.2. Participation In other International Programs	36
9.5. International Research Visitors	36
10. Dissemination	37
10.1. Promoting Scientific Activities	37
10.1.1. Scientific events selection	37
10.1.1.1. Member of the conference program committees	37
10.1.1.2. Reviewer	37
10.1.2. Journal	37
10.1.2.1. Member of the editorial boards	37
10.1.2.2. Reviewer - Reviewing activities	37
10.1.3. Invited talks	37
10.1.4. Scientific expertise	37
10.1.5. Research administration	38
10.2. Teaching - Supervision - Juries	38
10.2.1. Teaching	38
10.2.2. Supervision	38
10.2.3. Juries	39
10.3. Popularization	40
11. Bibliography	40

Project-Team HIEPACS

Creation of the Team: 2009 January 01, updated into Project-Team: 2010 January 01

Keywords:

Computer Science and Digital Science:

- 1.1.4. - High performance computing
- 1.1.5. - Exascale
- 6.2.5. - Numerical Linear Algebra
- 6.2.7. - High performance computing
- 7.1. - Parallel and distributed algorithms
- 7.2. - Discrete mathematics, combinatorics

Other Research Topics and Application Domains:

- 3.3.1. - Earth and subsoil
- 3.4.2. - Industrial risks and waste
- 4. - Energy
 - 4.1. - Fossile energy production
 - 4.1.1. - Oil, gas
 - 4.1.3. - Fusion
 - 5.2.4. - Aerospace
 - 5.5. - Materials
 - 9.4.1. - Computer science
 - 9.4.2. - Mathematics
 - 9.4.4. - Chemistry

1. Members

Research Scientists

- Luc Giraud [Team leader, Inria, Senior Researcher, HdR]
- Emmanuel Agullo [Inria, Researcher]
- Olivier Coulaud [Inria, Senior Researcher, HdR]
- Jean Roman [Inria, Senior Researcher, Direction for Science and half-time in **HIEPACS**, Professor at Bordeaux INP on secondment, HdR]

Faculty Members

- Aurélien Esnard [Univ. Bordeaux, Associate Professor]
- Mathieu Faverge [Bordeaux INP, Associate Professor]
- Abdou Guermouche [Univ. Bordeaux, Associate Professor]
- Pierre Ramet [Univ. Bordeaux, Associate Professor]

Engineers

- Patrick Dos Santos [Univ. Bordeaux, from Apr 2015]
- Matías Hastaran [Inria, until Oct 2015]
- Gabriel Hautreux [Inria, until Dec 2015]
- Quentin Khan [Inria, from Sept Feb 2015, granted by Inria & Institut Carnot]
- Julien Pedron [Univ. Bordeaux]
- Cyrille Piacibello [Inria, granted by Min. du Redressement Productif]

Florent Pruvost [Inria, SED development engineer 80 % time in **HIEPACS**]
Theophile Terraz [Inria, until Sep 2015]

PhD Students

Pierre Blanchard [ENS Cachan]
Nicolas Bouzat [Inria, from Oct 2015]
Bérenger Bramas [Inria, granted by Conseil Régional Aquitaine - Airbus Group Innovations]
Astrid Casadei [Univ. Bordeaux]
Jean-Marie Couteyen [Airbus Defence and Space, ANRT - CIFRE]
Arnaud Durocher [CEA, from Nov 2015, granted by Maison de la Simulation]
Arnaud Etcheverry [Inria, until Feb 2015]
Cyril Fournier [CERFACS, from Mar 2015]
Xavier Lacoste [Inria, until Feb 2015, ANR **ANEMOS** project]
Aurelien Falco [Inria, from Oct 2015, granted by Conseil Régional Aquitaine - Airbus Group Innovations]
Salli Moustafa [EDF, until Nov 2015, ANRT - CIFRE; Inria, Dec 2015]
Stojce Nakov [Inria, until Dec 2015, Total E&P Recherche Developpement]
Gregoire Pichon [Inria, from Oct 2015, DGA - Inria]
Louis Poirel [Inria, ANR **DEDALES** project]
Alexis Praga [CERFACS]
Maria Predari [Inria, Inria - Conseil Régional Aquitaine]
Fabien Rozar [CEA Cadarache, until Oct 2015, IRFM and Maison de la Simulation]
Mawussi Zounon [Inria, until Feb 2015]

Post-Doctoral Fellows

Romain Garnier [Inria, until Nov 2015, Inria - Conseil Régional Aquitaine]
Yuval Harness [Inria, Inria - Conseil Régional Aquitaine]
Matthieu Kuhn [Inria, **TECSER** project]
Emrullah-Fatih Yetkin [Inria, granted by **EXA2CT** project]

Visiting Scientists

Pierre Brenner [Airbus Defence and Space]
Hojat Ghorbanidehno [Stanford University, from Jun 2015 until Jul 2015]
Guillaume Latu [CEA Cadarache, IRFM]
Guillaume Sylvand [Airbus Group Innovation]

Administrative Assistant

Chrystel Plumejeau [Inria]

Others

Robin Cahierre [Inria, Internship from Jul 2015 until Sep 2015]
Aurelien Falco [Inria, Internship from Feb 2015 until Jul 2015]
Quentin Khan [Inria, Internship from Feb 2015 until Jul 2015]
Thibaud Lariviere [Inria, Internship from Jul 2015 until Aug 2015]
Loris Lucido [Inria, Internship from from May 2015 until Jul 2015]
Gregoire Pichon [Inria, Internship from Feb 2015 until Jul 2015]

2. Overall Objectives

2.1. Introduction

Over the last few decades, there have been innumerable science, engineering and societal breakthroughs enabled by the development of high performance computing (HPC) applications, algorithms and architectures. These powerful tools have provided researchers with the ability to computationally find efficient solutions for some of the most challenging scientific questions and problems in medicine and biology, climatology, nanotechnology, energy and environment. It is admitted today that *numerical simulation is the third pillar for*

the development of scientific discovery at the same level as theory and experimentation. Numerous reports and papers also confirmed that very high performance simulation will open new opportunities not only for research but also for a large spectrum of industrial sectors

An important force which has continued to drive HPC has been to focus on frontier milestones which consist in technical goals that symbolize the next stage of progress in the field. In the 1990s, the HPC community sought to achieve computing at a teraflop rate and currently we are able to compute on the first leading architectures at a petaflop rate. Generalist petaflop supercomputers are available and exaflop computers are foreseen in early 2020.

For application codes to sustain petaflops and more in the next few years, hundreds of thousands of processor cores or more are needed, regardless of processor technology. Currently, a few HPC simulation codes easily scale to this regime and major algorithms and codes development efforts are critical to achieve the potential of these new systems. Scaling to a petaflop and more involves improving physical models, mathematical modeling, super scalable algorithms that will require paying particular attention to acquisition, management and visualization of huge amounts of scientific data.

In this context, the purpose of the **HIEPACS** project is to contribute performing efficiently frontier simulations arising from challenging academic and industrial research. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on emerging hierarchical many-core, possibly heterogeneous, platforms. Through this approach, **HIEPACS** intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers. This research will be conducted on close collaboration in particular with European and US initiatives and likely in the framework of H2020 European collaborative projects.

The methodological part of **HIEPACS** covers several topics. First, we address generic studies concerning massively parallel computing, the design of high-end performance algorithms and software to be executed on future extreme scale platforms. Next, several research perspectives in scalable parallel linear algebra techniques are addressed, ranging from dense direct, sparse direct, iterative and hybrid approaches for large linear systems. Then we consider research plans for N-body interaction computations based on efficient parallel fast multipole methods and finally, we address research tracks related to the algorithmic challenges for complex code couplings in multiscale/multiphysic simulations.

Currently, we have one major multiscale application that is in *material physics*. We contribute to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modeling and our advanced numerical schemes will help in the design and efficient software implementation for very large parallel multiscale simulations. Moreover, the robustness and efficiency of our algorithmic research in linear algebra are validated through industrial and academic collaborations with different partners involved in various application fields. Finally, we are also involved in a few collaborative initiatives in various application domains in a co-design like framework. These research activities are conducted in a wider multidisciplinary context with colleagues in other academic or industrial groups where our contribution is related to our expertises. Not only these collaborations enable our knowledges to have a stronger impact in various application domains through the promotion of advanced algorithms, methodologies or tools, but in return they open new avenues for research in the continuity of our core research activities.

Thanks to the two Inria collaborative agreements such as with Airbus Group/Conseil Régional Aquitaine and with CEA, we have joint research efforts in a co-design framework enabling efficient and effective technological transfer towards industrial R&D. Furthermore, thanks to two ongoing associated teams, namely **MORSE** and **FASTLA** we contribute with world leading groups to the design of fast numerical solvers and their parallel implementations.

Our high performance software packages are integrated in several academic or industrial complex codes and are validated on very large scale simulations. For all our software developments, we use first the experimental

platform **PLAFRIM**, the various large parallel platforms available through GENCI in France (CCRT, CINES and IDRIS Computational Centers), and next the high-end parallel platforms that will be available via European and US initiatives or projects such that PRACE.

3. Research Program

3.1. Introduction

The methodological component of **HIEPACS** concerns the expertise for the design as well as the efficient and scalable implementation of highly parallel numerical algorithms to perform frontier simulations. In order to address these computational challenges a hierarchical organization of the research is considered. In this bottom-up approach, we first consider in Section 3.2 generic topics concerning high performance computational science. The activities described in this section are transversal to the overall project and their outcome will support all the other research activities at various levels in order to ensure the parallel scalability of the algorithms. The aim of this activity is not to study general purpose solution but rather to address these problems in close relation with specialists of the field in order to adapt and tune advanced approaches in our algorithmic designs. The next activity, described in Section 3.3, is related to the study of parallel linear algebra techniques that currently appear as promising approaches to tackle huge problems on extreme scale platforms. We highlight the linear problems (linear systems or eigenproblems) because they are in many large scale applications the main computational intensive numerical kernels and often the main performance bottleneck. These parallel numerical techniques, which are involved in the IPL **C2S@EXA**, will be the basis of both academic and industrial collaborations, some are described in Section 4.1, but will also be closely related to some functionalities developed in the parallel fast multipole activity described in Section 3.4. Finally, as the accuracy of the physical models increases, there is a real need to go for parallel efficient algorithm implementation for multiphysics and multiscale modeling in particular in the context of code coupling. The challenges associated with this activity will be addressed in the framework of the activity described in Section 3.5.

Currently, we have one major application (see Section 4.1) that is in material physics. We will collaborate to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modelling, our advanced numerical schemes will help in the design and efficient software implementation for very large parallel simulations. We also participate to a few co-design actions in close collaboration with some applicative groups. The objective of this activity is to instantiate our expertise in fields where they are critical for designing scalable simulation tools. We refer to Section 4.2 for a detailed description of these activities.

3.2. High-performance computing on next generation architectures

Participants: Emmanuel Agullo, Olivier Coulaud, Luc Giraud, Mathieu Favergé, Abdou Guermouche, Matías Hastaran, Xavier Lacoste, Guillaume Latu, Stojce Nakov, Florent Pruvost, Pierre Ramet, Jean Roman, Emrullah-Fatih Yetkin, Mawussi Zounon.

The research directions proposed in **HIEPACS** are strongly influenced by both the applications we are studying and the architectures that we target (i.e., massively parallel heterogeneous many-core architectures, ...). Our main goal is to study the methodology needed to efficiently exploit the new generation of high-performance computers with all the constraints that it induces. To achieve this high-performance with complex applications we have to study both algorithmic problems and the impact of the architectures on the algorithm design.

From the application point of view, the project will be interested in multiresolution, multiscale and hierarchical approaches which lead to multi-level parallelism schemes. This hierarchical parallelism approach is necessary to achieve good performance and high-scalability on modern massively parallel platforms. In this context, more specific algorithmic problems are very important to obtain high performance. Indeed, the kind of applications we are interested in are often based on data redistribution for example (e.g., code coupling applications). This well-known issue becomes very challenging with the increase of both the number of computational nodes and the amount of data. Thus, we have both to study new algorithms and to adapt the existing ones. In addition, some issues like task scheduling have to be restudied in this new context. It is important to note that the work developed in this area will be applied for example in the context of code coupling (see Section 3.5).

Considering the complexity of modern architectures like massively parallel architectures or new generation heterogeneous multicore architectures, task scheduling becomes a challenging problem which is central to obtain a high efficiency. Of course, this work requires the use/design of scheduling algorithms and models specifically to tackle our target problems. This has to be done in collaboration with our colleagues from the scheduling community like for example O. Beaumont (Inria **REALOPT** Project-Team). It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore architectures, it has appeared, in the last five years, that the best programming model is an approach mixing multi-threading within computational nodes and message passing between them. In the last five years, a lot of work has been developed in the high-performance computing community to understand what is critic to efficiently exploit massively multicore platforms that will appear in the near future. It appeared that the key for the performance is firstly the granularity of the computations. Indeed, in such platforms the granularity of the parallelism must be small so that we can feed all the computing units with a sufficient amount of work. It is thus very crucial for us to design new high performance tools for scientific computing in this new context. This will be developed in the context of our solvers, for example, to adapt to this new parallel scheme. Secondly, the larger the number of cores inside a node, the more complex the memory hierarchy. This remark impacts the behaviour of the algorithms within the node. Indeed, on this kind of platforms, NUMA effects will be more and more problematic. Thus, it is very important to study and design data-aware algorithms which take into account the affinity between computational threads and the data they access. This is particularly important in the context of our high-performance tools. Note that this work has to be based on an intelligent cooperative underlying run-time (like the tools developed by the Inria **STORM** Project-Team) which allows a fine management of data distribution within a node.

Another very important issue concerns high-performance computing using “heterogeneous” resources within a computational node. Indeed, with the deployment of the GPU and the use of more specific co-processors, it is important for our algorithms to efficiently exploit these new type of architectures. To adapt our algorithms and tools to these accelerators, we need to identify what can be done on the GPU for example and what cannot. Note that recent results in the field have shown the interest of using both regular cores and GPU to perform computations. Note also that in opposition to the case of the parallelism granularity needed by regular multicore architectures, GPU requires coarser grain parallelism. Thus, making both GPU and regular cores work all together will lead to two types of tasks in terms of granularity. This represents a challenging problem especially in terms of scheduling. From this perspective, we investigate new approaches for composing parallel applications within a runtime system for heterogeneous platforms.

In that framework, the **SOLHAR** project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computers equipped with accelerators. Several attempts have been made to accomplish the porting of these methods on such architectures; the proposed approaches are mostly based on a simple offloading of some computational tasks (the coarsest grained ones) to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. **SOLHAR** proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the **StarPU** tool developed in the **STORM** team. Although the **SOLHAR** project will focus on heterogeneous computers equipped with GPUs due to their wide availability and affordable cost, the research accomplished on algorithms, methods and programming models will be readily applicable to other accelerator devices. Our final goal would be to have high performance

solvers and tools which can efficiently run on all these types of complex architectures by exploiting all the resources of the platform (even if they are heterogeneous).

In order to achieve an advanced knowledge concerning the design of efficient computational kernels to be used on our high performance algorithms and codes, we will develop research activities first on regular frameworks before extending them to more irregular and complex situations. In particular, we will work first on optimized dense linear algebra kernels and we will use them in our more complicated direct and hybrid solvers for sparse linear algebra and in our fast multipole algorithms for interaction computations. In this context, we will participate to the development of those kernels in collaboration with groups specialized in dense linear algebra. In particular, we intend develop a strong collaboration with the group of Jack Dongarra at the University of Tennessee and collaborating research groups. The objectives will be to develop dense linear algebra algorithms and libraries for multicore architectures in the context the **PLASMA** project and for GPU and hybrid multicore/GPU architectures in the context of the **MAGMA** project. The framework that hosts all these research activities is the associate team **MORSE**.

A more prospective objective is to study the resiliency in the context of large-scale scientific applications for massively parallel architectures. Indeed, with the increase of the number of computational cores per node, the probability of a hardware crash on a core or of a memory corruption is dramatically increased. This represents a crucial problem that needs to be addressed. However, we will only study it at the algorithmic/application level even if it needed lower-level mechanisms (at OS level or even hardware level). Of course, this work can be performed at lower levels (at operating system) level for example but we do believe that handling faults at the application level provides more knowledge about what has to be done (at application level we know what is critical and what is not). The approach that we will follow will be based on the use of a combination of fault-tolerant implementations of the run-time environments we use (like for example **ULFM**) and an adaptation of our algorithms to try to manage this kind of faults. This topic represents a very long range objective which needs to be addressed to guaranty the robustness of our solvers and applications. In that respect, we are involved in a ANR-Blanc project entitles **RESCUE** jointly with two other Inria EPI, namely **ROMA** and **GRAND-LARGE** as well as in the **EXA2CT** FP7 project. The main objective of the **RESCUE** project is to develop new algorithmic techniques and software tools to solve the exascale resilience problem. Solving this problem implies a departure from current approaches, and calls for yet-to-be- discovered algorithms, protocols and software tools.

Finally, it is important to note that the main goal of **HIEPACS** is to design tools and algorithms that will be used within complex simulation frameworks on next-generation parallel machines. Thus, we intend with our partners to use the proposed approach in complex scientific codes and to validate them within very large scale simulations as well as designing parallel solution in co-design collaborations.

3.3. High performance solvers for large linear algebra problems

Participants: Emmanuel Agullo, Astrid Casadei, Olivier Coulaud, Mathieu Faverge, Romain Garnier, Luc Giraud, Abdou Guermouche, Yuval Harness, Matthieu Kuhn, Xavier Lacoste, Stojce Nakov, Julien Pedron, Gregoire Pichon, Louis Poirel, Florent Pruvost, Pierre Ramet, Jean Roman.

Starting with the developments of basic linear algebra kernels tuned for various classes of computers, a significant knowledge on the basic concepts for implementations on high-performance scientific computers has been accumulated. Further knowledge has been acquired through the design of more sophisticated linear algebra algorithms fully exploiting those basic intensive computational kernels. In that context, we still look at the development of new computing platforms and their associated programming tools. This enables us to identify the possible bottlenecks of new computer architectures (memory path, various level of caches, inter processor or node network) and to propose ways to overcome them in algorithmic design. With the goal of designing efficient scalable linear algebra solvers for large scale applications, various tracks will be followed in order to investigate different complementary approaches. Sparse direct solvers have been for years the methods of choice for solving linear systems of equations, it is nowadays admitted that classical approaches are not scalable neither from a computational complexity nor from a memory view point for large problems such as those arising from the discretization of large 3D PDE problems. We will continue to work on sparse

direct solvers on the one hand to make sure they fully benefit from most advanced computing platforms and on the other hand to attempt to reduce their memory and computational costs for some classes of problems where data sparse ideas can be considered. Furthermore, sparse direct solvers are a key building boxes for the design of some of our parallel algorithms such as the hybrid solvers described in the sequel of this section. Our activities in that context will mainly address preconditioned Krylov subspace methods; both components, preconditioner and Krylov solvers, will be investigated. In this framework, and possibly in relation with the research activity on fast multipole, we intend to study how emerging \mathcal{H} -matrix arithmetic can benefit to our solver research efforts.

3.3.1. *Parallel sparse direct solver*

Solving large sparse systems $Ax = b$ of linear equations is a crucial and time-consuming step, arising in many scientific and engineering applications. Consequently, many parallel techniques for sparse matrix factorization have been studied and implemented.

Sparse direct solvers are mandatory when the linear system is very ill-conditioned; such a situation is often encountered in structural mechanics codes, for example. Therefore, to obtain an industrial software tool that must be robust and versatile, high-performance sparse direct solvers are mandatory, and parallelism is then necessary for reasons of memory capability and acceptable solution time. Moreover, in order to solve efficiently 3D problems with more than 50 million unknowns, which is now a reachable challenge with new multicore supercomputers, we must achieve good scalability in time and control memory overhead. Solving a sparse linear system by a direct method is generally a highly irregular problem that induces some challenging algorithmic problems and requires a sophisticated implementation scheme in order to fully exploit the capabilities of modern supercomputers.

New supercomputers incorporate many microprocessors which are composed of one or many computational cores. These new architectures induce strongly hierarchical topologies. These are called NUMA architectures. In the context of distributed NUMA architectures, in collaboration with the Inria **STORM** team, we study optimization strategies to improve the scheduling of communications, threads and I/O. We have developed dynamic scheduling designed for NUMA architectures in the **PaStiX** solver. The data structures of the solver, as well as the patterns of communication have been modified to meet the needs of these architectures and dynamic scheduling. We are also interested in the dynamic adaptation of the computation grain to use efficiently multi-core architectures and shared memory. Experiments on several numerical test cases have been performed to prove the efficiency of the approach on different architectures.

In collaboration with the ICL team from the University of Tennessee, and the **STORM** team from Inria, we are evaluating the way to replace the embedded scheduling driver of the **PaStiX** solver by one of the generic frameworks, **ParSEC** or **StarPU**, to execute the task graph corresponding to a sparse factorization. The aim is to design algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with GPU accelerators. More generally, this work will be performed in the context of the associate team **MORSE** and the ANR **SOLHAR** project which aims at designing high performance sparse direct solvers for modern heterogeneous systems. This ANR project involves several groups working either on the sparse linear solver aspects (**HIEPACS** and **ROMA** from Inria and APO from IRIT), on runtime systems (**STORM** from Inria) or scheduling algorithms (**REALOPT** and **ROMA** from Inria). The results of these efforts will be validated in the applications provided by the industrial project members, namely CEA-CESTA and Airbus Group Innovations.

On the numerical side, we are studying how the data sparseness that might exist in some dense blocks appearing during the factorization can be exploited using different compression techniques based on \mathcal{H} -matrix (and variants) arithmetics. This research activity will be conducted in the framework of the **FASTLA** associate team and will naturally irrigate the hybrid solvers described below as well as closely interact with the sparse direct solver actions as well as the other research efforts where similar data sparseness might be exploited.

3.3.2. *Hybrid direct/iterative solvers based on algebraic domain decomposition techniques*

One route to the parallel scalable solution of large sparse linear systems in parallel scientific computing is the use of hybrid methods that hierarchically combine direct and iterative methods. These techniques inherit the

advantages of each approach, namely the limited amount of memory and natural parallelization for the iterative component and the numerical robustness of the direct part. The general underlying ideas are not new since they have been intensively used to design domain decomposition techniques; those approaches cover a fairly large range of computing techniques for the numerical solution of partial differential equations (PDEs) in time and space. Generally speaking, it refers to the splitting of the computational domain into sub-domains with or without overlap. The splitting strategy is generally governed by various constraints/objectives but the main one is to express parallelism. The numerical properties of the PDEs to be solved are usually intensively exploited at the continuous or discrete levels to design the numerical algorithms so that the resulting specialized technique will only work for the class of linear systems associated with the targeted PDE.

In that context, we intend to continue our effort on the design of algebraic non-overlapping domain decomposition techniques that rely on the solution of a Schur complement system defined on the interface introduced by the partitioning of the adjacency graph of the sparse matrix associated with the linear system. Although it is better conditioned than the original system the Schur complement needs to be preconditioned to be amenable to a solution using a Krylov subspace method. Different hierarchical preconditioners will be considered, possibly multilevel, to improve the numerical behaviour of the current approaches implemented in our software libraries **HIPS** and **MaPHYs**. This activity will be developed in the context of the ANR **DEDALES** project. In addition to this numerical studies, advanced parallel implementation will be developed that will involve close collaborations between the hybrid and sparse direct activities.

3.3.3. Linear Krylov solvers

Preconditioning is the main focus of the two activities described above. They aim at speeding up the convergence of a Krylov subspace method that is the complementary component involved in the solvers of interest for us. In that framework, we believe that various aspects deserve to be investigated; we will consider the following ones:

- preconditioned block Krylov solvers for multiple right-hand sides. In many large scientific and industrial applications, one has to solve a sequence of linear systems with several right-hand sides given simultaneously or in sequence (radar cross section calculation in electromagnetism, various source locations in seismic, parametric studies in general, ...). For “simultaneous” right-hand sides, the solvers of choice have been for years based on matrix factorizations as the factorization is performed once and simple and cheap block forward/backward substitutions are then performed. In order to effectively propose alternative to such solvers, we need to have efficient preconditioned Krylov subspace solvers. In that framework, block Krylov approaches, where the Krylov spaces associated with each right-hand side are shared to enlarge the search space will be considered. They are not only attractive because of this numerical feature (larger search space), but also from an implementation point of view. Their block-structures exhibit nice features with respect to data locality and re-usability that comply with the memory constraint of multicore architectures. We will continue the numerical study and design of the block GMRES variant that combines inexact breakdown detection, deflation at restart and subspace recycling. Beyond new numerical investigations, a software implementation to be included in our linear solver library will be developed in the context of the DGA **HiBOX** project.
- Extension or modification of Krylov subspace algorithms for multicore architectures: finally to match as much as possible to the computer architecture evolution and get as much as possible performance out of the computer, a particular attention will be paid to adapt, extend or develop numerical schemes that comply with the efficiency constraints associated with the available computers. Nowadays, multicore architectures seem to become widely used, where memory latency and bandwidth are the main bottlenecks; investigations on communication avoiding techniques will be undertaken in the framework of preconditioned Krylov subspace solvers as a general guideline for all the items mentioned above. This research activity will benefit from the FP7 **EXA2CT** project led by **HiEPACS** on behalf of the IPL **C2S@Exa** that involves two other Inria projects namely **ALPINES** and **SAGE**.

3.3.4. Eigensolvers

Many eigensolvers also rely on Krylov subspace techniques. Naturally some links exist between the Krylov subspace linear solvers and the Krylov subspace eigensolvers. We plan to study the computation of eigenvalue problems with respect to the following two different axes:

- Exploiting the link between Krylov subspace methods for linear system solution and eigensolvers, we intend to develop advanced iterative linear methods based on Krylov subspace methods that use some spectral information to build part of a subspace to be recycled, either through space augmentation or through preconditioner update. This spectral information may correspond to a certain part of the spectrum of the original large matrix or to some approximations of the eigenvalues obtained by solving a reduced eigenproblem. This technique will also be investigated in the framework of block Krylov subspace methods.
- In the context of the calculation of the ground state of an atomistic system, eigenvalue computation is a critical step; more accurate and more efficient parallel and scalable eigensolvers are required.

3.3.5. \mathcal{H} -matrix arithmetics to reduce the memory and computation complexity of sparse direct solvers

In the context of FastLA Associate Team, during the last 2 years, we are collaborating with Eric Darve, professor in the Institute for Computational and Mathematical Engineering and the Mechanical Engineering Department at Stanford, on the design of a new efficient sparse direct solvers.

Sparse direct solvers such as **PaStiX** are currently limited by their memory requirements and computational cost. They are competitive for small matrices but are often less efficient than iterative methods for large matrices in terms of memory. We are currently accelerating the dense algebra components of direct solvers using hierarchical matrices algebra. In the first step, we are targeting an $O(N^{4/3})$ solver. Preliminary benchmarks indicate that a speed up of 2x to 10x is possible (on the largest test cases).

Moreover, in a second step, we are looking into a new class of direct solvers with cost $O(N)$. These solvers have the potential to significantly change the capabilities of linear solvers to solve complex partial differential equations on large scale parallel machines. In particular, many existing iterative methods and preconditioners fail at large scale (size of matrix N and size of parallel cluster). Instead, this new generation of solvers has been shown to scale like $O(N)$ even for very large matrices. On parallel computers, the amount of communication is essentially optimal (through near-optimal low-rank compression methodologies), leading to very scalable methods.

Such improvements will allow these solvers to outperform current state-of-the-art methods such as algebraic multigrid methods. **PaStiX** is a key platform to support these developments since it has been highly optimized for multicore and heterogeneous platforms. This project, investigated in the PhD of Gregoire Pichon (granted by DGA), will leverage several codes written at Stanford to solve linear systems.

3.4. High performance Fast Multipole Method for N-body problems

Participants: Emmanuel Agullo, Bérenger Bramas, Arnaud Etcheverry, Olivier Coulaud, Cyrille Piacibello, Guillaume Sylvand.

In most scientific computing applications considered nowadays as computational challenges (like biological and material systems, astrophysics or electromagnetism), the introduction of hierarchical methods based on an octree structure has dramatically reduced the amount of computation needed to simulate those systems for a given accuracy. For instance, in the N-body problem arising from these application fields, we must compute all pairwise interactions among N objects (particles, lines, ...) at every timestep. Among these methods, the Fast Multipole Method (FMM) developed for gravitational potentials in astrophysics and for electrostatic (coulombic) potentials in molecular simulations solves this N-body problem for any given precision with $O(N)$ runtime complexity against $O(N^2)$ for the direct computation.

The potential field is decomposed in a near field part, directly computed, and a far field part approximated thanks to multipole and local expansions. We introduced a matrix formulation of the FMM that exploits the cache hierarchy on a processor through the Basic Linear Algebra Subprograms (BLAS). Moreover, we developed a parallel adaptive version of the FMM algorithm for heterogeneous particle distributions, which is very efficient on parallel clusters of SMP nodes. Finally on such computers, we developed the first hybrid MPI-thread algorithm, which enables to reach better parallel efficiency and better memory scalability. We plan to work on the following points in **HIEPACS**.

3.4.1. Improvement of calculation efficiency

Nowadays, the high performance computing community is examining alternative architectures that address the limitations of modern cache-based designs. GPU (Graphics Processing Units) and the Cell processor have thus already been used in astrophysics and in molecular dynamics. The Fast Multipole Method has also been implemented on GPU. We intend to examine the potential of using these forthcoming processors as a building block for high-end parallel computing in N-body calculations. More precisely, we want to take advantage of our specific underlying BLAS routines to obtain an efficient and easily portable FMM for these new architectures. Algorithmic issues such as dynamic load balancing among heterogeneous cores will also have to be solved in order to gather all the available computation power. This research action will be conducted on close connection with the activity described in Section 3.2.

3.4.2. Non uniform distributions

In many applications arising from material physics or astrophysics, the distribution of the data is highly non uniform and the data can grow between two time steps. As mentioned previously, we have proposed a hybrid MPI-thread algorithm to exploit the data locality within each node. We plan to further improve the load balancing for highly non uniform particle distributions with small computation grain thanks to dynamic load balancing at the thread level and thanks to a load balancing correction over several simulation time steps at the process level.

3.4.3. Fast multipole method for dislocation operators

The engine that we develop will be extended to new potentials arising from material physics such as those used in dislocation simulations. The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. Several approaches based on the FMM or based on spatial decomposition in boxes are proposed to speed-up the computation. In dislocation codes, the calculation of the interaction forces between dislocations is still the most CPU time consuming. This computation has to be improved to obtain faster and more accurate simulations. Moreover, in such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically balance the computational load are crucial to achieve high performance.

3.4.4. Fast multipole method for boundary element methods

The boundary element method (BEM) is a well known solution of boundary value problems appearing in various fields of physics. With this approach, we only have to solve an integral equation on the boundary. This implies an interaction that decreases in space, but results in the solution of a dense linear system with $O(N^3)$ complexity. The FMM calculation that performs the matrix-vector product enables the use of Krylov subspace methods. Based on the parallel data distribution of the underlying octree implemented to perform the FMM, parallel preconditioners can be designed that exploit the local interaction matrices computed at the finest level of the octree. This research action will be conducted on close connection with the activity described in Section 3.3. Following our earlier experience, we plan to first consider approximate inverse preconditioners that can efficiently exploit these data structures.

3.5. Efficient algorithmic for load balancing and code coupling in complex simulations

Participants: Astrid Casadei, Olivier Coulaud, Aurélien Esnard, Maria Predari, Pierre Ramet, Jean Roman.

Many important physical phenomena in material physics and climatology are inherently complex applications. They often use multi-physics or multi-scale approaches, that couple different models and codes. The key idea is to reuse available legacy codes through a coupling framework instead of merging them into a standalone application. There is typically one model per different scale or physics; and each model is implemented by a parallel code. For instance, to model a crack propagation, one uses a molecular dynamic code to represent the atomistic scale and an elasticity code using a finite element method to represent the continuum scale. Indeed, fully microscopic simulations of most domains of interest are not computationally feasible. Combining such different scales or physics is still a challenge to reach high performance and scalability. If the model aspects are often well studied, there are several open algorithmic problems, that we plan to investigate in the **HIEPACS** project-team.

3.5.1. *Efficient schemes for multiscale simulations*

As mentioned previously, many important physical phenomena, such as material deformation and failure (see Section 4.1), are inherently multiscale processes that cannot always be modeled via continuum model. Fully microscopic simulations of most domains of interest are not computationally feasible. Therefore, researchers must look at multiscale methods that couple micro models and macro models. Combining different scales such as quantum-atomistic or atomistic, mesoscale and continuum, are still a challenge to obtain efficient and accurate schemes that efficiently and effectively exchange information between the different scales. We are currently involved in two national research projects, that focus on multiscale schemes. More precisely, the models that we start to study are the quantum to atomic coupling (QM/MM coupling) in the ANR **NOSSI** and the atomic to dislocation coupling in the ANR **OPTIDIS**.

3.5.2. *Dynamic load balancing for massively parallel coupled codes*

In this context of code coupling, one crucial issue is undoubtedly the load balancing of the whole coupled simulation that remains an open question. The goal here is to find the best data distribution for the whole coupled simulation and not only for each standalone code, as it is most usually done. Indeed, the naive balancing of each code on its own can lead to an important imbalance and to a communication bottleneck during the coupling phase, that can drastically decrease the overall performance. Therefore, one argues that it is required to model the coupling itself in order to ensure a good scalability, especially when running on massively parallel architectures (tens of thousands of processors/cores). In other words, one must develop new algorithms and software implementation to perform a *coupling-aware* partitioning of the whole application.

Another related problem is the problem of resource allocation. This is particularly important for the global coupling efficiency and scalability, because each code involved in the coupling can be more or less computationally intensive, and there is a good trade-off to find between resources assigned to each code to avoid that one of them waits for the other(s). And what happens if the load of one code dynamically changes relatively to the other? In such a case, it could be convenient to dynamically adapt the number of resources used at runtime.

For instance, the conjugate heat transfer simulation in complex geometries (as developed by the CFD team of CERFACS) requires to couple a fluid/convection solver (AVBP) with a solid/conduction solver (AVTP). The AVBP code is much more CPU consuming than the AVTP code. As a consequence, there is an important computational imbalance between the two solvers. The use of new algorithms to correctly load balance coupled simulations with enhanced graph partitioning techniques appears as a promising way to reach better performances of coupled application on massively parallel computers.

3.5.3. *Graph partitioning for hybrid solvers*

Graph handling and partitioning play a central role in the activity described here but also in other numerical techniques detailed in Section 3.3.

The Nested Dissection is now a well-known heuristic for sparse matrix ordering to both reduce the fill-in during numerical factorization and to maximize the number of independent computation tasks. By using the block data structure induced by the partition of separators of the original graph, very efficient parallel block solvers have been designed and implemented according to supernodal or multifrontal approaches. Considering hybrid methods mixing both direct and iterative solvers such as **HIPS** or **MaPHYs**, obtaining a domain decomposition

leading to a good balancing of both the size of domain interiors and the size of interfaces is a key point for load balancing and efficiency in a parallel context. We intend to revisit some well-known graph partitioning techniques in the light of the hybrid solvers and design new algorithms to be tested in the **Scotch** package.

4. Application Domains

4.1. Material physics

Participants: Pierre Blanchard, Olivier Coulaud, Arnaud Etcheverry.

Due to the increase of available computer power, new applications in nano science and physics appear such as study of properties of new materials (photovoltaic materials, bio- and environmental sensors, ...), failure in materials, nano-indentation. Chemists, physicists now commonly perform simulations in these fields. These computations simulate systems up to billion of atoms in materials, for large time scales up to several nanoseconds. The larger the simulation, the smaller the computational cost of the potential driving the phenomena, resulting in low precision results. So, if we need to increase the precision, there are two ways to decrease the computational cost. In the first approach, we improve algorithms and their parallelization and in the second way, we will consider a multiscale approach.

A domain of interest is the material aging for the nuclear industry. The materials are exposed to complex conditions due to the combination of thermo-mechanical loading, the effects of irradiation and the harsh operating environment. This operating regime makes experimentation extremely difficult and we must rely on multi-physics and multi-scale modeling for our understanding of how these materials behave in service. This fundamental understanding helps not only to ensure the longevity of existing nuclear reactors, but also to guide the development of new materials for 4th generation reactor programs and dedicated fusion reactors. For the study of crystalline materials, an important tool is dislocation dynamics (DD) modeling. This multiscale simulation method predicts the plastic response of a material from the underlying physics of dislocation motion. DD serves as a crucial link between the scale of molecular dynamics and macroscopic methods based on finite elements; it can be used to accurately describe the interactions of a small handful of dislocations, or equally well to investigate the global behavior of a massive collection of interacting defects.

To explore i.e. to simulate these new areas, we need to develop and/or to improve significantly models, schemes and solvers used in the classical codes. In the project, we want to accelerate algorithms arising in those fields. We will focus on the following topics (in particular in the currently under definition **OPTIDIS** project in collaboration with CEA Saclay, CEA Ile-de-france and SIMaP Laboratory in Grenoble) in connection with research described at Sections 3.4 and 3.5.

- The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. In dislocation codes, the computation of interaction forces between dislocations is still the most CPU time consuming and has to be improved to obtain faster and more accurate simulations.
- In such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically construct a good load balancing are crucial to achieve high performance.
- From a physical and a simulation point of view, it will be interesting to couple a molecular dynamics model (atomistic model) with a dislocation one (mesoscale model). In such three-dimensional coupling, the main difficulties are firstly to find and characterize a dislocation in the atomistic region, secondly to understand how we can transmit with consistency the information between the two micro and meso scales.

4.2. Co-design for scalable numerical algorithms in scientific applications

Participants: Pierre Brenner, Jean-Marie Couteyen, Mathieu Faverge, Xavier Lacoste, Guillaume Latu, Salli Moustafa, Pierre Ramet, Fabien Rozar, Jean Roman.

The research activities concerning the ITER challenge are involved in the Inria Project Lab (IPL) **C2S@EXA**.

4.2.1. *MHD instabilities edge localized modes*

The numerical simulations tools designed for ITER challenges aim at making a significant progress in understanding active control methods of plasma edge MHD instabilities Edge Localized Modes (ELMs) which represent particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in ITER. Project is focused in particular on the numerical modeling study of such ELM control methods as Resonant Magnetic Perturbations (RMPs) and pellet ELM pacing both foreseen in ITER. The goals of the project are to improve understanding the related physics and propose possible new strategies to improve effectiveness of ELM control techniques. The tool for the nonlinear MHD modeling (code **JOREK**) will be largely developed within the present project to include corresponding new physical models in conjunction with new developments in mathematics and computer science strategy in order to progress in urgently needed solutions for ITER.

The fully implicit time evolution scheme in the **JOREK** code leads to large sparse linear systems that have to be solved at every time step. The MHD model leads to very badly conditioned matrices. In principle the **PaStiX** library can solve these large sparse problems using a direct method. However, for large 3D problems the CPU time for the direct solver becomes too large. Iterative solution methods require a preconditioner adapted to the problem. Many of the commonly used preconditioners have been tested but no satisfactory solution has been found. The research activities presented in Section 3.3 will contribute to design new solution techniques best suited for this context.

4.2.2. *Turbulence of plasma particules inside a tokamak*

In the context of the ITER challenge, the **GYSELA** project aims at simulating the turbulence of plasma particules inside a tokamak. Thanks to a better comprehension of this phenomenon, it would be possible to design a new kind of source of energy based of nuclear fusion. Currently, **GYSELA** is parallalized in a MPI/OpenMP way and can exploit the power of the current greatest supercomputers. To simulate faithfully the plasma physic, **GYSELA** handles a huge amount of data. In fact, the memory consumption is a bottleneck on very large simulations (449 K cores). In this context, mastering the memory consumption of the code becomes critical to consolidate its scalability and to enable the implementation of new numerical and physical features to fully benefit from the extreme scale architectures.

The scientific objectives of these research activities are first the design of advanced generic tools to manage and to better predict and limit the memory consumption peak in order to reduce the memory footprint of **GYSELA**, and second to design a set of tools that analyses the performance and the topology of the targeted architecture to optimize the deployment of Gysela runs. This will allow the design of new advanced numerical methods (for the gyroaverage operator, for the source and collision operators) and efficient scalable parallel algorithms in order to be able to deal with new physics in **GYSELA**. In particular the objective is to tackle kinetic electron configurations for more realistic simulations.

4.2.3. *SN Cartesian solver for nuclear core simulation*

As part of its activity, EDF R&D is developing a new nuclear core simulation code named COCAGNE that relies on a Simplified PN (SPN) method to compute the neutron flux inside the core for eigenvalue calculations. In order to assess the accuracy of SPN results, a 3D Cartesian model of PWR nuclear cores has been designed and a reference neutron flux inside this core has been computed with a Monte Carlo transport code from Oak Ridge National Lab. This kind of 3D whole core probabilistic evaluation of the flux is computationally very demanding. An efficient deterministic approach is therefore required to reduce the computation effort dedicated to reference simulations.

In this collaboration, we work on the parallelization (for shared and distributed memories) of the DOMINO code, a parallel 3D Cartesian SN solver specialized for PWR core reactivity computations which is fully integrated in the COCAGNE system.

4.2.4. 3D aerodynamics for unsteady problems with moving bodies

Aribus Defence and Space has developed for 20 years the FLUSEPA code which focuses on unsteady phenomenon with changing topology like stage separation or rocket launch. The code is based on a finite volume formulation with temporal adaptive time integration and supports bodies in relative motion. The temporal adaptive integration classifies cells in several temporal levels, zero being the level with the slowest cells and each level being twice as fast as the previous one. This repartition can evolve during the computation, leading to load-balancing issues in a parallel computation context. Bodies in relative motion are managed through a CHIMERA-like technique which allows building a composite mesh by merging multiple meshes. The meshes with the highest priorities recover the least ones, and at the boundaries of the covered mesh, an intersection is computed. Unlike classical CHIMERA technique, no interpolation is performed, allowing a conservative flow integration.

The main objective of this research is to design a new scalable version of FLUSEPA from a task-based parallelization over a runtime system in order to run efficiently on modern multicore parallel architectures very large 3D simulations (for example ARIANE 5 and 6 booster separation).

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

The paper entitled “Task-based multi frontal QR solver for GPU-accelerated multicore architectures” by Emmanuel Agullo (Inria, France); Alfredo Buttari (CNRS - IRIT Toulouse, France); Abdou Guermouche (Université de Bordeaux, France); Florent Lopez (Université Paul Sabatier, France) received the best paper award at HiPC 2015 .

BEST PAPER AWARD:

[28]

E. AGULLO, A. BUTTARI, A. GUERMOUCHE, F. LOPEZ. *Task-based multifrontal QR solver for GPU-accelerated multicore architectures*, in "High Performance Computing-HiPC", Bangalore, India, December 2015, Best paper, <https://hal.inria.fr/hal-01270145>

6. New Software and Platforms

6.1. Introduction

We describe in this section the software that we are developing. The first list will be the main milestones of our project. The other software developments will be conducted in collaboration with academic partners or in collaboration with some industrial partners in the context of their private R&D or production activities. For all these software developments, we will use first the various (very) large parallel platforms available through GENCI in France (CCRT, CINES and IDRIS Computational Centers), and next the high-end parallel platforms that will be available via European and US initiatives or projects such that PRACE.

6.2. Chameleon

Participant: Emmanuel Agullo [corresponding member].

Chameleon is part of the MORSE (Matrices Over Runtime Systems @ Exascale) project. The overall objective is to develop robust linear algebra libraries relying on innovative runtime systems that can fully benefit from the potential of those future large-scale complex machines.

6.3. MaPHyS

Participant: Emmanuel Agullo [corresponding member].

MaPHyS (Massively Parallel Hybrid Solver) is a software package that implements a parallel linear solver coupling direct and iterative approaches. The underlying idea is to apply to general unstructured linear systems domain decomposition ideas developed for the solution of linear systems arising from PDEs. The interface problem, associated with the so called Schur complement system, is solved using a block preconditioner with overlap between the blocks that is referred to as Algebraic Additive Schwarz.

The **MaPHyS** package is very much a first outcome of the research activity described in Section 3.3. Finally, **MaPHyS** is a preconditioner that can be used to speed-up the convergence of any Krylov subspace method. We foresee to either embed in **MaPHyS** some Krylov solvers or to release them as standalone packages, in particular for the block variants that will be some outcome of the studies discussed in Section 3.3.

MaPHyS can be found at <http://maphys.gforge.inria.fr>.

6.4. PaStiX

Participant: Pierre Ramet [corresponding member].

Complete and incomplete supernodal sparse parallel factorizations.

PaStiX (Parallel Sparse matriX package) is a scientific library that provides a high performance parallel solver for very large sparse linear systems based on block direct and block ILU(k) iterative methods. Numerical algorithms are implemented in single or double precision (real or complex): LLt (Cholesky), LDLt (Crout) and LU with static pivoting (for non symmetric matrices having a symmetric pattern).

The **PaStiX** library uses the graph partitioning and sparse matrix block ordering package **Scotch**. **PaStiX** is based on an efficient static scheduling and memory manager, in order to solve 3D problems with more than 50 million of unknowns. The mapping and scheduling algorithm handles a combination of 1D and 2D block distributions. This algorithm computes an efficient static scheduling of the block computations for our supernodal parallel solver which uses a local aggregation of contribution blocks. This can be done by taking into account very precisely the computational costs of the BLAS 3 primitives, the communication costs and the cost of local aggregations. We also improved this static computation and communication scheduling algorithm to anticipate the sending of partially aggregated blocks, in order to free memory dynamically. By doing this, we are able to reduce the aggregated memory overhead, while keeping good performance.

Another important point is that our study is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of multicore nodes. In particular, we now offer a high performance version with a low memory overhead for multicore node architectures, which fully exploits the advantage of shared memory by using an hybrid MPI-thread implementation.

Direct methods are numerically robust methods, but the very large three dimensional problems may lead to systems that would require a huge amount of memory despite any memory optimization. A studied approach consists in defining an adaptive blockwise incomplete factorization that is much more accurate (and numerically more robust) than the scalar incomplete factorizations commonly used to precondition iterative solvers. Such incomplete factorization can take advantage of the latest breakthroughs in sparse direct methods and particularly should be very competitive in CPU time (effective power used from processors and good scalability) while avoiding the memory limitation encountered by direct methods.

PaStiX is publicly available at <http://pastix.gforge.inria.fr> under the Inria CeCILL licence.

6.5. HIPS

Participant: Pierre Ramet [corresponding member].

Multilevel method, domain decomposition, Schur complement, parallel iterative solver.

HIPS (Hierarchical Iterative Parallel Solver) is a scientific library that provides an efficient parallel iterative solver for very large sparse linear systems.

The key point of the methods implemented in **HIPS** is to define an ordering and a partition of the unknowns that relies on a form of nested dissection ordering in which cross points in the separators play a special role (Hierarchical Interface Decomposition ordering). The subgraphs obtained by nested dissection correspond to the unknowns that are eliminated using a direct method and the Schur complement system on the remaining of the unknowns (that correspond to the interface between the sub-graphs viewed as sub-domains) is solved using an iterative method (GMRES or Conjugate Gradient at the time being). This special ordering and partitioning allows for the use of dense block algorithms both in the direct and iterative part of the solver and provides a high degree of parallelism to these algorithms. The code provides a hybrid method which blends direct and iterative solvers. **HIPS** exploits the partitioning and multistage ILU techniques to enable a highly parallel scheme where several subdomains can be assigned to the same process. It also provides a scalar preconditioner based on the multistage ILUT factorization.

HIPS can be used as a standalone program that reads a sparse linear system from a file ; it also provides an interface to be called from any C, C++ or Fortran code. It handles symmetric, unsymmetric, real or complex matrices. Thus, **HIPS** is a software library that provides several methods to build an efficient preconditioner in almost all situations.

HIPS is publicly available at <http://hips.gforge.inria.fr> under the Inria CeCILL licence.

6.6. MetaPart

Participant: Aurélien Esnard [corresponding member].

MetaPart is a library that addresses the challenge of (dynamic) load balancing for emerging complex parallel simulations, such as multi-physics or multi-scale coupling applications. First, it offers a uniform API over state-of-the-art (hyper-) graph partitioning software packages such as **Scotch**, PaToH, METIS, Zoltan, Mondriaan, etc. etc. Based upon this API, it provides a framework that facilitates the development and the evaluation of high-level partitioning methods, such as MxN repartitioning or coupling-aware partitioning (co-partitioning).

The framework is publicly available at Inria Gforge: <http://metapart.gforge.inria.fr>.

6.7. MPICPL

Participant: Aurélien Esnard [corresponding member].

MPICPL (MPI CouPLing) is a software library dedicated to the coupling of parallel legacy codes, that are based on the well-known MPI standard. It proposes a lightweight and comprehensive programming interface that simplifies the coupling of several MPI codes (2, 3 or more). MPICPL facilitates the deployment of these codes thanks to the *mpicplrun* tool and it interconnects them automatically through standard MPI inter-communicators. Moreover, it generates the universe communicator, that merges the world communicators of all coupled-codes. The coupling infrastructure is described by a simple XML file, that is just loaded by the *mpicplrun* tool.

MPICPL was developed by **HIEPACS** for the purpose of the ANR **NOSSI**. It uses advanced features of MPI2 standard. The framework is publicly available at Inria Gforge: <http://mpicpl.gforge.inria.fr>.

6.8. ScalFMM

Participant: Olivier Coulaud [corresponding member].

ScalFMM (Parallel Fast Multipole Library for Large Scale Simulations) is a software library to simulate N-body interactions using the Fast Multipole Method.

ScalFMM intends to offer all the functionalities needed to perform large parallel simulations while enabling an easy customization of the simulation components: kernels, particles and cells. It works in parallel in a shared/distributed memory model using OpenMP and MPI. The software architecture has been designed with two major objectives: being easy to maintain and easy to understand. There are two main parts: 1) the management of the octree and the parallelization of the method ; 2) the kernels. This new architecture allows us to easily add new FMM algorithm or kernels and new paradigm of parallelization. The code is extremely documented and the naming convention fully respected. Driven by its user-oriented philosophy, **ScalFMM** is using CMAKE as a compiler/installer tool. Even if **ScalFMM** is written in C++ it will support a C and fortran API soon.

The library offers two methods to compute interactions between bodies when the potential decays like $1/r$. The first method is the classical FMM based on spherical harmonic expansions and the second is the Black-Box method which is an independent kernel formulation (introduced by E. Darve at Stanford). With this method, we can now easily add new non oscillatory kernels in our library. For the classical method, two approaches are used to decrease the complexity of the operators. We consider either matrix formulation that allows us to use BLAS routines or rotation matrix to speed up the M2L operator.

The **ScalFMM** package is available at <http://scalmmm.gforge.inria.fr>

6.9. ViTE

Participant: Mathieu Faverge [corresponding member].

Visualization, Execution trace

ViTE is a trace explorer. It is a tool made to visualize execution traces of large parallel programs. It supports Pajé, a trace format created by Inria Grenoble, and OTF and OTF2 formats, developed by the University of Dresden and allows the programmer a simpler way to analyse, debug and/or profile large parallel applications. It is an open source software licenced under CeCILL-A.

The **ViTE** software is available at <http://vite.gforge.inria.fr> and has been developed in collaboration with the Inria Bordeaux - Sud-Ouest SED team, Telecom SudParis and Inria Grenoble.

In the same context we also contribute to the EZtrace and GTG libraries in collaboration with F. Trahay from Telecom SudParis. EZTrace (<http://eztrace.gforge.inria.fr>) is a tool that aims at generating automatically execution trace from HPC programs. It generates execution trace files thanks to the GTG library (<http://gtg.gforge.inria.fr>) that can be later interpreted by visualization tools such as **ViTE**.

6.10. Other software

For the materials physics applications, a lot of development will be done in the context of older ANR projects (**NOSSI** and **OPTIDIS**) in collaboration with LaBRI, CPMOH, IPREM, EPFL and with CEA Saclay and Bruyère-le-Châtel.

- **OptiDis**

Participant: Olivier Coulaud [corresponding member].

OptiDis is a new code for large scale dislocation dynamics simulations. Its aim is to simulate real life dislocation densities (up until $5 \cdot 10^{22}$ dislocations/ m^{-2}) in order to understand plastic deformation and study strain hardening. The main application is to observe and understand plastic deformation on irradiated zirconium. Zirconium alloys is the first containment barrier against the dissemination of radioactive elements. More precisely, with neutron irradiated zirconium alloys we are talking of channeling mechanism, which means to stick with the reality, more than tens of thousands of induced loops so 10^8 degrees of freedom in the simulation.

The code is based on Numodis code developed at CEA Saclay and the **Sca1FMM** library developed in our Inria project. The code is written in C++ language and using the last features of C++11. One of the main aspects is the hybrid parallelism MPI/OpenMP that gives the software the ability to scale on large cluster while the computation load rises. In order to achieve that, we use different levels of parallelism. First of all, the simulation box is spread over MPI processes, we then use a thinner level for threads, dividing the domain using an Octree representation. All these parts are driven by the **Sca1FMM** library. On the last level our data are stored in an adaptive structure absorbing dynamic of this kind of simulation and handling well task parallelism.

The two following packages are mainly designed and developed in the context of a US initiative led by ICL and to which we closely collaborate through the associate team **MORSE**.

- **PLASMA**

Participant: Mathieu Faverge [corresponding member].

The **PLASMA** (Parallel Linear Algebra for Scalable Multi-core Architectures) project aims at addressing the critical and highly disruptive situation that is facing the Linear Algebra and High Performance Computing community due to the introduction of multi-core architectures.

The **PLASMA** ultimate goal is to create software frameworks that enable programmers to simplify the process of developing applications that can achieve both high performance and portability across a range of new architectures.

The development of programming models that enforce asynchronous, out of order scheduling of operations is the concept used as the basis for the definition of a scalable yet highly efficient software framework for Computational Linear Algebra applications.

The **PLASMA** library is available at <http://icl.cs.utk.edu/plasma>.

- **PaRSEC/DPLASMA**

Participant: Mathieu Faverge [corresponding member].

PaRSEC Parallel Runtime Scheduling and Execution Controller, is a generic framework for architecture aware scheduling and management of micro-tasks on distributed many-core heterogeneous architectures. Applications we consider can be expressed as a Direct Acyclic Graph of tasks with labeled edges designating data dependencies. DAGs are represented in a compact problem-size independent format that can be queried on-demand to discover data dependencies in a totally distributed fashion. **PaRSEC** assigns computation threads to the cores, overlaps communications and computations and uses a dynamic, fully-distributed scheduler based on architectural features such as NUMA nodes and algorithmic features such as data reuse.

The framework includes libraries, a runtime system, and development tools to help application developers tackle the difficult task of porting their applications to highly heterogeneous and diverse environments.

DPLASMA (Distributed Parallel Linear Algebra Software for Multicore Architectures) is the leading implementation of a dense linear algebra package for distributed heterogeneous systems. It is designed to deliver sustained performance for distributed systems where each node featuring multiple sockets of multicore processors, and if available, accelerators like GPUs or Intel Xeon Phi. **DPLASMA** achieves this objective through the state of the art **PaRSEC** runtime, porting the **PLASMA** algorithms to the distributed memory realm.

The **PaRSEC** runtime and the **DPLASMA** library are available at <http://icl.cs.utk.edu/parsec>.

6.11. Platforms

6.11.1. *PlaFRIM: an experimental parallel computing platform*

PLAFRIM is an open experimental platform for research and development in modeling, simulations and high performance computing. This platform has been set up from 2009 under the leadership of Inria Bordeaux Sud-Ouest in collaboration with computer science and mathematics laboratories, respectively Labri and IMB with

a strong support in the region Aquitaine. Since mid-2015, this platform is now open to laboratories involved in the CPU cluster and SMIs located in the region Aquitaine.

It aggregates different kinds of computational resources for research and development purposes. The latest technologies in terms of processors, memories and architecture are added when they are available on the market. It is now more than 2,500 cores (excluding GPU and Xeon Phi) that are available for all research teams of Inria Bordeaux, Labri and IMB. Those computers are in particular used by all the engineers who work in HiePACS and are advised by F. Rue from the SED.

The PlaFRIM platform initiative is coordinated by O. Coulaud.

7. New Results

7.1. High-performance computing on next generation architectures

7.1.1. *Soft error sensitivity of PCG and reliability of detection mechanisms*

Soft errors can be defined as failures arising from several electricity fluctuations, cosmic particle effects on chip or any other unexpected problem while computations are in progress. If computational environment grows up to exascale, the rate of these types of error is likely to increase. These bit-flips may have a strong impact on iterative methods, that might diverge or converge to an unexpected final accuracy. Consequently, soft errors deserve to be examined in details especially in the perspective of extreme scale computing platforms. In this work, we investigate the combination of different numerical techniques to tackle the challenge of the detection. The first ingredient relies on checksum mechanisms, that are applied to secure the sparse matrix vector (SpMV) products. However, the checksum equalities are only valid in exact arithmetic while calculation are performed in finite precision. Another possibility is to monitor the residual deviation between the true and computed residual. Exploiting finite precision analysis of the round-off provides us with an upper bound on the residual norm deviation that can be used. Through intensive numerical experiments and statistical analysis we shown how round-off error analysis for the residual norm deviation can be an efficient and robust soft error detection criterion alternative to checksum approaches. This methodology has also be applied to other variants of CG, namely the pipelined and chronopolus/gear versions.

This research effort was conducted in collaboration with colleagues S. Cools and W. Vanroose from the Applied Mathematics Group of Antwerp university within the framework of the **EXA2CT** project. In this context, we also studied the impact of soft errors on a variant of the algorithm designed in their group (so-called pipelined CG). This study allowed to highlight some numerical instability in the baseline version of this variant of CG in the presence of round-off errors and we jointly proposed a correction of it that led a new both scalable and stable variant (see Section 7.2.5).

We have also designed a self-recovering CG algorithm which detects large magnituded faults with ABFT and smoothes low and average magnituded faults with deviation-based criteria.

7.1.2. *Resilience of parallel sparse hybrid solvers*

As the computational power of high performance computing (HPC) systems continues to increase by using a huge number of CPU cores or specialized processing units, extreme-scale applications are increasingly prone to faults. Consequently, the HPC community has proposed many contributions to design resilient HPC applications. These contributions may be system-oriented, theoretical or numerical. In this study we consider an actual fully-featured parallel sparse hybrid (direct/iterative) linear solver, **MaPHyS**, and we propose numerical remedies to design a resilient version of the solver. The solver being hybrid, we focus in this study on the iterative solution step, which is often the dominant step in practice. We furthermore assume that a separate mechanism ensures fault detection and that a system layer provides support for setting back the environment (processes, ...) in a running state. The present manuscript therefore focuses on (and only on) strategies for recovering lost data *after* the fault has been detected (a separate concern beyond the scope of this study), *once* the system is restored (another separate concern not studied here). The numerical remedies we propose are

twofold. Whenever possible, we exploit the natural data redundancy between processes from the solver to perform exact recovery through clever copies over processes. Otherwise, data that has been lost and no longer available on any process is recovered through a so-called interpolation-restart mechanism. This mechanism is derived from our earlier studies by carefully taking into account the properties of the target hybrid solver. These numerical remedies have been implemented in the **MaPHYs** parallel solver so that we can assess their efficiency on a large number of processing units (up to 12,288 CPU cores) for solving large-scale real-life problems.

These contributions will be presented at the international conference HiPC [42].

7.1.3. Hierarchical DAG scheduling for hybrid distributed systems

Accelerator-enhanced computing platforms have drawn a lot of attention due to their massive peak computational capacity. Despite significant advances in the programming interfaces to such hybrid architectures, traditional programming paradigms struggle mapping the resulting multi-dimensional heterogeneity and the expression of algorithm parallelism, resulting in sub-optimal effective performance. Task-based programming paradigms have the capability to alleviate some of the programming challenges on distributed hybrid many-core architectures. In this work we take this concept a step further by showing that the potential of task-based programming paradigms can be greatly increased with minimal modification of the underlying runtime combined with the right algorithmic changes. We propose two novel recursive algorithmic variants for one-sided factorizations and describe the changes to the **PaRSEC** task-scheduling runtime to build a framework where the task granularity is dynamically adjusted to adapt the degree of available parallelism and kernel efficiency according to runtime conditions. Based on an extensive set of results we show that, with one-sided factorizations, i.e. Cholesky and QR, a carefully written algorithm, supported by an adaptive task-based runtime, is capable of reaching a degree of performance and scalability never achieved before in distributed hybrid environments.

These contributions will be presented at the international conference IPDPS 2015 [34] in Hyderabad.

7.1.3.1. Comparison of Static and Dynamic Resource Allocation Strategies for Matrix Multiplication

The tremendous increase in the size and heterogeneity of supercomputers makes it very difficult to predict the performance of a scheduling algorithm. In this context, relying on purely static scheduling and resource allocation strategies, that make scheduling and allocation decisions based on the dependency graph and the platform description, is expected to lead to large and unpredictable makespans whenever the behavior of the platform does not match the predictions. For this reason, the common practice in most runtime libraries is to rely on purely dynamic scheduling strategies, that make short-sighted scheduling decisions at runtime based on the estimations of the duration of the different tasks on the different available resources and on the state of the machine. In this work, we considered the special case of Matrix Multiplication, for which a number of static allocation algorithms to minimize the amount of communications have been proposed. Through a set of extensive simulations, we analyzed the behavior of static, dynamic, and hybrid strategies, and we assessed the possible benefits of introducing more static knowledge and allocation decisions in runtime libraries. These contributions have been presented at the international conference SBAC-PAD 2015.

7.1.3.2. Scheduling Trees of Malleable Tasks for Sparse Linear Algebra

Scientific workloads are often described as directed acyclic task graphs. In this paper, we focus on the multifrontal factorization of sparse matrices, whose task graph is structured as a tree of parallel tasks. Among the existing models for parallel tasks, the concept of *malleable* tasks is especially powerful as it allows each task to be processed on a time-varying number of processors. Following the model advocated by Prasanna and Musicus for matrix computations, we considered malleable tasks whose speedup is p^α , where p is the fractional share of processors on which a task executes, and α ($0 < \alpha \leq 1$) is a parameter which does not depend on the task. We first motivated the relevance of this model for our application with actual experiments on multicore platforms. Then, we studied the optimal allocation proposed by Prasanna and Musicus for makespan minimization using optimal control theory. We largely simplified their proofs by resorting only to pure scheduling arguments. Building on the insight gained thanks to these new proofs, we extended the study to distributed multicore platforms. There, a task cannot be distributed among several distributed

nodes. In such a distributed setting (homogeneous or heterogeneous), we proved the NP-completeness of the corresponding scheduling problem, and proposed some approximation algorithms. We finally assessed the relevance of our approach by simulations on realistic trees. We showed that the average performance gain of our allocations with respect to existing solutions (that are thus unaware of the actual speedup functions) is up to 16% for $\alpha = 0.9$ (the value observed in the real experiments). These contributions have been presented at the international conference Europar 2015.

7.1.3.3. *Task-based multifrontal QR solver for GPU-accelerated multicore architectures*

Recent studies have shown the potential of task-based programming paradigms for implementing robust, scalable sparse direct solvers for modern computing platforms. Yet, designing task flows that efficiently exploit heterogeneous architectures remains highly challenging. In this work we first tackled the issue of data partitioning using a method suited for heterogeneous platforms. On the one hand, we designed task of sufficiently large granularity to obtain a good acceleration factor on GPU. On the other hand, we limited the size in order to both fit the GPU memory constraints and generate enough parallelism in the task graph. Secondly we handled the task scheduling with a strategy capable of taking into account workload and architecture heterogeneity at a reduced cost. Finally we proposed an original evaluation of the performance obtained in our solver on a test set of matrices. We showed that the proposed approach allows for processing extremely large input problems on GPU-accelerated platforms and that the overall performance is competitive with equivalent state of the art solvers designed and optimized for GPU-only use. These contributions have been presented at the international conference HiPC 2015 where they received the best paper award.

7.1.3.4. *Fast and Accurate Simulation of Multithreaded Sparse Linear Algebra Solvers*

The ever growing complexity and scale of parallel architectures imposes to rewrite classical monolithic HPC scientific applications and libraries as their portability and performance optimization only comes at a prohibitive cost. There is thus a recent and general trend in using instead a modular approach where numerical algorithms are written at a high level independently of the hardware architecture as Directed Acyclic Graphs (DAG) of tasks. A task-based runtime system then dynamically schedules the resulting DAG on the different computing resources, automatically taking care of data movement and taking into account the possible speed heterogeneity and variability. Evaluating the performance of such complex and dynamic systems is extremely challenging especially for irregular codes. In this work, we explained how we crafted a faithful simulation, both in terms of performance and memory usage, of the behavior of `qr_mumps`, a fully-featured sparse linear algebra library, on multi-core architectures. In our approach, the target high-end machines are calibrated only once to derive sound performance models. These models can then be used at will to quickly predict and study in a reproducible way the performance of such irregular and resource-demanding applications using solely a commodity laptop. These contributions have been presented at the international conference ICPADS 2015.

7.2. High performance solvers for large linear algebra problems

7.2.1. *Divide and conquer symmetric tridiagonal eigensolver for multicore architectures*

Computing eigenpairs of a symmetric matrix is a problem arising in many industrial applications, including quantum physics and finite-elements computation for automobiles. A classical approach is to reduce the matrix to tridiagonal form before computing eigenpairs of the tridiagonal matrix. Then, a back-transformation allows one to obtain the final solution. Parallelism issues of the reduction stage have already been tackled in different shared-memory libraries. In this work, we focus on solving the tridiagonal eigenproblem, and we describe a novel implementation of the Divide and Conquer algorithm. The algorithm is expressed as a sequential task-flow, scheduled in an out-of-order fashion by a dynamic runtime which allows the programmer to play with tasks granularity. The resulting implementation is between two and five times faster than the equivalent routine from the INTEL MKL library, and outperforms the best MRRR implementation for many matrices. These contributions have been presented at the international conference IPDPS 2015 [32] in Hyderabad.

7.2.2. *Blocking strategy optimizations for sparse direct linear solver on heterogeneous architectures*

Solving sparse linear systems is a problem that arises in many scientific applications, and sparse direct solvers are a time consuming and key kernel to those applications or more advanced solvers such as hybrid direct-iterative solvers. That is why optimizing their performance on modern architectures is a crucial problem. The preprocessing steps of sparse direct solvers: ordering and symbolic factorization, are two major steps that lead to a reduced amount of computation and memory, and to a better task granularity to reach a good level of performance when using BLAS kernels. With the advent of GPUs, the granularity of the symbolic factorization became more important than ever. In this work, we present a reordering strategy that increases the block granularity. This strategy relies on the symbolic factorization to refine the ordering produced by tools such as METIS or *Scotch*, and does not impact the number of operations required to solve the problem. We integrated this algorithm in the *PaStiX* solver and show a reduction of the number of off-diagonal blocks by two to three on a large spectrum of matrices. This improvement leads to an efficiency on GPUs raised by up to 40%. These contributions have been presented at the Sparse Days [51] in Saint-Girons.

7.2.3. *On the use of \mathcal{H} -Matrix Arithmetic in PaStiX: a Preliminary Study*

The objective is to investigate innovative lowrank approximations based on \mathcal{H} -matrix variants for direct solver and Schur complements. The intent is to improve scalability of those components involved in preconditioners and hybrid solvers by reducing the computational and memory costs of the dense calculation. The quality of hybrid ordering algorithms combining topdown (such as nested dissection) and bottomup (such as minimum degree) ordering techniques in the context of sparse linear solvers will be investigated.

In this work, we describe a preliminary fast direct solver using HODLR library to compress large blocks appearing in the symbolic structure of the *PaStiX* sparse direct solver. We present our general strategy before analyzing the practical gains in terms of memory and floating point operations with respect to a theoretical study of the problem. Finally, we discuss ways to enhance the overall performance of the solver.

Some contributions have already been presented at the Workshop on Fast Solvers [52] in Toulouse. This work is a joint effort between Professor Darve's group at Stanford and the Inria HiePACS team within *FASTLA*.

7.2.4. *Data sparse techniques for parallel hybrid solvers*

In this work we describe how data sparse techniques exploiting \mathcal{H} -matrix calculations can be implemented in a parallel hybrid sparse linear solver based on an algebraic non overlapping domain decomposition approach.

Various graph-based clustering techniques to approximate the local Schur complements are investigated, with the aim of optimally complying with the interface structure of the local interfaces of the subdomains. We consider strong-hierarchical (sH) matrix arithmetic as efficient means for obtaining low rank approximations in terms of workload distribution as well as memory consumption. We also show how sH-arithmetic can be utilized to form an effective global preconditioner for the iterative phase of the hybrid solver. Numerical and parallel experiments are presented to evaluate the advantages and drawbacks of the different variants.

This work is a joint effort between Professor Darve's group at Stanford and the Inria HiePACS team within *FASTLA*. Some intermediate progresses have already been presented [38], [37]

7.2.5. *Analysis of the rounding error accumulation in Conjugate Gradient to improve the maximal attainable accuracy of pipelined CG*

Pipelined Krylov solvers typically offer better scalability in the strong scaling limit compared to standard Krylov methods. The synchronization bottleneck is mitigated by overlapping time-consuming global communications with useful computations in the algorithm. However, to achieve this communication hiding strategy, pipelined methods feature multiple recurrence relations on additional auxiliary variables to update the guess for the solution. This paper aims to study the influence of rounding errors on the convergence of the pipelined Conjugate Gradient method. It is analyzed why rounding effects have a significantly larger impact on the maximal attainable accuracy of the pipelined CG algorithm compared to the traditional CG method.

Based on a rounding error model, we then propose an automated residual replacement strategy to reduce the effect of rounding errors on the final iterative solution. The resulting pipelined CG method with residual replacement improves the maximal attainable accuracy of pipelined CG while maintaining its efficient parallel performance.

This research effort was conducted in collaboration with colleagues S. Cools and W. Vanroose from the Applied Mathematics Group of Antwerp university within the framework of the **EXA2CT** project.

7.3. High performance Fast Multipole Method for N-body problems

7.3.1. Task-based Fast Multipole Method

Last year we have worked primarily on developing an efficient fast multipole method for heterogeneous architecture. Some of the accomplishments for this year include:

1. We have finalized the Uniform FMM (ufmm) based on polynomial interpolations combined with a hierarchical (data sparse) representation of a kernel matrix. The algorithm is close to the Black Box FMM by Fong and Darve developed with Chebyshev polynomials, however it uses an interpolation scheme based on an equispaced grid, which allows the use of FFT and consequently reduce both running time and memory footprint but has implications on accuracy and stability. The theory behind the Uniform FMM kernel is explained in a research report [63] along with numerical benchmarks on artificial test cases and presented in [44]. This new kernel was extended to be used for dislocation kernel.
2. Concerning the Group-Tree approach, we have shown in past studies its advantages of the task-based FMM and how the group-tree is well suited for runtime systems. In fact, it improves the locality, but it also reduces the number of dependencies which is an important asset to decrease the runtime overhead. These prospective task-based FMM can solve problems on heterogeneous architecture as presented in [36]. Therefore, we have continued this work and created a robust group-tree that has been included in ScalFMM and which is now available to the community. This data structure is generic and can be used with the different ScalFMM kernels. Moreover, we have extended our work and implemented a distributed task-based FMM above StarPU. The description of the data structure and some experimental studies will be presented in February 2016 during PhD defense of B. Bérenger.
3. With the advent of complex modern architectures, the low-level paradigms long sufficient to build high performance computing (HPC) numerical codes have met their limits. Achieving efficiency, ensuring portability, while preserving programming tractability on such hardware prompted the HPC community to design new, higher level paradigms. Indeed, several robust runtime systems proposed recently have shown the benefit of task-based parallelism models in terms of performance portability on complex platforms, on top of which full-featured numerical libraries have been ported successfully. However, the common weakness of these projects is to deeply tie applications to specific expert-only runtime system APIs. The OPENMP specification, which aims at providing a common parallel programming means for shared-memory platforms, appears a good candidate to address this issue thanks to the latest task-based constructs introduced as part of its revision 4.0. The goal of this joint work with **STORM** team is to assess the effectiveness and limits of this support for designing a high-performance numerical library like **ScalFMM** library, which implements state-of-the-art fast multipole methods (FMM) algorithms and that we have considerably re-designed with respect to the most advanced features provided by OPENMP 4.0. We show that OPENMP 4.0 allows for significant performance improvements over previous OPENMP revisions on recent multicore processors. We furthermore propose extensions to the OPENMP 4.0 standard and show how they could enhance FMM performance. To assess our statement, we have implemented this support within the **KLANG-OMP** source-to-source compiler that translates OPENMP directives into calls to the **StarPU** task-based runtime system. This study shows that we can take advantage of the advanced capabilities of a fully-featured runtime system without resorting to a specific, native runtime port, hence bridging the gap between the OPENMP standard and the very high performance that was so far reserved to expert-only runtime system APIs.

7.3.2. Time-domain boundary element method

The Time-domain Boundary Element Method (TD-BEM) has not been widely studied but represents an interesting alternative to its frequency counterpart. Usually based on inefficient Sparse Matrix Vector-product (SpMV), we investigate other approaches in order to increase the sequential flop-rate.

The TD-BEM formulation we is naturally expressed using sparse-matrix vector product (SpMV). We describe how the Flop-rate can be improved using a so-called multi-vectors/vector product, and we provide an efficient implementation of this operation using vectorization. We have extended our TD-BEM solver to support NVidia GPUs, and we have looked at different blocking schemes and their respective implementations. We have created a new blocking storage which matches our operators and allows to obtain a high Flop-rate. In addition, we provide a balancing heuristic to divide the work between the CPUs and the GPUs dynamically. The results have been published in [20], and our solver is now able to work on distributed heterogeneous nodes.

Our TD-BEM solver is efficient, but it still has a quadratic complexity which might become a problem for large problems. This high complexity motivates the study of an FMM based TD-BEM solver with the objective of being more competitive as the problem size increases. Therefore, we have implemented an FMM-based solver but while the complexity should be lower than the matrix approach, it remains unclear from which problem size. Moreover, we show in [PhD defense of B. Bérenger] different results and point-out that the memory cost is much more expensive for the FMM approach compare to the matrix one. The method has been discussed in [43] among other ScalFMM applications.

All the implementations should be in high quality in the Software Engineering sense since the resulting library is going to be used by industrial applications.

This work is developed in the framework of Bérenger Bramas's PhD and contributes to the EADS-ASTRIUM, Inria, Conseil Régional initiative.

7.3.3. Randomized algorithms for covariance matrices

7.3.3.1. Covariance kernel matrices

Random projection based Low Rank Approximation (LRA) algorithms such as the randomized SVD produce approximate matrix factorizations in quadratic instead of cubic time in N (N being the matrix size). This complexity can be further improved if fast matrix multiplication is available. A paper explaining our recent advances in fast randomized LRA of covariance kernel matrices using FMM is available as a research report [63] and presented in [44]. In particular, the fast multipole acceleration of the randomized SVD allowed for generating Gaussian random fields on arbitrary grids in linear running time and memory requirements. The code is available in the open source C++ project FMR: <https://gforge.inria.fr/projects/fmr>, it relies heavily on the ScalFMM library for data structures and fast matrix multiplication.

7.3.3.2. New applications: Data Assimilation and Taxonomy

Many applications like data assimilation (e.g. Kalman Filtering or variational approaches) or biology (e.g. taxonomy) involve covariance matrices that are only known in algebraic form, as opposed to kernel matrices that can be explicitly build given a kernel function. In a joint project (called FastMDS) with Alain Franc (INRA, Inria PLEIADE) addressing fast methods for the classification of biological species (taxonomy) our randomized SVD algorithm was used in order to accelerate a MultiDimensionalScaling (MDS) algorithm. The MDS is a widely used method in machine learning and data analysis that aim at visualizing the information contained in a distance matrix. Our MDS algorithm is applied to DNA sequences coming from various sources (e.g. Leman's lake), it consists in forming an euclidian image of the sample by taking the square root of a covariance matrix computed from the distance matrix. The randomized SVD approach lead to promising results, since it allowed to treat up to 100.000 samples in a few seconds. Since the covariance matrix still needs to be loaded in memory, storage might become problematic for larger samples. Therefore we are now considering matrix-free methods in order to decrease the memory requirements but also hierarchical algorithms in order to compute the MDS in near-linear time. The following methods are currently under investigation:

- Random column selection based LRA methods such as the Nystrom method or blocked variant of the Nystrom method (BBF, see Wang, Darve, Mahoney).
- Random projection based LRA powered by general H2-methods.

All these techniques are considered since they apply well, when the relevant information is spread uniformly among the data, just like in our data sets.

7.4. Efficient algorithmic for load balancing and code coupling in complex simulations

7.4.1. Dynamic load balancing for massively parallel coupled codes

In the field of scientific computing, load balancing is a major issue that determines the performance of parallel applications. Nowadays, simulations of real-life problems are becoming more and more complex, involving numerous coupled codes, representing different models. In this context, reaching high performance can be a great challenge. In the PhD of Maria Predari (started in october 2013), we develop new graph partitioning techniques, called co-partitioning, that address the problem of load balancing for two coupled codes: the key idea is to perform a *coupling-aware* partitioning, instead of partitioning these codes independently, as it is usually done. However, our co-partitioning technique requires to use graph partitioning with *fixed vertices*, that raises serious issues with state-of-the-art software, that are classically based on the well-known recursive bisection paradigm (RB). Indeed, the RB method often fails to produce partitions of good quality. To overcome this issue, we propose a *new* direct k -way greedy graph growing algorithm, called KGGGP, that overcomes this issue and succeeds to produce partition with better quality than RB while respecting the constraint of fixed vertices. Experimental results compare KGGGP against state-of-the-art methods for graphs available from the popular DIMACS'10 collection. This work will be presented in the 24th Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP 2016).

7.5. Application Domains

7.5.1. Material physics

7.5.1.1. Molecular Vibrational Spectroscopy

Quantum chemistry eigenvalue problem is a big challenge in recent research. Here we are interested in solving eigenvalue problems coming from the molecular vibrational analysis. These problems are challenging because the size of the vibrational Hamiltonian matrix to be diagonalized is exponentially increasing with the size of the molecule we are studying. So, for molecules bigger than 10 atoms the actual existent algorithms suffer from a curse of dimensionality or computational time. We propose a new variational algorithm (namely residue-based adaptive vibrational configuration interaction) intended for the resolution of the vibrational Schrödinger equation. The main advantage of this approach is to efficiently reduce the dimension of the active space generated into the configuration interaction (CI) process. This adaptive algorithm is developed with the use of three correlated conditions i.e. a suitable starting space ; a criterion for convergence, and a procedure to expand the approximate space. The speed of the algorithm was increased with the use of a posteriori error estimator (residue) to select the most relevant direction to increase the space. Two examples have been selected for benchmark. In the case of Formalde hydemolecule (H_2CO) with a dimension space of 6, we mainly study the performance of RA-VCI algorithm: comparison with the variation-perturbation method, choice of the initial space, residual contributions. For Acetonitrile molecule (CH_3CN) with dimension space of 12 the active space computed by our algorithm is divided by 20 compared to the computations done by Avila et. al using the same potential energy surface. This work was presented in [54], [53].

7.5.1.2. Dislocations

7.5.1.2.1. Direct evaluation of the anisotropic elastic force field

The anisotropic elastic force field created by dislocations is not explicitly given, in fact it is only known in integral form using Green's or Stroh's formalism. The approach considered in OptiDis is based on Stroh's formalism, i.e. we compute the stress field using tensorial angular functions known as Stroh matrices. A benefit of using Stroh's formalism is that it only requires the evaluation of a single line integral for the force field and no integration for the stress field, while Green's formalism involve double and single line integral respectively. The evaluation of Stroh matrices in arbitrary directions is not affordable, therefore spherical harmonic expansions were considered in order to approximate the stress field efficiently. Until now the integration of the stress field on target dislocations was performed numerically using simple quadratures, although the quadrature size required to evaluate the force field at a given precision may explode as segments get closer and computation may become untractable. In order to avoid this behaviour, we developed semi-analytical expressions of the force field based on the analytic integration of the expansions of the stress field (in spherical harmonics). This new method is an adaptation of Aubry et al. approach to Stroh's formalism, in the sense that it also provides optimized recursive formulae to efficiently evaluate these semi-analytic expressions. Numerous verifications and further improvements of the expressions are required before implementing it inside OptiDis.

7.5.1.2.2. Parallel dislocation dynamics simulation

We have focused on the improvements of our hybrid MPI-OpenMP parallelism of the OptiDis code. More precisely, we have continued the development of parallel algorithm to add/remove element in the cache-conscious data structure. This data structured combined with an octree manages efficiently large set of data (segments and nodes) during all the steps of the algorithm. Moreover, we have tuned and improved our hybrid MPI-OpenMP parallelism to run simulations with large number of radiation induced defects forming our dislocation network. To obtain a good scalability, we have introduced a better load balancing at thread level as well as process level. By combining efficient data structure and hybrid parallelism we obtained a speedup of 112 on 160 cores for a simulation of half a million of segments.

All this work was developped in the Phd of A. Etchevery.

7.5.2. Co-design for scalable numerical algorithms in scientific applications

7.5.2.1. MHD instabilities edge localized modes

The last contribution of Xavier Lacoste's thesis deals with the integration of our work in **JOEK**, a production controlled plasma fusion simulation code from CEA Cadarache. We described a generic finite element oriented distributed matrix assembly and solver management API. The goal of this API is to optimize and simplify the construction of a distributed matrix which, given as an input to **PaStiX**, can improve the memory scaling of the application. Experiments exhibit that using this API we could reduce the memory consumption by moving to a distributed matrix input and improve the performance of the factorized matrix assembly by reducing the volume of communication. All this study is related to **PaStiX** integration inside **JOEK** but the same API could be used to produce a distributed assembly for another solver or/and another finite elements based simulation code.

7.5.2.2. Turbulence of plasma particles inside a tokamak

Concerning the **GyseLA** global non-linear electrostatic code, the efforts during the period have concentrated on predicting memory requirement and on the gyroaverage operator.

The Gysela program uses a mesh of 5 dimensions of the phase space (3 dimensions in configuration space and 2 dimensions in velocity space). On the large cases, the memory consumption already reaches the limit of the available memory on the supercomputers used in production (Tier-1 and Tier-0 typically). Furthermore, to implement the next features of Gysela (e.g. adding kinetic electrons in addition to ions), the needs of memory will dramatically increase, the main unknown will represents hundreds of TB. In this context, two tools were created to analyze and decrease the memory consumption. The first one is a tool that plots the memory consumption of the code during a run. This tool helps the developer to localize where the memory peak is

located. The second tool is a prediction tool to compute the peak memory in offline mode (for production use mainly). A post processing stage combined with some specific traces generated on purpose during runtime allow the analysis of the memory consumption. Low-level primitives are called to generate these traces and to model memory consumption : they are included in the libMTM library (Modeling and Tracing Memory). Thanks to this work on memory consumption modeling, we have decreased the memory peak of the Gysela code up to 50 % on a large case using 32,768 cores and memory scalability improvement has been shown using these tools up to 65k cores.

The main unknown of the Gysela is a distribution function that represents either the density of the guiding centers, either the density of the particles in a tokamak (depending of the location in the code). The switch between these two representations is done thanks to the gyroaverage operator. In the actual version of Gysela, the computation of this operator is achieved thanks to the so-called Padé approximation. In order to improve the precision of the gyroaveraging, a new implementation based on interpolation methods has been done (mainly by researchers from the Inria Tonus project-team and IPP Garching). We have performed the integration of this new implementation in Gysela and also some parallel benchmarks. However, the new gyroaverage operator is approximatively 10 times slower than the original one. Investigations and optimizations on this operator are still a work in progress.

This work has been carried on in the framework of Fabien Rozar's PhD in collaboration with CEA Cadarache (defended in November 2015). A new PhD (Nicolas Bouzat) has started in October 2015 and the scientific objectives of this work will be first to consolidate the parallel version of the gyroaverage operator, in particular by designing a complete MPI+OpenMP parallel version, and then to design new numerical methods for the gyroaverage, source and collision operators to deal with new physics in Gysela. The objective is to tackle kinetic electron configurations for more realistic simulations.

7.5.2.3. SN Cartesian solver for nuclear core simulation

High-fidelity nuclear power plant core simulations require solving the Boltzmann transport equation. In discrete ordinate methods, the most computationally demanding operation of this equation is the sweep operation. Considering the evolution of computer architectures, we propose in this work, as a first step toward heterogeneous distributed architectures, a hybrid parallel implementation of the sweep operation on top of the generic task-based runtime system: **PaRSEC**. Such an implementation targets three nested levels of parallelism: message passing, multi-threading, and vectorization. A theoretical performance model was designed to validate the approach and help the tuning of the multiple parameters involved in such an approach. The proposed parallel implementation of the Sweep achieves a sustained performance of 6.1 Tflop/s, corresponding to 33.9% of the peak performance of the targeted supercomputer. This implementation compares favorably with state-of-art solvers such as PARTISN; and it can therefore serve as a building block for a massively parallel version of the neutron transport solver DOMINO developed at EDF.

The main contribution has been presented at the international conference IPDPS 2015 [31] in Hyderabad.

7.5.2.4. 3D aerodynamics for unsteady problems with moving bodies

In the first part of our research work concerning the parallel aerodynamic code FLUSEPA, a first OpenMP-MPI version based on the previous one has been developed. By using an hybrid approach based on a domain decomposition, we achieved a faster version of the code and the temporal adaptive method used without bodies in relative motion has been tested successfully for real complex 3D-cases using up to 400 cores. Moreover, an asynchronous strategy for computing bodies in relative motion and mesh intersections has been developed and has been used for actual 3D-cases. A journal article (for JCP) to sum-up this part of the work is under redaction and a presentation at ISC at the "2nd International Workshop on High Performance Computing Simulation in Energy/Transport Domains" on July 2015 is scheduled.

This intermediate version exhibited synchronization problems for the aerodynamic solver due to the time integration used by the code. To tackle this issue, a task-based version over the runtime system **StarPU** is currently under development and evaluation. This year was mainly devoted to the realisation of this version. Task generation function have been designed in order to maximize asynchronism in execution. Those functions respect the data pattern access of the code and led to the refactorization of the actual kernels. A task-based version is now available for the aerodynamic solver and is available for both shared and distributed memory.

This work has been presented as a poster during the SIAM CSE' 15 conference and at the Parallel CFD' 15 and HPCSET' 15 conferences.

The next steps will be to validate the correction of this task-based version and to work on the performance of this new version on actual cases. Later, the task description should be extended to the motion and intersection operations.

This work is carried on in the framework of Jean-Marie Couteyen's PhD in collaboration with Airbus Defence and Space.

7.5.2.5. Spectral recycling strategies for the solution of nonlinear eigenproblems in thermoacoustics

In this work we consider the numerical solution of large nonlinear eigenvalue problems that arise in thermoacoustic simulations involved in the stability analysis of large combustion devices. We briefly introduce the physical modeling that leads to a nonlinear eigenvalue problem that is solved using a nonlinear fixed point iteration scheme. Each step of this nonlinear method requires the solution of a complex non-Hermitian linear eigenvalue problem. We review a set of state of the art eigensolvers and discuss strategies to recycle spectral information from one nonlinear step to the next. More precisely, we consider the Jacobi-Davidson algorithm, the Implicitly Restarted Arnoldi method, the Krylov-Schur solver and its block-variant, as well as the subspace iteration method with Chebyshev acceleration. On a small test example we study the relevance of the different approaches and illustrate on a large industrial test case the performance of the parallel solvers best suited to recycle spectral information for large scale thermoacoustic stability analysis.

The results of this work conducted in collaboration with S. Moreau (Sherbrooke University) and Y. Saad (University of Minnesota Twin-cities) are detailed in [22]

7.5.2.6. A conservative 2-D advection model towards large-scale parallel calculation

To exploit the possibilities of parallel computers, we designed a large-scale bidimensional atmospheric advection model named Pangolin. As the basis for a future chemistry-transport model, a finite-volume approach for advection was chosen to ensure mass preservation and to ease parallelization. To overcome the pole restriction on time steps for a regular latitude-longitude grid, Pangolin uses a quasi-area-preserving reduced latitude-longitude grid. The features of the regular grid are exploited to reduce the memory footprint and enable effective parallel performances. In addition, a custom domain decomposition algorithm is presented. To assess the validity of the advection scheme, its results are compared with state-of-the-art models on algebraic test cases. Finally, parallel performances are shown in terms of strong scaling and confirm the efficient scalability up to a few hundred cores

The results of this work are detailed in [21].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Airbus Defence and Space research and development contract:

- Design of a parallel version of the FLUSEPA software (Jean-Marie Couteyen (PhD); Pierre Brenner, Jean Roman).

CEA DPTA research and development contract:

- The objective was to evaluate if our ScalFMM library could be used to compute electrostatic interactions in molecular dynamics code (Stamp) of the CEA.

CEA-CESTA research and development contract:

- Performance analysis of the recent improvements in PaStiX sparse direct solver for matrices coming from different applications developed at CEA-CESTA.

CEA Cadarache (ITER) research and development contract:

- Peta and exaflop algorithms for turbulence simulations of fusion plasmas (Fabien Rozar (PhD); Guillaume Latu, Jean Roman).

EDF R & D - SINETICS research and development contract:

- Design of a massively parallel version of the SN method for neutronic simulations (Moustafa Salli (PhD); Mathieu Faverge, Pierre Ramet, Jean Roman).

TOTAL research and development contracts:

- Parallel hybrid solver for massively heterogeneous manycore platforms (Stojce Nakov (PhD); Emmanuel Agullo, Luc Giraud, Abdou Guermouche, Jean Roman).

8.2. Bilateral Grants with Industry

Airbus Group Innovations research and development contract:

- Design and implementation of temporal FMM calculation (B. Bramas (PhD); Olivier Coulaud, Guillaume Sylvand).
- Design and implementation of FMM and block Krylov solver for BEM applications. The HiBOX project is led by the SME IMACS and funded by the DGA Rapid programme (C. Piacibello (Engineer), Olivier Coulaud, Luc Giraud).

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Innovative simulation methods for large scale numeric prototypes on emerging architectures computers

Participants: Emmanuel Agullo, Olivier Coulaud, Aurélien Esnard, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Pierre Ramet, Jean Roman.

Grant: Regional council

Dates: 2013 – 2015

Partners: EPIs **REALOPT**, **STORM** from Inria Bordeaux Sud-Ouest, CEA-CESTA and l'Institut pluridisciplinaire de recherche sur l'environnement et les matériaux (IPREM) .

Overview: Numerical simulation is now integrated into all the design levels and the scientific studies for both academic and industrial contexts. Given the increasing size and sophistication of the simulations carried out, the use of parallel computing is inescapable. The complexity of such achievements requires collaboration of multidisciplinary teams capable of mastering all the necessary scientific skills for each component constituting the chain of expertise. In this project we consider each of these elements as well as efficient methods for parallel codes coupling. All these works are intended to contribute to the design of large scale parallel multi-physics simulations. In addition to this research human activities the regional council also support some innovative computing equipment that will be embedded in the PlaFRIM experimental platform, project led by O. Coulaud.

9.2. National Initiatives

9.2.1. Inria Project Lab

9.2.1.1. C2S@Exa - Computer and Computational Sciences at Exascale

Since January 2013, the team is participating to the **C2S@EXA** Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. At the current state of the art in technologies and methodologies, a multidisciplinary approach is required to overcome the challenges raised by the development of highly scalable numerical simulation software that can exploit computing platforms offering several hundreds of thousands of cores. Hence, the main objective of **C2S@EXA** is the establishment of a continuum of expertise in the computer science and numerical mathematics domains, by gathering researchers from Inria project-teams whose research and development activities are tightly linked to high performance computing issues in these domains. More precisely, this collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

9.2.2. ANR

9.2.2.1. SOLHAR: SOLvers for Heterogeneous Architectures over Runtime systems

Participants: Emmanuel Agullo, Mathieu Faverge, Abdou Guermouche, Xavier Lacoste, Pierre Ramet, Jean Roman, Guillaume Sylvand.

Grant: ANR-MONU

Dates: 2013 – 2017

Partners: Inria (**REALOPT**, **STORM** Bordeaux Sud-Ouest et **ROMA** Rhone-Alpes), IRIT/INPT, CEA-CESTA et Airbus Group Innovations.

Overview:

During the last five years, the interest of the scientific computing community towards accelerating devices has been rapidly growing. The reason for this interest lies in the massive computational power delivered by these devices. Several software libraries for dense linear algebra have been produced; the related algorithms are extremely rich in computation and exhibit a very regular pattern of access to data which makes them extremely good candidates for GPU execution. On the contrary, methods for the direct solution of sparse linear systems have irregular, indirect memory access patterns that adversely interact with typical GPU throughput optimizations.

This project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with accelerators. The ultimate aim of this project is to achieve the implementation of a software package providing a solver based on direct methods for sparse linear systems of equations. To date, the approaches proposed to achieve this objective are mostly based on a simple offloading of some computational tasks to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems. The development of a production-quality, sparse direct solver requires a considerable research effort along three distinct axes:

- linear algebra: algorithms have to be adapted or redesigned in order to exhibit properties that make their implementation and execution on heterogeneous computing platforms efficient and reliable. This may require the development of novel methods for defining data access patterns that are more suitable for the dynamic scheduling of computational tasks on processing units with considerably different capabilities as well as techniques for guaranteeing a reliable and robust behavior and accurate solutions. In addition, it will be necessary to develop novel and efficient accelerator

implementations of the specific dense linear algebra kernels that are used within sparse, direct solvers;

- runtime systems: tools such as the **StarPU** runtime system proved to be extremely efficient and robust for the implementation of dense linear algebra algorithms. Sparse linear algebra algorithms, however, are commonly characterized by complicated data access patterns, computational tasks with extremely variable granularity and complex dependencies. Therefore, a substantial research effort is necessary to design and implement features as well as interfaces to comply with the needs formalized by the research activity on direct methods;
- scheduling: executing a heterogeneous workload with complex dependencies on a heterogeneous architecture is a very challenging problem that demands the development of effective scheduling algorithms. These will be confronted with possibly limited views of dependencies among tasks and multiple, and potentially conflicting objectives, such as minimizing the makespan, maximizing the locality of data or, where it applies, minimizing the memory consumption.

Given the wide availability of computing platforms equipped with accelerators and the numerical robustness of direct solution methods for sparse linear systems, it is reasonable to expect that the outcome of this project will have a considerable impact on both academic and industrial scientific computing. This project will moreover provide a substantial contribution to the computational science and high-performance computing communities, as it will deliver an unprecedented example of a complex numerical code whose parallelization completely relies on runtime scheduling systems and which is, therefore, extremely portable, maintainable and evolvable towards future computing architectures.

9.2.2.2. *SONGS: Simulation Of Next Generation Systems*

Participant: Abdou Guermouche.

Grant: ANR 11 INFRA 13

Dates: 2011 – 2015

Partners: Inria (Bordeaux Sud-Ouest, Nancy - Grand Est, Rhone-Alpes, Sophia Antipolis - Méditerranée), I3S, LSIIT

Overview:

The last decade has brought tremendous changes to the characteristics of large scale distributed computing platforms. Large grids processing terabytes of information a day and the peer-to-peer technology have become common even though understanding how to efficiently exploit such platforms still raises many challenges. As demonstrated by the USS SimGrid project funded by the ANR in 2008, simulation has proved to be a very effective approach for studying such platforms. Although even more challenging, we think the issues raised by petaflop/exaflop computers and emerging cloud infrastructures can be addressed using similar simulation methodology.

The goal of the **SONGS** project is to extend the applicability of the SimGrid simulation framework from Grids and Peer-to-Peer systems to Clouds and High Performance Computation systems. Each type of large-scale computing system will be addressed through a set of use cases and lead by researchers recognized as experts in this area.

Any sound study of such systems through simulations relies on the following pillars of simulation methodology: Efficient simulation kernel; Sound and validated models; Simulation analysis tools; Campaign simulation management.

9.2.2.3. *ANEMOS: Advanced Numeric for ELMs : Modeling and Optimized Schemes*

Participants: Xavier Lacoste, Guillaume Latu, Pierre Ramet.

Grant: ANR-MN

Dates: 2012 – 2016

Partners: Univ. Nice, CEA/IRFM, CNRS/MDS.

Overview: The main goal of the project is to make a significant progress in understanding of active control methods of plasma edge MHD instabilities Edge Localized Modes (ELMs) which represent particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in ITER. The project is focused in particular on the numerical modelling study of such ELM control methods as Resonant Magnetic Perturbations (RMPs) and pellet ELM pacing both foreseen in ITER. The goals of the project are to improve understanding of the related physics and propose possible new strategies to improve effectiveness of ELM control techniques. The tool for the non-linear MHD modeling is the **JOREK** code which was essentially developed within previous ANR **ASTER**. **JOREK** will be largely developed within the present project to include corresponding new physical models in conjunction with new developments in mathematics and computer science strategy. The present project will put the non-linear MHD modeling of ELMs and ELM control on the solid ground theoretically, computationally, and applications-wise in order to progress in urgently needed solutions for ITER.

Regarding our contributions, the **JOREK** code is mainly composed of numerical computations on 3D data. The toroidal dimension of the tokamak is treated in Fourier space, while the poloidal plane is decomposed in Bezier patches. The numerical scheme used involves a direct solver on a large sparse matrix as a main computation of one time step. Two main costs are clearly identified: the assembly of the sparse matrix, and the direct factorization and solve of the system that includes communications between all processors. The efficient parallelization of **JOREK** is one of our main goals, to do so we will reconsider: data distribution, computation distribution or GMRES implementation. The quality of the sparse solver is also crucial, both in term of performance and accuracy. In the current release of **JOREK**, the memory scaling is not satisfactory to solve problems listed above, since at present as one increases the number of processes for a given problem size, the memory footprint on each process does not reduce as much as one can expect. In order to access finer meshes on available supercomputers, memory savings have to be done in the whole code. Another key point for improving parallelization is to carefully profile the application to understand the regions of the code that do not scale well. Depending on the timings obtained, strategies to diminish communication overheads will be evaluated and schemes that improve load balancing will be initiated. **JOREK** uses **PaStiX** sparse matrix library for matrix inversion. However, large number of toroidal harmonics and particular thin structures to resolve for realistic plasma parameters and ITER machine size still require more aggressive optimisation in numeric dealing with numerical stability, adaptive meshes etc. However many possible applications of **JOREK** code we proposed here which represent urgent ITER relevant issues related to ELM control by RMPs and pellets remain to be solved.

9.2.2.4. *RESCUE: Résilience des applications SCientifiques*

Participants: Emmanuel Agullo, Luc Giraud, Abdou Guermouche, Jean Roman, Mawussi Zounon.

Grant: ANR-Blanc (computer science theme)

Dates: 2010 – 2015

Partners: Inria EPI **ROMA** (leader) and GRAND LARGE.

Overview: The advent of exascale machines will help solve new scientific challenges only if the resilience of large scientific applications deployed on these machines can be guaranteed. With 10,000,000 core processors, or more, the time interval between two consecutive failures is anticipated to be smaller than the typical duration of a checkpoint, i.e., the time needed to save all necessary application and system data. No actual progress can then be expected for a large-scale parallel application. Current fault-tolerant techniques and tools can no longer be used. The main objective of the **RESCUE** project is to develop new algorithmic techniques and software tools to solve the exascale resilience problem. Solving this problem implies a departure from current approaches, and calls for yet-to-be-discovered algorithms, protocols and software tools.

This proposed research follows three main research thrusts. The first thrust deals with novel checkpoint protocols. This thrust will include the classification of relevant fault categories and the development of a software package for fault injection into application execution at runtime. The main research activity will be the design and development of scalable and light-weight checkpoint and migration protocols, with on-the-fly storing of key data, distributed but coordinated decisions, etc. These protocols will be validated via a prototype implementation integrated with the public-domain MPICH project. The second thrust entails the development of novel execution models, i.e., accurate stochastic models to predict (and, in turn, optimize) the expected performance (execution time or throughput) of large-scale parallel scientific applications. In the third thrust, we will develop novel parallel algorithms for scientific numerical kernels. We will profile a representative set of key large-scale applications to assess their resilience characteristics (e.g., identify specific patterns to reduce checkpoint overhead). We will also analyze execution trade-offs based on the replication of crucial kernels and on decentralized ABFT (Algorithm-Based Fault Tolerant) techniques. Finally, we will develop new numerical methods and robust algorithms that still converge in the presence of multiple failures. These algorithms will be implemented as part of a software prototype, which will be evaluated when confronted with realistic faults generated via our fault injection techniques.

We firmly believe that only the combination of these three thrusts (new checkpoint protocols, new execution models, and new parallel algorithms) can solve the exascale resilience problem. We hope to contribute to the solution of this critical problem by providing the community with new protocols, models and algorithms, as well as with a set of freely available public-domain software prototypes.

9.2.2.5. *DEDALES: Algebraic and Geometric Domain Decomposition for Subsurface/Groundwater Flows*

Participants: Emmanuel Agullo, Luc Giraud, Mathieu Faverge, Louis Poirel.

Grant: ANR-14-CE23-0005

Dates: 2014 – 2018

Partners: Inria EPI POMDAPI (leader); Université Paris 13 - Laboratoire Analyse, Géométrie et Applications; Maison de la Simulation; Andra.

Overview: Project **DEDALES** aims at developing high performance software for the simulation of two phase flow in porous media. The project will specifically target parallel computers where each node is itself composed of a large number of processing cores, such as are found in new generation many-core architectures. The project will be driven by an application to radioactive waste deep geological disposal. Its main feature is phenomenological complexity: water-gas flow in highly heterogeneous medium, with widely varying space and time scales. The assessment of large scale model is of major importance and issue for this application, and realistic geological models have several million grid cells. Few, if at all, software codes provide the necessary physical features with massively parallel simulation capabilities. The aim of the **DEDALES** project is to study, and experiment with, new approaches to develop effective simulation tools with the capability to take advantage of modern computer architectures and their hierarchical structure. To achieve this goal, we will explore two complementary software approaches that both match the hierarchical hardware architecture: on the one hand, we will integrate a hybrid parallel linear solver into an existing flow and transport code, and on the other hand, we will explore a two level approach with the outer level using (space time) domain decomposition, parallelized with a distributed memory approach, and the inner level as a subdomain solver that will exploit thread level parallelism. Linear solvers have always been, and will continue to be, at the center of simulation codes. However, parallelizing implicit methods on unstructured meshes, such as are required to accurately represent the fine geological details of the heterogeneous media considered, is notoriously difficult. It has also been suggested that time level parallelism could be a useful avenue to provide an extra degree of parallelism, so as to exploit the very large number of computing elements that will be part of these next generation computers. Project **DEDALES** will show that space-time DD methods can provide this extra level, and can usefully be combined with parallel linear solvers at the subdomain level. For all tasks, realistic test cases will be used to show the validity and the parallel scalability of the chosen approach. The most demanding models will be at the frontier of what is currently feasible for the size of models.

9.2.2.6. *TECSER: Novel high performance numerical solution techniques for RCS computations*

Participants: Emmanuel Agullo, Luc Giraud, Matthieu Kuhn.

Grant: ANR-14-ASTRID

Dates: 2014 – 2017

Partners: Inria EPI NACHOS (leader), Corida, HiePACS; Airbus Group Innovations, Nucléides.

Overview: the objective of the TECSER projet is to develop an innovative high performance numerical methodology for frequency-domain electromagnetics with applications to RCS (Radar Cross Section) calculation of complicated structures. This numerical methodology combines a high order hybridized DG method for the discretization of the frequency-domain Maxwell in heterogeneous media with a BEM (Boundary Element Method) discretization of an integral representation of Maxwell's equations in order to obtain the most accurate treatment of boundary truncation in the case of theoretically unbounded propagation domain. Beside, scalable hybrid iterative/direct domain decomposition based algorithms are used for the solution of the resulting algebraic system of equations.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. HPC4E

Title: HPC for Energy

Programm: H2020

Duration: 2015 - 2018

Coordinator: Barcelona Supercomputing Center

Inria contact: Stephane Lanteri

Objectives: This project has three general objectives and a large list of specific technical objectives related with research in each technology:

1. The main objective is to develop beyond the state of the art high performance simulation tools that can help the energy industry to respond future energy demands and also to carbon related environmental issues using the state of the art HPC systems.
2. Improve the cooperation between energy industries from EU and Brazil. The project includes relevant energy industrial partners from Brazil and EU, which will benefit from the project's results. They guarantee that TRL of the project technologies will be very high
3. Improve the cooperation between the leading research centres in EU and Brazil in HPC applied to energy industry. This includes sharing supercomputing infrastructures between Brazil and EU. The cross fertilization between energy related problems and other scientific fields will be beneficial at both sides of the Atlantic.

9.3.1.2. EXA2CT

Type: FP7

Defi: Special action

Instrument: Specific Targeted Research Project

Objectif: Exascale computing platforms, software and applications

Duration: September 2013 - August 2016

Coordinator: IMEC, Belgium

Partner: Particular specializations and experience of the partners are:

- Applications:
 - NAG - long experience in consultancy for HPC applications
 - Intel France - collaboration with industry on the migration of software for future HPC systems

- TS-SFR - long experience in consultancy for HPC applications in Aerospace and Oil & Gas
- Algorithms – primarily numerical:
 - UA - broad experience in numerical solvers, with some taken up by the PETSc numerical library and other work published in high-ranking journals such as Science.
 - USI - expertise in parallel many-core algorithms for real-world applications on emerging architectures
 - Inria - expertise on large scale parallel numerical algorithms
 - IT4I - experience in the development of scalable solvers for large HPC systems (e.g. PRACE)
- Programming Models & Runtime Environments:
 - Imec - leads the programming model research within the Flanders ExaScience Lab
 - UVSQ - specialized in code optimization and performance evaluation in the area of HPC
 - TS-SFR - leading the BMBF funded GASPI project
 - Fraunhofer - developed a GASPI runtime environment used in industrial applications
- Hardware Optimization:
 - Intel France - investigates workloads for new hardware architectures within the context of the Exascale Computing Research centre

Inria contact: Luc Giraud

Abstract: The EXA2CT project brings together experts at the cutting edge of the development of solvers, related algorithmic techniques, and HPC software architects for programming models and communication. We will produce modular open source proto-applications that demonstrate the algorithms and programming techniques developed in the project, to help boot-strap the creation of genuine exascale codes.

Numerical simulation is a crucial part of science and industry in Europe. The advancement of simulation as a discipline relies on increasingly compute intensive models that require more computational resources to run. This is the driver for the evolution to exascale. Due to limits in the increase in single processor performance, exascale machines will rely on massive parallelism on and off chip, with a complex hierarchy of resources. The large number of components and the machine complexity introduce severe problems for reliability and programmability.

9.4. International Initiatives

We are involved in the Inria@SiliconValley initiative through the associate team FASTLA described below.

9.4.1. Inria Associate Teams not involved in an Inria International Labs

9.4.1.1. MORSE

Title: Matrices Over Runtime Systems @ Exascale

International Partner (Institution - Laboratory - Researcher):

KAUST Supercomputing Laboratory (USA)

Duration: 2014 - 2016

See also: <http://icl.cs.utk.edu/projectsdev/morse/index.html>

The goal of Matrices Over Runtime Systems at Exascale (MORSE) project is to design dense and sparse linear algebra methods that achieve the fastest possible time to an accurate solution on large-scale multicore systems with GPU accelerators, using all the processing power that future high end systems can make available. To develop software that will perform well on petascale and exascale systems with thousands of nodes and millions of cores, several daunting challenges have to be overcome, both by the numerical linear algebra and the runtime system communities. By designing a research framework for describing linear algebra algorithms at a high level of abstraction, the MORSE team will enable the strong collaboration between research groups in linear algebra, runtime systems and scheduling needed to develop methods and libraries that fully benefit from the potential of future large-scale machines. Our project will take a pioneering step in the effort to bridge the immense software gap that has opened up in front of the High-Performance Computing (HPC) community.

9.4.1.2. FASTLA

Title: Fast and Scalable Hierarchical Algorithms for Computational Linear Algebra

International Partner (Institution - Laboratory - Researcher):

Stanford University (USA)

Lawrence Berkeley National Laboratory (USA)

Duration: 2014 - 2016

See also: http://people.bordeaux.inria.fr/coulaud/projets/FastLA_Website/

In this project, we propose to study fast and scalable hierarchical numerical kernels and their implementations on heterogeneous manycore platforms for two major computational kernels in intensive challenging applications. Namely, fast multipole methods (FMM) and sparse hybrid linear solvers, that appear in many intensive numerical simulations in computational sciences. Regarding the FMM we plan to study novel generic formulations based on \mathcal{H} -matrices techniques, that will be eventually validated in the field of material physics: the dislocation dynamics. For the hybrid solvers, new parallel preconditioning approaches will be designed and the use of \mathcal{H} -matrices techniques will be first investigated in the framework of fast and monitored approximations on central components. Finally, the innovative algorithmic design will be essentially focused on heterogeneous manycore platforms. The partners, Inria HiePACS, Lawrence Berkeley Nat. Lab and Stanford University, have strong, complementary and recognized experiences and backgrounds in these fields.

9.4.2. Participation In other International Programs

9.4.2.1. HOSCAR

We are involved in the Inria-CNPq **HOSCAR** project led by Stéphane Lanteri.

The general objective of the project is to setup a multidisciplinary Brazil-France collaborative effort for taking full benefits of future high-performance massively parallel architectures. The targets are the very large-scale datasets and numerical simulations relevant to a selected set of applications in natural sciences: (i) resource prospection, (ii) reservoir simulation, (iii) ecological modeling, (iv) astronomy data management, and (v) simulation data management. The project involves computer scientists and numerical mathematicians divided in 3 fundamental research groups: (i) numerical schemes for PDE models (Group 1), (ii) scientific data management (Group 2), and (iii) high-performance software systems (Group 3).

The final annual meeting has been organized in Inria Sophia, on September 21-24, 2015, while a follow-up of the project will exist as a H2020 project entitled HPC4E (HPC for Energy) to be started in 2016 with an enlarged partnership.

9.5. International Research Visitors

9.5.1. Visits to International Teams

9.5.1.1. Research stays abroad

Mathieu Faverge has been invited to KAUST University from October to December 2015 in the context of the associate team **MORSE**.

Pierre Blanchard participated to the Gene Golub SIAM Summer school on Randomized Numerical Linear Algebra held in Delph, Greece in June 2015.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific events selection

10.1.1.1. Member of the conference program committees

Luc Giraud has been member of the scientific program committee of the international conferences HiPC'15, IPDPS'16 and PDSEC'15.

Jean Roman has been member of the scientific program committee of the international conferences IEEE PDP'15 and PDP'16.

10.1.1.2. Reviewer

Furthermore, the **HIEPACS** members have contributed to the reviewing process of several international conferences: CCGRID 2015, IEEE IPDPS 2016,

10.1.2. Journal

10.1.2.1. Member of the editorial boards

Luc Giraud is member of the SIAM J. Matrix Analysis and Applications editorial board.

10.1.2.2. Reviewer - Reviewing activities

The **HIEPACS** members have contributed to the reviewing process of several international journals (ACM Trans. on Mathematical Software, Advances in Computational Mathematics, IEEE Trans. on Parallel and Distributed Systems, Journal of Parallel and Distributed Computing, Parallel Computing, SIAM J. Scientific Comp., ...).

10.1.3. Invited talks

Luc Giraud gave an invited talk at the 2015 **Salishan Conference on High-Speed Computing** (April 27 - 30, 2015) as well as to the seminar of the Laboratoire Jean Kuntzmann (LJK) in Grenoble (Nov. 2015).

Mathieu Faverge gave an invited talk at an EDF seminar on High Programming Productivity for High Performance Computing via Runtime Systems (December 15th, 2015).

10.1.4. Scientific expertise

Luc Giraud was a member of the evaluation committee of the "Software for Exascale Computing" (SPPEXA) program funded by the funding agencies from France (ANR), Germany (DFG), and Japan (JST). He also acted as expert for projects submitted to the Israel Science Foundation.

Jean Roman is member of the "Scientific Board" of the CEA-DAM. As representative of Inria, he is member of the board of ETP4HPC (European Technology Platform for High Performance Computing), of the French Information Group for PRACE, of the Technical Group of GENCI and of the Scientific Advisory Board of the Maison de la Simulation.

Pierre Ramet is Scientific Advisor at CEA-DAM (French Department of Energy) since October 2015. He is member of the evaluation committee at GENCI since 2008. He is also member of the Scientific Board of :

- the Scientific Computing axis of the Cluster of Excellence CPU from Bordeaux University since 2014,
- the Mesocentre in Bordeaux University since 2010.

10.1.5. Research administration

Jean Roman is a member of the Direction for Science at Inria : he is the Deputy Scientific Director of the Inria research domain entitled *Applied Mathematics, Computation and Simulation* and is in charge at the national level of the Inria activities concerning High Performance Computing.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Undergraduate level/Licence

1. A. Esnard: Operating system programming, 36h, University Bordeaux I; Using network, 23h, University Bordeaux I.
He is also in charge of the computer science certificate for Internet (C2i) at the University Bordeaux I.
2. M. Faverge: Programming Environment, 26h, L3; Numerical Algorithmic, 30h, L3; C Projects, 20h, L3, ENSEIRB-MatMeca, France
3. P. Ramet: System programming 24h, Databases 32h, Objet programming 48h, Distributed programming 32h, Cryptography 32h at Bordeaux University.

Post graduate level/Master

1. O. Coulaud: Paradigms for parallel computing, 24h, ENSEIRB-MatMeca, Talence; Méthodes hiérarchiques, 8h, ENSEIRB-MatMeca, Talence.
2. E. Agullo: Operating systems, 24h, University Bordeaux I; Dense linear algebra kernels, 8h, ENSEIRB-MatMeca; Numerical Algorithms, 30h; ENSEIRB-MatMeca, Talence.
3. A. Esnard: Network management, 27h, University Bordeaux I; Network security, 27h, University Bordeaux I; Programming distributed applications, 35h, ENSEIRB-MatMeca, Talence.
4. M. Faverge: System Programming, 74h, M1; Load Balancing and Scheduling, 19h, M2, ENSEIRB-MatMeca, Talence.
He is also in charge of the second year of Embedded Electronic Systems option at ENSEIRB-MatMeca, Talence.
5. P. Ramet: Scheduling, 8h; Numerical Algorithmic, 30h; ENSEIRB-MatMeca, Talence.
He also give classes on Cryptography, 30h, Ho Chi Minh City, Vietnam.
6. L. Giraud: Introduction to intensive computing and related programming tools, 20h, INSA Toulouse; Introduction to high performance computing and applications, 20h, ISAE-ENSICA; On mathematical tools for numerical simulations, 10h, ENSEIHT Toulouse; Parallel sparse linear algebra, 11h, ENSEIRB-MatMeca, Talence.
7. A. Guermouche: Network management, 92h, University Bordeaux I; Network security, 64h, University Bordeaux I; Operating system, 24h, University Bordeaux I.
8. J. Roman: Parallel sparse linear algebra, 10h, ENSEIRB-MatMeca, Talence; Parallel algorithms, 22h, ENSEIRB-MatMeca, Talence.

10.2.2. Supervision

Defended PhD thesis

1. Astrid Casadei, *Optimisations des solveurs linéaires creux hybrides basés sur une approche par complément de Schur et décomposition de domaine*, defended on October 19th, advisors: F. Pellegrini and P. Ramet.
2. Arnaud Etchevery, *Simulation de la dynamique des dislocations à très grande échelle*, defended on November 23th, advisors: O. Coulaud and G. Sylvand.

3. Xavier Lacoste, *Scheduling and memory optimizations for sparse direct solver on multi-core/multi-gpu cluster systems*, defended on February 18th, advisors: F. Pellegrini and P. Ramet.
4. Stojce Nakov, *On the design of sparse hybrid linear solvers for modern parallel architectures*, defended on December 14th, advisors: E. Agullo and J. Roman.
5. Alexis Praga, *Un modèle de transport chimie atmosphérique à grande échelle adapté aux calculateurs massivement parallèles*, defended on January 30th, advisors: D. Cariolle (CERFACS) and L. Giraud.
6. Fabien Rozar, *Contributions à l'amélioration de l'extensibilité de simulations parallèles de plasmas turbulents*, defended on November 5th, advisors: G. Latu and J. Roman.
7. Salli Moustafa, *Massively parallel Cartesian discrete ordinates method for neutron transport simulation*, defended on December 15th, advisors: P. Ramet and J. Roman.
8. Mawussi Zounon, *On numerical resilience in linear algebra*, defended on April 1st, advisors: E. Agullo and L. Giraud.

PhD in progress :

1. Pierre Blanchard, *Fast and accurate methods for dislocation dynamics*, starting Oct. 2013, advisors: O. Coulaud and E. Darve (Stanford Univ.).
2. Bérenger Bramas, *Optimization of time domain BEM solvers*, starting Jan 2013, advisors: O. Coulaud and G. Sylvand.
3. Nicolas Bouzat, *Fine grain algorithms and deployment methods for exascale plasma physic applications*, starting October 2015, advisors: G. Latu, M. Mehrenberger and J. Roman.
4. Jean-Marie Couteyen, *Parallélisation et passage à l'échelle du code FLUSEPA*, starting Feb 2013, advisors : P. Brenner (Airbus Defence and Space) and J. Roman.
5. Arnaud Durocher, *Passage à l'échelle des simulations de Dynamique des Dislocations sur plateforme hétérogène pour l'étude des mécanismes de fluage dans les matériaux du nucléaire*, starting Nov. 2015, advisors: O. Coulaud and L. Dupuy (CEA-DEN)
6. Aurélien Falco, *High performance solver for BEM-FEM coupling*, starting December 2015, advisors: E. Agullo, L. Giraud and G. Sylvand.
7. Grégoire Pichon, *Utilisation de techniques de compression \mathcal{H} -matrices pour solveur direct creux parallèle dans le cadre des applications FEM*, starting October 2015, advisors: L. Giraud and P. Ramet.
8. Cyrille Fournier, *New parallel programming paradigm for LES calculation at large scale*, starting March 2015, advisors: L. Giraud and G. Staffelbach (CERFACS).
9. Maria Predari, *Dynamic Load Balancing for Massively Parallel Coupled Codes*, starting Oct. 2013, advisors: A. Esnard and J. Roman.
10. Louis Poirel, *Two level hybrid linear solver*, starting Nov. 2014, advisors: E. Agullo, M. Favrege and L. Giraud.

10.2.3. Juries

- HDR of M. Chau (INP Toulouse) entitled "Algorithmes Parallèles Asynchrones et Applications en Calcul Scientifique" defended December 2015. L. Giraud (referee).
- PhD of J. Herrmann (ENS Lyon) entitled "Memory-aware Algorithms and Scheduling Techniques for Matrix Computations" defended November 2015. L. Giraud (examinator).
- Phd of E. Cieren (Université Bordeaux) entitled "Molecular Dynamics for Exascale supercomputers" defended October 2015. O. Coulaud (examinator).

- Phd of P. Pei Li (Université Bordeaux) entitled "Système unifié de transformation de code et d'exécution pour un passage aux architectures multicœurs hétérogènes" defended December 2015. J. Roman (examinator).

10.3. Popularization

In the context of HPC-PME initiative, we started a collaboration with ALGO'TECH INFORMATIQUE and we have organised one of the first PhD-consultant action implemented by Xavier Lacoste led by Pierre Ramet. ALGO'TECH is one of the most innovative SMEs (small and medium sized enterprises) in the field of cabling embedded systems, and more broadly, automatic devices. The main target of the project is to validate the possibility to use the sparse linear solvers of our team in the area of electromagnetic simulation tools developed by ALGO'TECH.

The **HIEPACS** members have organized the PATC training session on Parallel Linear algebra at CINES in Montpellier April 9-10, 2015.

11. Bibliography

Major publications by the team in recent years

- [1] E. AGULLO, B. BRAMAS, O. COULAUD, E. DARVE, M. MESSNER, T. TAKAHASHI. *Task-Based FMM for Multicore Architectures*, in "SIAM Journal on Scientific Computing", 2014, vol. 36, n^o 1, pp. 66-93 [DOI : 10.1137/130915662], <https://hal.inria.fr/hal-00911856>
- [2] E. AGULLO, J. DONGARRA, B. HADRI, H. LTAIEF. *Tile QR factorization with parallel panel processing for multicore architectures*, in "SIAM Conference on Parallel Processing for Scientific Computing (PP10)", United States Seattle, 2010
- [3] E. AGULLO, L. GIRAUD, Y.-F. JING. *Block GMRES method with inexact breakdowns and deflated restarting*, in "SIAM Journal on Matrix Analysis and Applications", November 2014, vol. 35, n^o 4, pp. 1625-1651, <https://hal.inria.fr/hal-01067159>
- [4] A. CASADEI, P. RAMET, J. ROMAN. *An improved recursive graph bipartitioning algorithm for well balanced domain decomposition*, in "21st annual IEEE International Conference on High Performance Computing (HiPC 2014)", Goa, India, December 2014, <https://hal.inria.fr/hal-01100962>
- [5] J. DONGARRA, M. FAVERGE, T. HÉRAULT, M. JACQUELIN, J. LANGOU, Y. ROBERT. *Hierarchical QR factorization algorithms for multi-core clusters*, in "Parallel Computing", 2013, vol. 39, n^o 4-5, pp. 212-232 [DOI : 10.1016/J.PARCO.2013.01.003], <http://hal.inria.fr/hal-00809770>
- [6] L. GIRAUD, A. HAIDAR, Y. SAAD. *Sparse approximations of the Schur complement for parallel algebraic hybrid linear solvers in 3D*, in "Numerical Mathematics: Theory, Methods and Applications", August 2010, vol. 3, n^o 3, pp. 276-294
- [7] P. KOVAL, D. FOERSTER, O. COULAUD. *A Parallel Iterative Method for Computing Molecular Absorption Spectra*, in "Journal of Chemical Theory and Computation", 2010, vol. 6, n^o 9, pp. 2654-2668 [DOI : 10.1021/CT100280x]
- [8] X. LACOSTE, M. FAVERGE, P. RAMET, S. THIBAUT, G. BOSILCA. *Taking advantage of hybrid systems for sparse direct solvers via task-based runtimes*, in "HCW'2014 workshop of IPDPS", Phoenix, United States, IEEE, May 2014, <https://hal.inria.fr/hal-00987094>

- [9] S. MOUSTAFA, M. FAVERGE, L. PLAGNE, P. RAMET. *3D Cartesian Transport Sweep for Massively Parallel Architectures with PARSEC*, in "29th IEEE International Parallel & Distributed Processing Symposium", Hyderabad, India, May 2015, pp. 581-590 [DOI : 10.1109/IPDPS.2015.75], <https://hal.inria.fr/hal-01078362>
- [10] M. PREDARI, A. ESNARD. *Coupling-Aware Graph Partitioning Algorithms: Preliminary Study*, in "HiPC-21th International Conference on High Performance Computing", Goa, India, December 2014 [DOI : 10.1109/HIPC.2014.7116879], <https://hal.inria.fr/hal-01069578>
- [11] F. ROZAR, G. LATU, J. ROMAN, V. GRANDGIRARD. *Toward memory scalability of GYSELA code for extreme scale computers*, in "Concurrency and Computation: Practice and Experience", November 2014, pp. 1-16 [DOI : 10.1002/CPE.3429], <https://hal.inria.fr/hal-01111720>

Publications of the year

Doctoral Dissertations and Habilitation Theses

- [12] A. CASADEI. *Optimizations of hybrid sparse linear solvers relying on Schur complement and domain decomposition approaches*, Université de Bordeaux, October 2015, <https://tel.archives-ouvertes.fr/tel-01228520>
- [13] A. ETCHEVERY. *Simulation de la dynamique des dislocations à très grande échelle*, Université de Bordeaux, November 2015
- [14] X. LACOSTE. *Scheduling and memory optimizations for sparse direct solver on multi-core/multi-gpu duster systems*, Université de Bordeaux, February 2015, <https://tel.archives-ouvertes.fr/tel-01222565>
- [15] S. MOUSTAFA. *Massively parallel Cartesian discrete ordinates method for neutron transport simulation*, Université de Bordeaux, December 2015
- [16] S. NAKOV. *On the design of sparse hybrid linear solvers for modern parallel architectures*, Université de Bordeaux, November 2015
- [17] A. PRAGA. *A large-scale atmospheric chemistry-transport model for massively parallel architectures*, Université Toulouse III - Paul Sabatier, January 2015, <https://tel.archives-ouvertes.fr/tel-01178394>
- [18] F. ROZAR. *Contributions à l'amélioration de l'extensibilité de simulations parallèles de plasmas turbulents*, Université de Bordeaux, December 2015
- [19] M. ZOUNON. *On numerical resilience in linear algebra*, Université de Bordeaux, April 2015, <https://tel.archives-ouvertes.fr/tel-01231838>

Articles in International Peer-Reviewed Journals

- [20] B. BRAMAS, O. COULAUD, G. SYLVAND. *Time-domain BEM for the wave equation on distributed-heterogeneous architectures: A blocking approach*, in "Parallel Computing", July 2015, n^o 49, 16 p. [DOI : 10.1016/J.PARCO.2015.07.005], <https://hal.inria.fr/hal-01200727>
- [21] A. PRAGA, D. CARIOLLE, L. GIRAUD. *Pangolin v1.0, a conservative 2-D advection model towards large-scale parallel calculation*, in "Geoscientific Model Development", February 2015, vol. 8, pp. 205 - 220 [DOI : 10.5194/GMD-8-205-2015], <https://hal.inria.fr/hal-01117048>

- [22] P. SALAS, L. GIRAUD, Y. SAAD, S. MOREAU. *Spectral recycling strategies for the solution of nonlinear eigenproblems in thermoacoustics*, in "Numerical Linear Algebra with Applications", 2015, vol. 22, n^o 6, pp. 1039-1058 [DOI : 10.1002/NLA.1995], <https://hal.inria.fr/hal-01238263>
- [23] C. STEINER, M. MEHRENBERGER, N. CROUSEILLES, V. GRANDGIRARD, G. LATU, F. ROZAR. *Gyroaveraging operator for a polar mesh*, in "European Physical Journal D", 2015, vol. 69, n^o 1, 221 p. [DOI : 10.1140/EPJD/E2014-50211-7], <https://hal.inria.fr/hal-01090681>

Invited Conferences

- [24] E. AGULLO, L. GIRAUD, P. SALAS, E. F. YETKIN, M. ZOUNON. *On Numerical Resiliency in Numerical Linear Algebra Solvers*, in "Salishan Conference on High-Speed Computing", Salishan, United States, DOE laboratories, April 2015, <https://hal.archives-ouvertes.fr/hal-01162627>
- [25] B. REPS, G. PIETER, K. MEERBERGEN, E. AGULLO, E. F. YETKIN, L. GIRAUD, W. VANROOSE. *Communication Avoiding and Hiding in preconditioned Krylov solvers*, in "High Performance Computing in Science and Engineering: HPCSE'15", Karolinka, Czech Republic, IT4Innovations National Supercomputing Center VSB-Technical University of Ostrava, Czech Republic, May 2015, <https://hal.archives-ouvertes.fr/hal-01162638>

International Conferences with Proceedings

- [26] E. AGULLO, O. BEAUMONT, L. EYRAUD-DUBOIS, J. HERRMANN, S. KUMAR, L. MARCHAL, S. THIBAUT. *Bridging the Gap between Performance and Bounds of Cholesky Factorization on Heterogeneous Platforms*, in "Heterogeneity in Computing Workshop 2015", Hyderabad, India, May 2015, <https://hal.inria.fr/hal-01120507>
- [27] E. AGULLO, O. BEAUMONT, L. EYRAUD-DUBOIS, S. KUMAR. *Are Static Schedules so Bad ? A Case Study on Cholesky Factorization*, in "30th IEEE International Parallel & Distributed Processing Symposium, IPDPS'16", Chicago, IL, United States, IEEE, May 2016, <https://hal.inria.fr/hal-01223573>

- [28] *Best Paper*
E. AGULLO, A. BUTTARI, A. GUERMOUCHE, F. LOPEZ. *Task-based multifrontal QR solver for GPU-accelerated multicore architectures*, in "High Performance Computing-HiPC", Bangalore, India, December 2015, Best paper, <https://hal.inria.fr/hal-01270145>.

- [29] O. BEAUMONT, L. EYRAUD-DUBOIS, A. GUERMOUCHE, T. LAMBERT. *Comparison of Static and Dynamic Resource Allocation Strategies for Matrix Multiplication*, in "26th IEEE International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD), 2015", Florianopolis, Brazil, October 2015, <https://hal.inria.fr/hal-01163936>
- [30] A. GUERMOUCHE, L. MARCHAL, B. SIMON, F. VIVIEN. *Scheduling Trees of Malleable Tasks for Sparse Linear Algebra*, in "European Conference on Parallel Processing (Euro-Par)", Vienna, Austria, 2015, <https://hal.inria.fr/hal-01160104>
- [31] S. MOUSTAFA, M. FAVERGE, L. PLAGNE, P. RAMET. *3D Cartesian Transport Sweep for Massively Parallel Architectures with PARSEC*, in "29th IEEE International Parallel & Distributed Processing Symposium", Hyderabad, India, May 2015, pp. 581-590 [DOI : 10.1109/IPDPS.2015.75], <https://hal.inria.fr/hal-01078362>

- [32] G. PICHON, A. HAIDAR, M. FAVERGE, J. KURZAK. *Divide and Conquer Symmetric Tridiagonal Eigensolver for Multicore Architectures*, in "29th IEEE International Parallel & Distributed Processing Symposium", Hyderabad, India, May 2015, <https://hal.inria.fr/hal-01078356>
- [33] L. STANISIC, E. AGULLO, A. BUTTARI, A. GUERMOUCHE, A. LEGRAND, F. LOPEZ, B. VIDEAU. *Fast and Accurate Simulation of Multithreaded Sparse Linear Algebra Solvers*, in "The 21st IEEE International Conference on Parallel and Distributed Systems", Melbourne, Australia, December 2015, <https://hal.inria.fr/hal-01180272>
- [34] W. WU, A. BOUTEILLER, G. BOSILCA, M. FAVERGE, J. DONGARRA. *Hierarchical DAG Scheduling for Hybrid Distributed Systems*, in "29th IEEE International Parallel & Distributed Processing Symposium", Hyderabad, India, May 2015, <https://hal.inria.fr/hal-01078359>

Conferences without Proceedings

- [35] E. AGULLO, H. BARUCQ, L. BOILLOT, G. BOSILCA, H. CALANDRA, J. DIAZ. *Portable task-based programming for seismic wave propagation simulation in time domain*, in "HOSCAR – 5th Brazil-French workshop on High performance cOmputing and SCientific dAta management dRiven by highly demanding applications (Inria-CNPq)", SOPHIA ANTIPOLIS, France, September 2015, <https://hal.inria.fr/hal-01208461>
- [36] E. AGULLO, B. BRAMAS, O. COULAUD, E. DARVE, M. MESSNER, T. TAKAHASHI. *Task-Based Parallelization of the Fast Multipole Method on NVIDIA GPUs and Multicore Processors*, in "Computational Science and Engineering (CSE)", Salt Lake City, United States, SIAM, March 2015, <https://hal.inria.fr/hal-01135258>
- [37] E. AGULLO, E. DARVE, L. GIRAUD, Y. HARNESS. *Data sparse techniques for parallel hybrid solvers*, in "SIAM Conference on Applied Linear Algebra", Atlanta, United States, April 2015, <https://hal.inria.fr/hal-01256230>
- [38] E. AGULLO, E. DARVE, Y. HARNESS, L. GIRAUD. *H-matrix techniques for parallel hybrid solvers*, in "Workshop on Fast Direct Solvers", Toulouse, France, June 2015, <https://hal.inria.fr/hal-01215344>
- [39] E. AGULLO, A. FALCO, L. GIRAUD, B. LIZÉ, G. SYLVAND. *H-Matrix Solver for FEM/BEM*, in "Workshop on Fast Direct Solvers", Toulouse, France, June 2015, <https://hal.inria.fr/hal-01215345>
- [40] E. AGULLO, L. GIRAUD, P. SALAS, E. F. YETKIN, M. ZOUNON. *On Resiliency in Krylov Solvers*, in "PACS'15: Plateform for Advanced Scientific Computing Conference", Zurich, Switzerland, June 2015, <https://hal.archives-ouvertes.fr/hal-01162618>
- [41] E. AGULLO, L. GIRAUD, E. F. YETKIN. *Reliability of Checksum based Detection for Soft Errors in Conjugate Gradient Variants*, in "SIAM conference on computational science and engineering", Salt Lake city, Utah, United States, March 2015, <https://hal.inria.fr/hal-01200706>
- [42] E. AGULLO, L. GIRAUD, M. ZOUNON. *On the resilience of parallel sparse hybrid solvers*, in "22nd annual IEEE International Conference on High Performance Computing (HiPC 2015)", Bangalore, India, December 2015, <https://hal.inria.fr/hal-01256316>

- [43] P. BLANCHARD, B. BRAMAS, O. COULAUD, E. DARVE, L. DUPUY, A. ETCHEVERRY, G. SYLVAND. *ScalFMM: A Generic Parallel Fast Multipole Library*, in "Computational Science and Engineering (CSE)", Salt Lake City, United States, SIAM, March 2015, <https://hal.inria.fr/hal-01135253>
- [44] P. BLANCHARD, O. COULAUD, E. DARVE, B. BRAMAS. *Hierarchical Randomized Low-Rank Approximations*, in "SIAM Conference on Applied Linear Algebra (SIAM LA)", Atlanta, United States, SIAM, October 2015, <https://hal.archives-ouvertes.fr/hal-01255724>
- [45] L. BOILLOT, E. AGULLO, G. BOSILCA, H. CALANDRA, H. BARUCQ, J. DIAZ. *Portable task-based programming for elastodynamics*, in "Rice - Oil & Gas HPC Workshop", HOUSTON, United States, March 2015, <https://hal.inria.fr/hal-01128750>
- [46] L. BOILLOT, G. BOSILCA, E. AGULLO, H. CALANDRA. *Portable task-based programming for Seismic Imaging*, in "MATHIAS – TOTAL Symposium on Mathematics", Paris, France, October 2015, <https://hal.inria.fr/hal-01223339>
- [47] A. CASADEI, P. RAMET, J. ROMAN. *Towards a recursive graph bipartitioning algorithm for well balanced domain decomposition*, in "Mini-Symposium on "Partitioning for Complex Objectives" at SIAM CSE'15 conference", Salt Lake City, United States, March 2015, <https://hal.inria.fr/hal-01100985>
- [48] A. CASADEI, P. RAMET, J. ROMAN. *Towards a recursive graph bipartitioning algorithm for well balanced domain decomposition*, in "Mini-Symposium on "Combinatorial Issues in Sparse Matrix Computation" at ICIAM'15 conference", Beijing, China, August 2015, <https://hal.inria.fr/hal-01100990>
- [49] J.-M. COUTEYEN, J. ROMAN, P. BRENNER. *MPMD parallelization of an aerodynamic code with bodies in relative motion*, in "2nd International Workshop on High Performance Computing Simulation in Energy/Transport Domains (HPCSET 2015)", Frankfurt, Germany, July 2015, <https://hal.inria.fr/hal-01255460>
- [50] J.-M. COUTEYEN, J. ROMAN, P. BRENNER. *Task-based parallelization of a CFD code over a Runtime System*, in "27th International Conference on Parallel Computational Fluid Dynamics", Montreal, Canada, May 2015, <https://hal.inria.fr/hal-01255450>
- [51] M. FAVERGE, G. PICHON, P. RAMET, J. ROMAN. *Blocking strategy optimizations for sparse direct linear solver on heterogeneous architectures*, in "Sparse Days", Saint Girons, France, June 2015, <https://hal.inria.fr/hal-01187881>
- [52] M. FAVERGE, G. PICHON, P. RAMET, J. ROMAN. *On the use of H-Matrix Arithmetic in PaStiX: a Preliminary Study*, in "Workshop on Fast Direct Solvers", Toulouse, France, June 2015, <https://hal.inria.fr/hal-01187882>
- [53] R. GARNIER, V. LE BRIS, D. BÉGUÉ, O. COULAUD, I. BARAILLE, M. ODUNLAMI. *Optimisation of the variational method for vibrational Hamiltonian eigenvalues computation*, in "59th SOURIAU COLLOQUIUM: Colloque International de Théories Variationnelles", Seignosse, France, June 2015, <https://hal.archives-ouvertes.fr/hal-01179654>
- [54] R. GARNIER, V. LE BRIS, M. ODUNLAMI, D. BÉGUÉ, I. BARAILLE, O. COULAUD. *Efficient basis selection for the computation of vibrational spectrum*, in "10th European Conference on Computational Chemistry", Fulda, Germany, August 2015, <https://hal.archives-ouvertes.fr/hal-01200748>

- [55] X. LACOSTE, M. FAVERGE, P. RAMET. *A task-based sparse direct solver suited for large scale hierarchical/heterogeneous architectures*, in "Mini-Symposium on "Task-based Scientific Computing Applications" at SIAM CSE'15 conference", Salt Lake City, United States, March 2015, <https://hal.inria.fr/hal-01100979>
- [56] X. LACOSTE, M. FAVERGE, P. RAMET. *On the design of parallel linear solvers for large scale problems*, in "Mini-Symposium on Recent advances in matrix computations for extreme-scale computers at ICIAM'15 conference", Beijing, China, August 2015, <https://hal.inria.fr/hal-01100987>
- [57] G. PICHON, E. DARVE, M. FAVERGE, P. RAMET, J. ROMAN. *Exploiting H-Matrices in Sparse Direct Solvers*, in "SIAM Conference on Parallel Processing for Scientific Computing", Paris, France, April 2016, <https://hal.inria.fr/hal-01251812>
- [58] G. PICHON, M. FAVERGE, P. RAMET, J. ROMAN. *Impact of Blocking Strategies for Sparse Direct Solvers on Top of Generic Runtimes*, in "SIAM Conference on Parallel Processing for Scientific Computing", Paris, France, April 2016, <https://hal.inria.fr/hal-01251808>

Research Reports

- [59] E. AGULLO, A. BUTTARI, A. GUERMOUCHE, F. LOPEZ. *Task-based multifrontal QR solver for GPU-accelerated multicore architectures*, IRIT, Toulouse, June 2015, n^o IRI/RT-2015-02-FR-r1, <https://hal.archives-ouvertes.fr/hal-01166312>
- [60] E. AGULLO, L. GIRAUD, P. SALAS, M. ZOUNON. *Interpolation-restart strategies for resilient eigensolvers*, Inria Bordeaux, June 2015, n^o 8625, <https://hal.inria.fr/hal-01201748>
- [61] E. AGULLO, L. GIRAUD, M. ZOUNON. *On the resilience of a parallel sparse hybrid solver*, Inria Bordeaux ; Inria, June 2015, n^o RR-8744, <https://hal.inria.fr/hal-01165186>
- [62] M. ALAYA, M. FAVERGE, X. LACOSTE, A. PÉRÉ-LAPERNE, J. PÉRÉ-LAPERNE, P. RAMET, T. TERRAZ. *Simul'Elec and PASTIX interface specifications*, Inria Bordeaux ; AlgoTech ; Inria, April 2015, n^o RT-0458, <https://hal.inria.fr/hal-01142204>
- [63] P. BLANCHARD, O. COULAUD, E. DARVE. *Fast hierarchical algorithms for generating Gaussian random fields*, Inria Bordeaux Sud-Ouest, November 2015, <https://hal.inria.fr/hal-01228519>
- [64] S. COOLS, E. F. YETKIN, E. AGULLO, L. GIRAUD, W. VANROOSE. *Analysis of rounding error accumulation in Conjugate Gradients to improve the maximal attainable accuracy of pipelined CG*, Inria Bordeaux Sud-Ouest, January 2016, n^o RR-8849, <https://hal.inria.fr/hal-01262716>

Other Publications

- [65] T. COJEAN, A. GUERMOUCHE, A. HUGO, R. NAMYST, P.-A. WACRENIER. *Exploiting two-level parallelism by aggregating computing resources in task-based applications over accelerator-based machines*, July 2015, working paper or preprint, <https://hal.inria.fr/hal-01181135>
- [66] J. COUTEYEN CARPAYE, J. ROMAN, P. BRENNER. *FLUSEPA - a Navier-Stokes Solver for Unsteady Problems with Bodies in Relative Motion : Toward a Task-Based Parallel Version over a Runtime System*, March 2015, SIAM CSE, Poster, <https://hal.inria.fr/hal-01255440>

- [67] M. PREDARI, A. ESNARD. *Graph Operators for Coupling-aware Graph Partitioning Algorithms*, July 2015, CIMI HPC Semester Workshop2: Innovative clustering methods for large graphs and block methods, <https://hal.inria.fr/hal-01203006>
- [68] M. PREDARI, A. ESNARD. *New graph partitioning techniques for load balancing of coupled simulation*, September 2015, womENCourage 2015, Poster, <https://hal.inria.fr/hal-01258036>