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Activity Report 2019

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

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1. Team, Visitors, External Collaborators

Research Scientists

Luc Giraud [Team leader, Inria, Senior Researcher, HDR]
Jean Roman [Inria, Senior Researcher, until Jan 2020, HDR]
Emmanuel Agullo [Inria, Researcher]
Olivier Beaumont [Inria, Senior Researcher, from Apr 2019, HDR]
Olivier Coulaud [Inria, Senior Researcher, HDR]
Lionel Eyraud-Dubois [Inria, Researcher, from Apr 2019]

Faculty Members

Aurélien Esnard [Univ de Bordeaux, Associate Professor]
Mathieu Faverge [Institut National Polytechnique de Bordeaux, Associate Professor]
Abdou Guermouche [Univ Bordeaux I, Associate Professor, HDR]
Jean Rene Poirier [INP Toulouse, Associate Professor, in delegation until Jul 2019, HDR]
Pierre Ramet [Univ de Bordeaux, Associate Professor, HDR]

Post-Doctoral Fellows

Mohammad Issa [Inria, Post-Doctoral Fellow, from Dec 2019]
Cristobal Samaniego Alvarado [Inria, Post-Doctoral Fellow, until Apr 2019]
Nick Schenkels [Inria, Post-Doctoral Fellow]

PhD Students

Tobias Castanet [Univ de Bordeaux, PhD Student, from Dec 2019]
Aurélien Falco [Inria, PhD Student, until May 2019]
Marek Felsoci [Inria, PhD Student, from Oct 2019]
Martina Iannacito [Inria, PhD Student, from Oct 2019]
Esragul Korkmaz [Inria, PhD Student]
Romain Peressoni [Univ de Bordeaux, PhD Student, from Oct 2019]
Alena Shilova [Inria, PhD Student, from Apr 2019]
Nicolas Venkovic [CERFACS, PhD Student]
Mathieu Verite [Inria, PhD Student, from Sep 2019]
Yanfei Xiang [Inria, PhD Student, from Nov 2019]

Technical staff

Cyril Bordage [Inria, Engineer, until Mar 2019]
Tony Delarue [Inria, Engineer, from Oct 2019]
Pierre Esterie [Inria, Engineer]
Gilles Marait [Inria, Engineer]

Interns and Apprentices

Lucas Barros de Assis [Inria, from Jun 2019 until Sep 2019]
Tony Delarue [Inria, from Feb 2019 until Aug 2019]
Van Gia Thinh Nguyen [Inria, from Jun 2019 until Sep 2019]
Romain Peressoni [Inria, from Mar 2019 until Aug 2019]
Richard Sartori [Inria, from Mar 2019 until Sep 2019]
Mathieu Verite [Inria, from Jul 2019 until Aug 2019]

Administrative Assistant

Chrystel Plumejeau [Inria]

Visiting Scientists

Jesus Camara [Universidad de Murcia]
Rocio Carratala Saez [Universitat Jaume I, from Jun 2019 until Aug 2019]
Lucas Fron Ortin [ENSEEIHT, Jul 2019]
Grégoire Pichon [Universitat Jaume I, from Jun 2019 until Aug 2019]

External Collaborators

Jean René Poirier [INP Toulouse, from Sep 2019, HDR]
Guillaume Sylvand [Airbus Central R & T]

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 conduced on close collaboration in particular with European and US initiatives and likely in the framework of EuroHPC 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 prospectives in scalable parallel linear algebra techniques are addressed, ranging from dense direct, sparse direct, iterative and hybrid approaches for large linear systems. We are also interested in the general problem of minimizing memory consumption and data movements, by changing algorithms and possibly performing extra computations, in particular in the context of Deep Neural Networks. Then we consider research on 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 multi-disciplinary context with colleagues in other academic or industrial groups where our contribution is related to our expertises. Not only these collaborations enable our expertise 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/Conseil Régional Grande 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 the past associate team FASTLA we contribute with world leading groups at Berkeley National Lab and Stanford University 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 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 Beaumont, Olivier Coulaud, Pierre Esterie, Lionel Eyraud-Dubois, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Gilles Marait, Pierre Ramet, Jean Roman, Nick Schenkels, Alena Shilova, Mathieu Verite.

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. With the recent addition of colleagues from the scheduling community (O. Beaumont and L. Eyraud-Dubois), the team is better equipped than ever to design scheduling algorithms and models specifically tailored to our target problems. It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore and heterogeneous 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 behavior 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 the context of scaling up, and particularly in the context of minimizing energy consumption, it is generally acknowledged that the solution lies in the use of heterogeneous architectures, where each resource is particularly suited to specific types of tasks, and in a fine control at the algorithmic level of data movements and the trade-offs to be made between computation and communication. In this context, we are particularly interested in the optimization of the training phase of deep convolutional neural networks which consumes a lot of memory and for which it is possible to exchange computations for data movements and memory occupation. We are also interested in the complexity introduced by resource heterogeneity itself, both from a theoretical point of view on the complexity of scheduling problems and from a more practical point of view on the implementation of specific kernels in dense or sparse linear algebra.

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. A new solver has emerged from the associate team, Chameleon. While PLASMA and MAGMA focus on multicore and GPU architectures, respectively, Chameleon makes the most out of heterogeneous architectures thanks to task-based dynamic runtime systems.

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.

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, Olivier Coulaud, Tony Delarue, Mathieu Faverge, Aurélien Falco, Marek Felsoci, Luc Giraud, Abdou Guermouche, Esragul Korkmaz, Gilles Marait, Van Gia Thinh Nguyen, Jean Rene Poirier, Pierre Ramet, Jean Roman, Cristobal Samaniego Alvarado, Guillaume Sylvand, Nicolas Venkovic, Yanfei Xiang.

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 solvers

For the solution of large sparse linear systems, we design numerical schemes and software packages for direct and hybrid parallel solvers. 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. 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 block low-rank compression techniques.

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 ANR SOLHARIS 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 (HIEPACS 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 Central R & T.

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 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 precondition 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 library MaPHyS. This activity will be developed further developped in the H2020 EoCoE2 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 libray Fabulous originately developed in the context of the DGA HiBox project and further developped in the LynCs (Linear Algebra, Krylov-subspace methods, and multi-grid solvers for the discovery of New Physics) sub-project of Prace-6IP.
- 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.

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 though 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. *Fast Solvers for FEM/BEM Coupling*

In this research project, we are interested in the design of new advanced techniques to solve large mixed dense/sparse linear systems, the extensive comparison of these new approaches to the existing ones, and the application of these innovative ideas on realistic industrial test cases in the domain of aeroacoustics (in collaboration with Airbus Central R & T).

- The use of $\mathcal{H}$-matrix solvers on these problems has been investigated in the context of the PhD of A. Falco. Airbus CR&T, in collaboration with Inria Bordeaux Sud-Ouest, has developed a task-based $\mathcal{H}$-matrix solver on top of the runtime engine StarPU. Ideas coming from the field of sparse direct solvers (such as nested dissection or symbolic factorization) have been tested within $\mathcal{H}$-matrices.
- The question of parallel scalability of task-based tools is an active subject of research, using new communication engine such as NewMadeleine, that will be investigated during this project, in conjunction with new algorithmic ideas on the task-based writing of $\mathcal{H}$-matrix algorithms.
- Naturally, comparison with existing tools will be performed on large realistic test cases. Coupling schemes between these tools and the hierarchical methods used in $\mathcal{H}$-matrix will be developed and benched as well.

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

Participants: Emmanuel Agullo, Olivier Coulaud, Pierre Esterie, 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 Mutipole 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 conduced 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 conduced on close connection with the activity described in Section 3.3. Following our earlier experience, we plan to first consider approximate inverse preconditionners that can efficiently exploit these data structures.

3.5. Load balancing algorithms for complex simulations

Participants: Cyril Bordage, Aurélien Esnard, Pierre Ramet.

Many important physical phenomena in material physics and climatology are inherently complex applications. They often use multi-physics or multi-scale approaches, which 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.

Another prominent example is found in the field of aeronautic propulsion: 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). As the AVBP code is much more CPU consuming than the AVTP code, there is an important computational imbalance between the two solvers.

In this context, 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 stand-alone 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, which can drastically decrease the overall performance. Therefore, we argue 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). What does furthermore happen if the load of one code dynamically changes relatively to the other one? In such a case, it could be convenient to dynamically adapt the number of resources used during the execution.

There are several open algorithmic problems that we investigate in the HIEPACS project-team. All these problems uses a similar methodology based upon the graph model and are expressed as variants of the classic graph partitioning problem, using additional constraints or different objectives.

3.5.1. Dynamic load-balancing with variable number of processors

As a preliminary step related to the dynamic load balancing of coupled codes, we focus on the problem of dynamic load balancing of a single parallel code, with variable number of processors. Indeed, if the workload varies drastically during the simulation, the load must be redistributed regularly among the processors. Dynamic load balancing is a well studied subject but most studies are limited to an initially fixed number of processors. Adjusting the number of processors at runtime allows one to preserve the parallel code efficiency or keep running the simulation when the current memory resources are exceeded. We call this problem, *MxN graph repartitioning*.

We propose some methods based on graph repartitioning in order to re-balance the load while changing the number of processors. These methods are split in two main steps. Firstly, we study the migration phase and we build a “good” migration matrix minimizing several metrics like the migration volume or the number of exchanged messages. Secondly, we use graph partitioning heuristics to compute a new distribution optimizing the migration according to the previous step results.

3.5.2. Load balancing of coupled codes

As stated above, the load balancing of coupled code is a major issue, that determines the performance of the complex simulation, and reaching high performance can be a great challenge. In this context, we develop new graph partitioning techniques, called *co-partitioning*. They 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 classically done. More precisely, we propose to enrich the classic graph model with *inter-edges*, which represent the coupled code interactions. We describe two new algorithms, and compare them to the naive approach. In the preliminary experiments we perform on synthetically-generated graphs, we notice that our algorithms succeed to balance the computational load in the coupling phase and in some cases they succeed to reduce the coupling communications costs. Surprisingly, we notice that our algorithms do not degrade significantly the global graph edge-cut, despite the additional constraints that they impose.

Besides this, 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, such as `Scotch`, for real-life graphs available from the popular *DIMACS’10* collection.

3.5.3. Load balancing strategies for hybrid sparse linear solvers

Graph handling and partitioning play a central role in the activity described here but also in other numerical techniques detailed in sparse linear algebra Section. 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 super-nodal or multi-frontal approaches. Considering hybrid methods mixing both direct and iterative solvers such as 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: Olivier Coulaud, Pierre Esterie.

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 acheive 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 of algorithms in scientific applications

Participants: Emmanuel Agullo, Aurélien Falco, Olivier Beaumont, Lionel Eyraud-Dubois, Mathieu Faverge, Marek Felsoci, Luc Giraud, Gilles Marait, Van Gia Thinh Nguyen, Pierre Ramet, Guillaume Sylvand, Alena Shilova.

4.2.1. High performance simulation for ITER tokamak

Scientific simulation for ITER tokamak modeling provides a natural bridge between theory and experimentation and is also an essential tool for understanding and predicting plasma behavior. Recent progresses in numerical simulation of fine-scale turbulence and in large-scale dynamics of magnetically confined plasma have been enabled by access to petascale supercomputers. These progresses would have been unreachable without new computational methods and adapted reduced models. In particular, the plasma science community has developed codes for which computer runtime scales quite well with the number of processors up to thousands cores. The research activities of HIEPACS concerning the international ITER challenge have started in the Inria Project Lab C2S@EXA in collaboration with CEA-IRFM and were related to two complementary studies: a first one concerning the turbulence of plasma particles inside a tokamak (in the context of GYSELA code) and a second one concerning the MHD instability edge localized modes (in the context of JOREK code). The activity concerning GYSELA was completed at the end of 2018.

Other numerical simulation tools designed for the ITER challenge aim at making a significant progress in understanding active control methods of plasma edge MHD instability Edge Localized Modes (ELMs) which represent a particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in the tokamak. The goal is to improve the understanding of the related physics and to propose possible new strategies to improve effectiveness of ELM control techniques. The simulation tool used (JOREK code) is related to non linear MHD modeling and is based on a fully implicit time evolution scheme that leads to 3D large very badly conditioned sparse linear systems to be solved at every time step. In this context, the use of PaStiX library to solve efficiently these large sparse problems by a direct method is a challenging issue.

This activity continues within the context of the EOCOE2 project, in which the PaStiX solver is identified to allow the processing of very larger linear systems for the nuclear fusion code TOKAM3X from CEA-IRFM. Contrary to the JOREK code, the problem to be treated corresponds to the complete 3D volume of the plasma torus. The objective is to be competitive, for complex geometries, compared to an Algebraic MultiGrid approach designed by one partner of EOCOE2.

4.2.2. Numerical and parallel scalable hybrid solvers in large scale calculations

Parallel and numerically scalable hybrid solvers based on a fully algebraic coarse space correction have been theoretically studied and various advanced parallel implementations have been designed. Their parallel scalability has been initially investigated on large scale problems within the EOCOE project thanks to a close collaboration with the BSC and the integration of MaPHyS within the Alya software. This activity will further develop in the EOCOE2 project. The performance has also been assessed on PRACE Tier-0 machine within a PRACE Project Access through a collaboration with CERFACS and Laboratoire de Physique des Plasmas at Ecole Polytechnique for the calculation of plasma propulsion. A comparative parallel scalability study with the Algebraic MultiGrid from Petsc has been conducted in that framework.

4.2.3. Aeroacoustics Simulation

This domains is in the context of a long term collaboration with Airbus Research Centers. Wave propagation phenomena intervene in many different aspects of systems design at Airbus. They drive the level of acoustic vibrations that mechanical components have to sustain, a level that one may want to diminish for comfort reason (in the case of aircraft passengers, for instance) or for safety reason (to avoid damage in the case of a payload in a rocket fairing at take-off). Numerical simulations of these phenomena plays a central part in the upstream design phase of any such project. Airbus Central R & T has developed over the last decades an in-depth knowledge in the field of Boundary Element Method (BEM) for the simulation of wave propagation in homogeneous media and in frequency domain. To tackle heterogeneous media (such as the jet engine flows, in the case of acoustic simulation), these BEM approaches are coupled with volumic finite elements (FEM). We end up with the need to solve large (several millions unknowns) linear systems of equations composed of a dense part (coming for the BEM domain) and a sparse part (coming from the FEM domain). Various parallel solution techniques are available today, mixing tools created by the academic world (such as the Mumps and Pastix sparse solvers) as well as parallel software tools developed in-house at Airbus (dense solver SPIDO, multipole solver, $\mathcal{H}$-matrix solver with an open sequential version available online). In the current state of knowledge and technologies, these methods do not permit to tackle the simulation of aeroacoustics problems at the highest acoustic frequencies (between 5 and 20 kHz, upper limits of human audition) while considering the whole complexity of geometries and phenomena involved (higher acoustic frequency implies smaller mesh sizes that lead to larger unknowns number, a number that grows like f^2 for BEM and f^3 for FEM, where f is the studied frequency). The purpose of the study in this domain is to develop advanced solvers able to tackle this kind of mixed dense/sparse linear systems efficiently on parallel architectures.

4.2.4. Optimization for Deep Convolutional Neural Networks

The training phase of Deep Convolutional Neural Networks represents nowadays a significant share of the computations performed on HPC supercomputers. It introduces several new problems concerning resource allocation and scheduling issues, because of the specific pattern of task graphs induced by the stochastic gradient descent and because memory consumption is particularly critical when performing training. As of today, the most classical parallelization methods consists in partitioning mini-batches, images, filters,... but all these methods induce high synchronization and communication costs, and only very partially resolve memory issues. Within the framework of the Inria IPL on HPC Big Data and Learning convergence, we are working on re-materialization techniques and on the use of model parallelism, in particular to be able to build on the research that has been carried out in a more traditional HPC framework on the exploitation of resource heterogeneity and dynamic runtime scheduling.

5. Highlights of the Year

5.1. Highlights of the Year

- HIEPACS was extremely pleased to welcome two new permanent Inria members, namely O. Beaumont and L. Eyraud-Dubois, whose scientific expertises clearly strengthen the impact of the team on the HPC research.
- We are very delighted to report that seven new PhD students have joined the team this year on research topics covering the full range of those adressed by the team. These PhD students, with gender parity, come from different places in France (Bordeaux, Strasbourg) as well as other places worldwide (China, Italy and Russia). This cultural and scientific variety will surely lead to a nice and fruitful blend and will contribute to the stimulating research atmosphere within the team.
- In June 2019, we organized the 14th Scheduling for Large Scale Systems Workshop, in the campus of Victoire in Bordeaux. 48 participants from all over the world registered to the workshop and gave 36 presentations over 3 days, covering topics like Numerical Algorithms, Resilience, Performance Evaluation, Job and DAG Scheduling.

- Inria's Autumn school, November 4-8 2019, Inria Bordeaux Sud-Ouest co-organized by E. Agullo (HIEPACS), H. Beaugendre (CARDAMON) and J. Diaz (MAGIQUE3D)

  The school aimed at simulating a physical problem, from its modeling to its implementation in a high performance computing (HPC) framework. The school offered both plenary courses and hands-on sessions that involved many members of the three teams. The physical problem considered was the harmonic wave propagation.

  The first day was dedicated to the modeling of the problem and its discretization using a Discontinuous Galerkin scheme. The following two days were dedicated to linear algebra for solving large sparse systems. Background on direct, iterative and hybrid methods for sparse linear systems were discussed. Hands-on on related parallel solvers were then be proposed. Has followed a session dedicated to advanced parallel schemes using task-based paradigms, including a hands-on with the starpu runtime system. The ultimate hands-on session was devoted to the use of parallel profiling tools. The school was closed with plenary talks illustrating the usage of such a workflow in an industrial context.

  The hands-on session were conducted on the Federative Platform for Research in Computer Science and Mathematics (PlaFRIM) machine in a guix-hpc reproducible environment

  The school was attended by about 40 participants mostly PhDs and postdocs from Inria teams.

6. New Software and Platforms

6.1. AVCI

Adaptive vibrational configuration interaction

KEYWORDS: Vibrational spectra - Eigen value

FUNCTIONAL DESCRIPTION: A-VCI is a theoretical vibrational spectroscopy algorithm developed to effectively reduce the number of vibrational states used in the configuration-interaction (CI) process. It constructs a nested basis for the discretization of the Hamiltonian operator inside a large CI approximation space and uses an a-posteriori error estimator (residue) to select the most relevant directions to expand the discretization space.

The Hamiltonian operator consists of 3 operators: a harmonic oscillator sum, the potential energy surface operator and the Coriolis operators. In addition, the code can compute the intensity of eigenvectors.

The code can handle molecules up to 10 atoms, which corresponds to solving an eigenvalue problem in a 24-dimensional space.

- Partner: IPREM
- Contact: Olivier Coulaud

6.2. Chameleon

KEYWORDS: Runtime system - Task-based algorithm - Dense linear algebra - HPC - Task scheduling

SCIENTIFIC DESCRIPTION: 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.

We expect advances in three directions based first on strong and closed interactions between the runtime and numerical linear algebra communities. This initial activity will then naturally expand to more focused but still joint research in both fields.

1. Fine interaction between linear algebra and runtime systems. On parallel machines, HPC applications need to take care of data movement and consistency, which can be either explicitly managed at the level of the application itself or delegated to a runtime system. We adopt the latter approach in order to better keep up with hardware trends whose complexity is growing exponentially. One major task in this project is to define a proper interface between HPC applications and runtime systems in order to maximize productivity and expressivity. As mentioned in the next section, a widely used approach consists in abstracting the application as a DAG that the runtime system is in charge of scheduling. Scheduling such a DAG over a set of heterogeneous processing units introduces a lot of new challenges, such as predicting accurately the execution time of each type of task over each kind of unit, minimizing data transfers between memory banks, performing data prefetching, etc. Expected advances: In a nutshell, a new runtime system API will be designed to allow applications to provide scheduling hints to the runtime system and to get real-time feedback about the consequences of scheduling decisions.

2. Runtime systems. A runtime environment is an intermediate layer between the system and the application. It provides low-level functionality not provided by the system (such as scheduling or management of the heterogeneity) and high-level features (such as performance portability). In the framework of this proposal, we will work on the scalability of runtime environment. To achieve scalability it is required to avoid all centralization. Here, the main problem is the scheduling of the tasks. In many task-based runtime environments the scheduler is centralized and becomes a bottleneck as soon as too many cores are involved. It is therefore required to distribute the scheduling decision or to compute a data distribution that impose the mapping of task using, for instance the so-called “owner-compute” rule. Expected advances: We will design runtime systems that enable an efficient and scalable use of thousands of distributed multicore nodes enhanced with accelerators.

3. Linear algebra. Because of its central position in HPC and of the well understood structure of its algorithms, dense linear algebra has often pioneered new challenges that HPC had to face. Again, dense linear algebra has been in the vanguard of the new era of petascale computing with the design of new algorithms that can efficiently run on a multicore node with GPU accelerators. These algorithms are called “communication-avoiding” since they have been redesigned to limit the amount of communication between processing units (and between the different levels of memory hierarchy). They are expressed through Direct Acyclic Graphs (DAG) of fine-grained tasks that are dynamically scheduled. Expected advances: First, we plan to investigate the impact of these principles in the case of sparse applications (whose algorithms are slightly more complicated but often rely on dense kernels). Furthermore, both in the dense and sparse cases, the scalability on thousands of nodes is still limited, new numerical approaches need to be found. We will specifically design sparse hybrid direct/iterative methods that represent a promising approach.

Overall end point. The overall goal of the MORSE associate team is to enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

FUNCTIONAL DESCRIPTION: Chameleon is a dense linear algebra software relying on sequential task-based algorithms where sub-tasks of the overall algorithms are submitted to a Runtime system. A Runtime system such as StarPU is able to manage automatically data transfers between not shared memory area (CPUs-GPUs, distributed nodes). This kind of implementation paradigm allows to design high performing linear algebra algorithms on very different type of architecture: laptop, many-core nodes, CPUs-GPUs, multiple nodes. For example, Chameleon is able to perform a Cholesky factorization (double-precision) at 80 TFlop/s on a dense matrix of order 400 000 (i.e. 4 min 30 s).

RELEASE FUNCTIONAL DESCRIPTION: Chameleon includes the following features:

- BLAS 3, LAPACK one-sided and LAPACK norms tile algorithms - Support QUARK and StarPU runtime systems and PaRSEC since 2018 - Exploitation of homogeneous and heterogeneous platforms through the use of BLAS/LAPACK CPU kernels and cuBLAS/MAGMA CUDA kernels - Exploitation of clusters of interconnected nodes with distributed memory (using OpenMPI)

- Participants: Cédric Castagnede, Samuel Thibault, Emmanuel Agullo, Florent Pruvost and Mathieu Faverge

- Partners: Innovative Computing Laboratory (ICL) - King Abdullha University of Science and Technology - University of Colorado Denver
- Contact: Emmanuel Agullo
- URL: https://gitlab.inria.fr/solverstack/chameleon

6.3. Diodon

KEYWORDS: Dimensionality reduction - Data analysis

FUNCTIONAL DESCRIPTION: Most of dimension reduction methods inherited from Multivariate Data Analysis, and currently implemented as element in statistical learning for handling very large datasets (the dimension of spaces is the number of features) rely on a chain of pretreatments, a core with a SVD for low rank approximation of a given matrix, and a post-treatment for interpreting results. The costly part in computations is the SVD, which is in cubic complexity. Diodon is a list of functions and drivers which implement (i) pre-treatments, SVD and post-treatments on a large diversity of methods, (ii) random projection methods for running the SVD which permits to bypass the time limit in computing the SVD, and (iii) an implementation in C++ of the SVD with random projection at prescribed rank or precision, connected to MDS.

- Contact: Alain Franc

6.4. DPLASMA

Distributed Parallel Linear Algebra Software for Multicore Architectures

FUNCTIONAL DESCRIPTION: DPLASMA 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.

- Contact: Mathieu Faverge
- URL: http://icl.cs.utk.edu/parsec/index.html

6.5. Fabulous

Fast Accurate Block Linear krylOv Solver

KEYWORDS: Numerical algorithm - Block Krylov solver

SCIENTIFIC DESCRIPTION: Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides

FUNCTIONAL DESCRIPTION: Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides. The library implements block variants of minimal norm residual variants with partial convergence management and spectral information recycling. The package already implements regular block-GMRES (BGMRES), Inexact Breakdown BGMRES (IB-BMGRES), Inexact Breakdown BGMRES with Deflated Restarting (IB-BGMRES-DR), Block Generalized Conjugate Residual with partial convergence management. The C++ library relies on callback mechanisms to implement the calculations (matrix-vector, dot-product, ...) that depend on the parallel data distribution selected by the user.

- Participants: Emmanuel Agullo, Luc Giraud, Gilles Marait and Cyrille Piacibello
- Contact: Luc Giraud
- Publication: Block GMRES method with inexact breakdowns and deflated restarting
- URL: https://gitlab.inria.fr/solverstack/fabulous/

6.6. MAPHYS

Massively Parallel Hybrid Solver

KEYWORD: Parallel hybrid direct/iterative solution of large linear systems

FUNCTIONAL DESCRIPTION: MaPHySis 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. A fully algebraic coarse space is available for symmetric positive definite problems, that insures the numerical scalability of the preconditioner.

The parallel implementation is based on MPI+thread. Maphys relies on state-of-the art sparse and dense direct solvers.

MaPHySis essentially a preconditioner that can be used to speed-up the convergence of any Krylov subspace method and is coupled with the ones implemented in the Fabulous package.

- Participants: Emmanuel Agullo, Luc Giraud, Matthieu Kuhn, Gilles Marait and Louis Poirel
- Contact: Emmanuel Agullo
- Publications: Hierarchical hybrid sparse linear solver for multicore platforms - Robust coarse spaces for Abstract Schwarz preconditioners via generalized eigenproblems
- URL: https://gitlab.inria.fr/solverstack/maphys

6.7. MetaPart

KEYWORDS: High performance computing - HPC - Parallel computing - Graph algorithmics - Graph - Hypergraph

FUNCTIONAL DESCRIPTION: MetaPart is a framework for graph or hypergraph manipulation that addresses different problems, like partitioning, repartitioning, or co-partitioning, ... MetaPart is made up of several projects, such as StarPart, LibGraph or CoPart. StarPart is the core of the MetaPart framework. It offers a wide variety of graph partitioning methods (Metis, Scotch, Zoltan, Patoh, ParMetis, Kahip, ...), which makes it easy to compare these different methods and to better adjust the parameters of these methods. It is built upon the LibGraph library, that provides basic graph and hypergraph routines. The Copart project is a library used on top of StarPart, that provides co-partitioning algorithms for the load-blancing of parallel coupled simulations.

- Participant: Aurélien Esnard
- Contact: Aurélien Esnard
- URL: https://gitlab.inria.fr/metapart

6.8. MPICPL

MPI CouPLing

KEYWORDS: MPI - Coupling software

FUNCTIONAL DESCRIPTION: MPICPL 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 programing 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.

- Participant: Aurélien Esnard
- Contact: Aurélien Esnard
- URL: https://gitlab.inria.fr/esnard/mpicpl

6.9. OptiDis

KEYWORDS: Dislocation dynamics simulation - Fast multipole method - Large scale - Collision

FUNCTIONAL DESCRIPTION: OptiDis is a new code for large scale dislocation dynamics simulations. Its purpose is to simulate real life dislocation densities (up to 5.1022 dislocations/m-2) in order to understand plastic deformation and study strain hardening. The main application is to observe and understand plastic deformation of irradiated zirconium. Zirconium alloys are the first containment barrier against the dissemination of radioactive elements. More precisely, with neutron irradiated zirconium alloys we are talking about channeling mechanism, which means to stick with the reality, more than tens of thousands of induced loops, i. e. 100 million degrees of freedom in the simulation. The code is based on Numodis code developed at CEA Saclay and the ScalFMM library developed in HiePACS project. The code is written in C++ language and using the last features of C++11/14. 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 distributed over MPI processes, then we use a thinner level for threads, dividing the domain by an Octree representation. All theses parts are controlled by the ScalFMM library. On the last level, our data are stored in an adaptive structure that absorbs the dynamics of this type of simulation and manages the parallelism of tasks..

- Participant: Olivier Coulaud
- Contact: Olivier Coulaud
- URL: http://optidis.gforge.inria.fr/

6.10. PaStiX

Parallel Sparse matriX package

KEYWORDS: Linear algebra - High-performance calculation - Sparse Matrices - Linear Systems Solver - Low-Rank compression

SCIENTIFIC DESCRIPTION: 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 handle a combination of 1D and 2D block distributions. A dynamic scheduling can also be applied to take care of NUMA architectures while taking into account very precisely the computational costs of the BLAS 3 primitives, the communication costs and the cost of local aggregations.

FUNCTIONAL DESCRIPTION: PaStiX 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) methods. It can handle low-rank compression techniques to reduce the computation and the memory complexity. Numerical algorithms are implemented in single or double precision (real or complex) for LLt, LDLt and LU factorization with static pivoting (for non symmetric matrices having a symmetric pattern). The PaStiX library uses the graph partitioning and sparse matrix block ordering packages Scotch or Metis.

The PaStiX solver is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of multicore nodes with GPU accelerators or KNL processors. In particular, we provide 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.

The solver also provides some low-rank compression methods to reduce the memory footprint and/or the time-to-solution.

- Participants: Tony Delarue, Grégoire Pichon, Mathieu Faverge, EsragÜl Korkmaz and Pierre Ramet
- Partners: Université Bordeaux 1 - INP Bordeaux
- Contact: Pierre Ramet
- URL: https://gitlab.inria.fr/solverstack/pastix

6.11. pmtool

KEYWORDS: Scheduling - Task scheduling - StarPU - Heterogeneity - GPGPU - Performance analysis

FUNCTIONAL DESCRIPTION: Analyse post-mortem the behavior of StarPU applications. Provide lower bounds on makespan. Study the performance of different schedulers in a simple context. Provide implementations of many scheduling algorithms from the literature

NEWS OF THE YEAR: Included many new algorithms, in particular online algorithms Better integration with StarPU by accepting .rec files as input

- Participant: Lionel Eyraud-Dubois
- Contact: Lionel Eyraud-Dubois
- Publications: Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs - Fast Approximation Algorithms for Task-Based Runtime Systems
- URL: https://gitlab.inria.fr/eyrauddu/pmtool

6.12. rotor

Re-materializing Optimally with pyTORch

KEYWORDS: Deep learning - Optimization - Python - GPU - Automatic differentiation

FUNCTIONAL DESCRIPTION: Allows to train very large convolutional networks on limited memory by optimally selecting which activations should be kept and which should be recomputed. This code is meant to replace the checkpoint.py utility available in pytorch, by providing more efficient rematerialization strategies. The algorithm is easier to tune: the only required parameter is the available memory, instead of the number of segments.

- Contact: Lionel Eyraud-Dubois

6.13. ScalFMM

Scalable Fast Multipole Method

KEYWORDS: N-body - Fast multipole method - Parallelism - MPI - OpenMP

SCIENTIFIC DESCRIPTION: ScalFMM is a software library to simulate N-body interactions using the Fast Multipole Method. 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 @ 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.

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 is two main parts:

the management of the octree and the parallelization of the method the kernels. This new architecture allow us to easily add new FMM algorithm or kernels and new paradigm of parallelization.

FUNCTIONAL DESCRIPTION: Compute N-body interactions using the Fast Multipole Method for large number of objects

- Participants: Bramas Bérenger, Olivier Coulaud and Pierre Estérie
- Contact: Olivier Coulaud
- URL: https://gitlab.inria.fr/solverstack/ScalFMM

6.14. VITE

Visual Trace Explorer

KEYWORDS: Visualization - Execution trace

FUNCTIONAL DESCRIPTION: 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.

- Participant: Mathieu Faverge
- Contact: Mathieu Faverge
- URL: http://vite.gforge.inria.fr/

6.15. PlaFRIM

Plateforme Fédérative pour la Recherche en Informatique et Mathématiques

KEYWORDS: High-Performance Computing - Hardware platform

FUNCTIONAL DESCRIPTION: PlaFRIM is an experimental platform for research 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.

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 1,000 cores (excluding GPU and Xeon Phi) that are available for all research teams of Inria Bordeaux, Labri and IMB. This computer is in particular used by all the engineers who work in HiePACS and are advised by F. Rue from the SED.

- Contact: Olivier Coulaud
- URL: https://www.plafrim.fr/en/home/

7. New Results

7.1. High-performance computing on next generation architectures

7.1.1. Memory optimization for the training phase of deep convolutional networks

Training Deep Neural Networks is known to be an expensive operation, both in terms of computational cost and memory load. Indeed, during training, all intermediate layer outputs (called activations) computed during the forward phase must be stored until the corresponding gradient has been computedin the backward phase. These memory requirements sometimes prevent to consider larger batch sizes and deeper networks, so that they can limit both convergence speed and accuracy. Recent works have proposed to offload some of the computed forward activations from the memory of the GPU to the memory of the CPU. This requires to determine which activations should be offloaded and when these transfers from and to the memory of the GPU should take place. In [28], We prove that this problem is NP-hard in the strong sense, and we propose two heuristics based on relaxations of the problem. We perform extensive experimental evaluation on standard Deep Neural Networks. We compare the performance of our heuristics against previous approaches from the literature, showing that they achieve much better performance in a wide variety of situations.

In [23], we also introduce a new activation checkpointing method which allows to significantly decrease memory usage when training Deep Neural Networks with the back-propagation algorithm. Similarly to checkpointing techniques coming from the literature on Automatic Differentiation, it consists in dynamically selecting the forward activations that are saved during the training phase, and then automatically recomputing missing activations from those previously recorded. We propose an original computation model that combines two types of activation savings: either only storing the layer inputs, or recording the complete history of operations that produced the outputs (this uses more memory, but requires fewer recomputations in the backward phase), and we provide an algorithm to compute the optimal computation sequence for this model. This paper also describes a PyTorch implementation that processes the entire chain, dealing with any sequential DNN whose internal layers may be arbitrarily complex and automatically executing it according to the optimal checkpointing strategy computed given a memory limit. Through extensive experiments, we show that our implementation consistently outperforms existing checkpointing approaches for a large class of networks, image sizes and batch sizes.

In [4], [24], we consider the problem of optimally scheduling the backpropagation of Deep Join Networks. Deep Learning training memory needs can prevent the user to consider large models and large batch sizes. In this work, we propose to use techniques from memory-aware scheduling and Automatic Differentiation (AD) to execute a backpropagation graph with a bounded memory requirement at the cost of extra recomputations. The case of a single homogeneous chain, i.e. the case of a network whose all stages are identical and form a chain, is well understood and optimal solutions have been proposed in the AD literature. The networks encountered in practice in the context of Deep Learning are much more diverse, both in terms of shape and heterogeneity. In this work, we define the class of backpropagation graphs, and extend those on which one can compute in polynomial time a solution that minimizes the total number of recomputations. In particular we consider join graphs which correspond to models such as Siamese or Cross Modal Networks.

7.1.2. Sizing and Partitioning Strategies for Burst-Buffers to Reduce IO Contention

Burst-Buffers are high throughput and small size storage which are being used as an intermediate storage between the PFS (Parallel File System) and the computational nodes of modern HPC systems. They can allow to hinder to contention to the PFS, a shared resource whose read and write performance increase slower than processing power in HPC systems. A second usage is to accelerate data transfers and to hide the latency to the PFS. In this work, we concentrate on the first usage. We propose a model for Burst-Buffers and application transfers. We consider the problem of dimensioning and sharing the Burst-Buffers between several applications. This dimensioning can be done either dynamically or statically. The dynamic allocation considers that any application can use any available portion of the Burst-Buffers. The static allocation considers that when a new application enters the system, it is assigned some portion of the Burst-Buffers, which cannot be used by the other applications until that application leaves the system and its data is purged from it. We show that the general sharing problem to guarantee fair performance for all applications is an NP-Complete problem. We propose a polynomial time algorithms for the special case of finding the optimal buffer size such that no application is slowed down due to PFS contention, both in the static and dynamic cases. Finally, we provide evaluations of our algorithms in realistic settings. We use those to discuss how to minimize the overhead of the static allocation of buffers compared to the dynamic allocation. More information on these results can be found in [9].

7.1.3. Efficient Ordering of Kernel Submission on GPUs

In distributed memory systems, it is paramount to develop strategies to overlap the data transfers between memory nodes with the computations in order to exploit their full potential. In [11], we consider the problem of determining the order of data transfers between two memory nodes for a set of independent tasks with the objective of minimizing the makespan. We prove that, with limited memory capacity, the problem of obtaining the optimal data transfer order is NP-complete. We propose several heuristics to determine this order and discuss the conditions that might be favorable to different heuristics. We analyze our heuristics on traces obtained by running two molecular chemistry kernels, namely, Hartree–Fock (HF) and Coupled Cluster Singles Doubles (CCSD), on 10 nodes of an HPC system. Our results show that some of our heuristics achieve significant overlap for moderate memory capacities and resulting in makespans that are very close to the lower bound.

Concurrent kernel execution is a relatively new feature in modern GPUs, which was designed to improve hardware utilization and the overall system throughput. However, the decision on the simultaneous execution of tasks is performed by the hardware with a leftover policy, that assigns as many resources as possible for one task and then assigns the remaining resources to the next task. This can lead to unreasonable use of resources. In [30], we tackle the problem of co-scheduling for GPUs with and without preemption, with the focus on determining the kernels submission order to reduce the number of preemptions and the kernels makespan, respectively. We propose a graph-based theoretical model to build preemptive and non-preemptive schedules. We show that the optimal preemptive makespan can be computed by solving a Linear Program in polynomial time, and we propose an algorithm based on this solution which minimizes the number of preemptions. We also propose an algorithm that transforms a preemptive solution of optimal makespan into a non-preemptive solution with the smallest possible preemption overhead. We show, however, that finding the minimal amount of preemptions among all preemptive solutions of optimal makespan is a NP-hard problem, and computing the optimal non-preemptive schedule is also NP-hard. In addition, we study the non-preemptive problem, without searching first for a good preemptive solution, and present a Mixed Integer Linear Program solution to this problem. We performed experiments on real-world GPU applications and our approach can achieve optimal makespan by preempting 6 to 9% of the tasks. Our non-preemptive approach, on the other side, obtains makespan within 2.5% of the optimal preemptive schedules, while previous approaches exceed the preemptive makespan by 5 to 12%.

7.1.4. Scheduling Tasks on Two Types of Resources

We consider the problem of scheduling task graphs on two types of unrelated resources, which arises in the context of task-based runtime systems on modern platforms containing CPUs and GPUs. In [10], we focus on an algorithm named HeteroPrio, which was originally introduced as an efficient heuristic for a particular application. HeteroPrio is an adaptation of the well known list scheduling algorithm, in which the tasks are picked by the resources in the order of their acceleration factor. This algorithm is augmented with a spoliation mechanism: a task assigned by the list algorithm can later on be reassigned to a different resource if it allows to finish this task earlier. We propose here the first theoretical analysis of the HeteroPrio algorithm in the presence of dependencies. More specifically, if the platform contains m and n processors of each type, we show that the worst-case approximation ratio of HeteroPrio is between $1 + \max(m/n, n/m)$ and $2 + \max(m/n, n/m)$. Our proof structure allows to precisely identify the necessary conditions on the spoliation strategy to obtain such a guarantee. We also present an in-depth experimental analysis, comparing several such spoliation strategies, and comparing HeteroPrio with other algorithms from the literature. Although the worst case analysis shows the possibility of pathological behavior, HeteroPrio is able to produce, in very reasonable time, schedules of significantly better quality.

The evolution in the design of modern parallel platforms leads to revisit the scheduling jobs on distributed heterogeneous resources. We contribute to [31], a survey whose goal is to present the main existing algorithms, to classify them based on their underlying principles and to propose unified implementations to enable their fair comparison, both in terms of running time and quality of schedules, on a large set of common benchmarks that we made available for the community [27]. Beyond this comparison, our goal is also to understand the main difficulties that heterogeneity conveys and the shared principles that guide the design of efficient algorithms.

7.1.5. Data-Locality Aware Tasks Scheduling with Replicated Inputs

In [5], we consider the influence on data-locality of the replication of data files, as automatically performed by Distributed File Systems such as HDFS. Replication is known to have a crucial impact on data locality in addition to system fault tolerance. Indeed, intuitively, having more replicas of the same input file gives more opportunities for this task to be processed locally, i.e. without any input file transfer. Given the practical importance of this problem, a vast literature has been proposed to schedule tasks, based on a random placement of replicated input files. Our goal in this paper is to study the performance of these algorithms, both in terms of makespan minimization (minimize the completion time of the last task when non-local processing is forbidden) and communication minimization (minimize the number of non-local tasks when no idle time on resources is allowed). In the case of homogenous tasks, we are able to prove, using models based on "balls into bins" and "power of two choices" problems, that the well known good behavior of classical strategies can be theoretically grounded. Going further, we even establish that it is possible, using semi-matchings theory, to find the optimal solution in very small time. We also use known graph-orientation results to prove that this optimal solution is indeed near-perfect with strong probability. In the more general case of heterogeneous tasks, we propose heuristics solutions both in the clairvoyant and non-clairvoyant cases (i.e. task length is known in advance or not), and we evaluate them through simulations, using actual traces of a Hadoop cluster.

7.2. High performance solvers for large linear algebra problems

7.2.1. Deflation and preconditioning strategies for sequences of sampled stochastic elliptic equations

We are interested in the quantification of uncertainties in discretized elliptic partial differential equations with random coefficients. In sampling-based approaches, this relies on solving large numbers of symmetric positive definite linear systems with different matrices. In this work, we investigate recycling Krylov subspace strategies for the iterative solution of sequences of such systems. The linear systems are solved using deflated conjugate gradient (CG) methods, where the Krylov subspace is augmented with approximate eigenvectors of the previously sampled operator. These operators are sampled by Markov chain Monte Carlo, which leads to sequences of correlated matrices. First, the following aspects of eigenvector approximation, and their effect on deflation, are investigated: (i) projection technique, and (ii) restarting strategy of the eigen-search space. Our numerical experiments show that these aspects only impact convergence behaviors of deflated CG at the early stages of the sampling sequence. Second, unlike sequences with multiple right-hand sides and a constant operator, our experiments with multiple matrices show the necessity to orthogonalize the iterated residual of the linear system with respect to the deflation subspace, throughout the sampling sequence. Finally, we observe a synergistic effect of deflation and block-Jacobi (bJ) preconditioning. While the action of bJ preconditioners leaves a trail of isolated eigenvalues in the spectrum of the preconditioned operator, for 1D problems, the corresponding eigenvectors are well approximated by the recycling strategy. Then, up to a certain number of blocks, deflated CG methods with bJ preconditioners achieve similar convergence behaviors to those observed with CG when using algebraic multigrid (AMG) as a preconditioner.

This work, developed in the framework of the PhD thesis of Nicolas Venkovic in collaboration with P. Mycek (Cerfacs) and O. Le Maitre (CMAP, Ecole Polytechnique), will be presented at the next Copper Mountain conference on iterative methods.

7.2.2. Robust preconditionners via generalized eigenproblems for hybrid sparse linear solvers

The solution of large sparse linear systems is one of the most time consuming kernels in many numerical simulations. The domain decomposition community has developed many efficient and robust methods in the last decades. While many of these solvers fall into the abstract Schwarz (aS) framework, their robustness has originally been demonstrated on a case-by-case basis. In this work, we propose a bound for the condition number of all deflated aS methods provided that the coarse grid consists of the assembly of local components that contain the kernel of some local operators. We show that classical results from the literature on particular instances of aS methods can be retrieved from this bound. We then show that such a coarse grid correction can be explicitly obtained algebraically via generalized eigenproblems, leading to a condition number independent of the number of domains. This result can be readily applied to retrieve or improve the bounds previously obtained via generalized eigenproblems in the particular cases of Neumann-Neumann (NN), Additive Schwarz (AS) and optimized Robin but also generalizes them when applied with approximate local solvers. Interestingly, the proposed methodology turns out to be a comparison of the considered particular aS method with generalized versions of both NN and AS for tackling the lower and upper part of the spectrum, respectively. We furthermore show that the application of the considered grid corrections in an additive fashion is robust in the AS case although it is not robust for aS methods in general. In particular, the proposed framework allows for ensuring the robustness of the AS method applied on the Schur complement (AS/S), either with deflation or additively, and with the freedom of relying on an approximate local Schur complement. Numerical experiments illustrate these statements.

More information on these results can be found in [3]

7.2.3. Rank Revealing QR Methods for Sparse Block Low Rank Solvers

In the context of the ANR Sashimi project and the Phd of Esragul Korkmaz, we have investigated several compression methods of dense blocks appearing inside sparse matrix solvers to reduce the memory consumption, as well as the time to solution.

Solving linear equations of type Ax=b for large sparse systems frequently emerges in science and engineering applications, which creates the main bottleneck. In spite that the direct methods are costly in time and memory consumption, they are still the most robust way to solve these systems. Nowadays, increasing the amount of computational units for the supercomputers became trendy, while the memory available per core is reduced. Therefore, when solving these linear equations, memory reduction becomes as important as time reduction. While looking for the lowest possible compression rank, Singular Value Decomposition (SVD) gives the best result. It is however too costly as the whole factorization is computed to find the resulting rank. In this respect, rank revealing QR decomposition variants are less costly, but can introduce larger ranks. Among these variants, column pivoting or matrix rotation can be applied on the matrix A, such that the most important information in the matrix is gathered to the leftmost columns and the remaining unnecessary information can be omitted. For reducing the communication cost of the classical QR decomposition with column pivoting, blocking versions with randomization are suggested as an alternative solution to find the pivots. In these randomized variants, the matrix A is projected on a much lower dimensional matrix by using an independent and identically distributed Gaussian matrix so that the pivoting/rotational matrix can be computed on the lower dimensional matrix. In addition, to avoid unnecessary updates of the trailing matrix at each iteration, a truncated randomized method is suggested and shown to be more efficient for larger matrix sizes. Thanks to these methods, closer results to SVD can be obtained and the cost of compression can be reduced.

A comparison of all these methods in terms of complexity, numerical stability and performance have been presented at the national conference COMPAS'2019 [18], and at the international workshop SparseDay'2019 [19].

7.2.4. Accelerating Krylov linear solvers with agnostic lossy data compression

In the context of the Inria International Lab JLESC we have an ongoing collaboration with Argonne National Laboratory on the use of agnostic compression techniques to reduce the memory footprint of iterative linear solvers. Krylov methods are among the most efficient and widely used algorithms for the solution of large linear systems. Some of these methods can, however, have large memory requirements. Despite the fact that modern high-performance computing systems have more and more memory available, the memory used by applications remains a major concern when solving large scale problems. This is one of the reasons why interest in lossy data compression techniques has grown tremendously in the last two decades: it can reduce the amount of information that needs to be stored and communicated. Recently, it has also been shown that Krylov methods allow for some inexactness in the matrix-vector product that is typically required in each iteration. We showed that the loss of accuracy caused by compressing and decompressing the solution of the preconditioning step in the flexible generalized minimal residual method can be interpreted as an inexact matrix-vector product. This allowed us to find a bound on the maximum compression error in each iteration based on the theory of inexact Krylov methods. We performed a series of numerical experiment in order to validate our results. A number of “relaxed compression strategies” was also considered in order to achieve higher compression ratios.

The results of this joint effort will be presented to the next SIAM conférence on Parallel processing SIAM-PP'20.

7.2.5. Energy Analysis of a Solver Stack for Frequency-Domain Electromagnetics

High-performance computing aims at developing models and simulations for applications in numerous scientific fields. Yet, the energy consumption of these HPC facilities currently limits their size and performance, and consequently the size of the tackled problems. The complexity of the HPC software stacks and their various optimizations makes it difficult to finely understand the energy consumption of scientific applications. To highlight this difficulty on a concrete use-case, we perform in [8] an energy and power analysis of a software stack for the simulation of frequency-domain electromagnetic wave propagation. This solver stack combines a high order finite element discretization framework of the system of three-dimensional frequency-domain Maxwell equations with an algebraic hybrid iterative-direct sparse linear solver. This analysis is conducted on the KNL-based PRACE-PCP system. Our results illustrate the difficulty in predicting how to trade energy and runtime.

7.2.6. Exploiting Parameterized Task-graph in Sparse Direct Solvers

Task-based programming models have been widely studied in the context of dense linear algebra, but remains less studied for the more complex sparse solvers. In this talk [17], we have presented the use of two different programming models: Sequential Task Flow from StarPU, and Parameterized Task Graph from PaRSEC to parallelize the factorization step of the PaStiX sparse direct solver. We have presented how those programming models have been used to integrate more complex and finer parallelism to take into account new architectures with many computational units. Efficiency of such solutions on homogeneous and heterogeneous architectures with a spectrum of matrices from different applications have been shown. We also have presented how such solutions enable, without extra cost to the programmer, better performance on irregular computations such as in the block low-rank implementation of the solver.

7.2.7. Block Low-rank Algebraic Clustering for Sparse Direct Solvers

In these talks [20], [21], we adressed the Block Low-Rank (BLR) clustering problem, to cluster unknowns within separators appearing during the factorization of sparse matrices. We have shown that methods considering only intra-separators connectivity (i.e., k-way or recursive bissection) as well as methods managing only interaction between separators have some limitations. The new strategy we proposed consider interactions between a separator and its children to pre-select some interactions while reducing the number of off-diagonal blocks. We demonstrated how this method enhance the BLR strategies in the sparse direct supernodal solver PaStiX, and discuss how it can be extended to low-rank formats with more than one level of hierarchy.

7.2.8. Leveraging Task-Based Polar Decomposition Using PARSEC on Massively Parallel Systems

In paper [13], we describe how to leverage a task-based implementation of the polar decomposition on massively parallel systems using the PARSEC dynamic runtime system. Based on a formulation of the iterative QR Dynamically-Weighted Halley (QDWH) algorithm, our novel implementation reduces data traffic while exploiting high concurrency from the underlying hardware architecture. First, we replace the most time-consuming classical QR factorization phase with a new hierarchical variant, customized for the specific structure of the matrix during the QDWH iterations. The newly developed hierarchical QR for QDWH exploits not only the matrix structure, but also shortens the length of the critical path to maximize hardware occupancy. We then deploy PARSEC to seamlessly orchestrate, pipeline, and track the data dependencies of the various linear algebra building blocks involved during the iterative QDWH algorithm. PARSEC enables to overlap communications with computations thanks to its asynchronous scheduling of fine-grained computational tasks. It employs look-ahead techniques to further expose parallelism, while actively pursuing the critical path. In addition, we identify synergistic opportunities between the task-based QDWH algorithm and the PARSEC framework. We exploit them during the hierarchical QR factorization to enforce a locality-aware task execution. The latter feature permits to minimize the expensive inter-node communication, which represents one of the main bottlenecks for scaling up applications on challenging distributed-memory systems. We report numerical accuracy and performance results using well and ill-conditioned matrices. The benchmarking campaign reveals up to 2X performance speedup against the existing state-of-the-art implementation for the polar decomposition on 36,864 cores.

7.3. Parallel Low-Rank Linear System and Eigenvalue Solvers Using Tensor Decompositions

It is common to accelerate the boundary element method by compression techniques (FMM, $\mathcal{H}$-matrix/ACA) that enable a more accurate solution or a solution in higher frequency. In this article, we present a compression method based on a transformation of the linear system into the tensor-train format by the quantization technique. The method is applied to a scattering problem on a canonical object with a regular mesh and improves the performance obtained from existing methods. This method has been presented at the 22nd International Conference on the Computation of Electromagnetic Field, (COMPUMAG 2019) [12] and an extented version is accepted in IEEE TRANSACTIONS ON MAGNETICS.

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

7.4.1. StarPart Redesign

In the context of the french ICARUS project (FUI), which focuses the development of high-fidelity calculation tools for the design of hot engine parts (aeronautics & automotive), we are looking to develop new load-balancing algorithms to optimize the complex numerical simulations of our industrial and academic partners (Turbomeca, Siemens, Cerfacs, Onera, ...). Indeed, the efficient execution of large-scale coupled simulations on powerful computers is a real challenge, which requires revisiting traditional load-balancing algorithms based on graph partitioning. A thesis on this subject has already been conducted in the Inria HiePACS team in 2016, which has successfully developed a co-partitioning algorithm that balances the load of two coupled codes by taking into account the coupling interactions between these codes. This work was initially integrated into the StarPart platform. The necessary extension of our algorithms to parallel & distributed (increasingly dynamic) versions has led to a complete redesign of StarPart, which has been the focus of our efforts this year (as in the previous year). The StarPart framework provides the necessary building blocks to develop new graph algorithms in the context of HPC, such as those we are targeting. The strength of StarPart lies in the fact that it is a light runtime system applied to the issue of "graph computing". It provides a unified data model and a uniform programming interface that allows easy access to a dozen partitioning libraries, including Metis, Scotch, Zoltan, etc. Thus, it is possible, for example, to load a mesh from an industrial test case provided by our partners (or an academic graph collection as DIMACS'10) and to easily compare the results for the different partitioners integrated in StarPart.

Alongside this work, we are beginning to work on the application of learning techniques to the problem of graph partitioning. Recent work on GCNs (Graph Convolutional Networks) is an interesting approach that we will explore.

7.5. Application Domains

7.5.1. Material physics

7.5.1.1. EigenSolver

The adaptive vibrational configuration interaction algorithm has been introduced as a new eigennvalues method for large dimension problem. It is based on the construction of nested bases for the discretization of the Hamiltonian operator according to a theoretical criterion that ensures the convergence of the method. It efficiently reduce the dimension of the set of basis functions used and then we are able solve vibrationnal eigenvalue problem up to the dimension 15 (7 atoms). Beyond this molecule size, two major issues appear. First, the size of the approximation domain increases exponentially with the number of atoms and the density of eigenvalues in the target area.

This year we have worked on two main areas. First of all, not all the eigenvalues that are calculated are determined by spectroscopy and therefore do not interest chemists. Only eigenvalues with an intensity are relevant. Also, we have set up a selection of interesting eigenvalues using the intensity operator. This requires calculating the scalar product between the smallest eigenvalues and the dipole moment applied to an eigenvector to evaluate its intensity. In addition, to get closer to the experimental values, we introduced the Coriolis operator into the Hamiltonian. A document is being written on these last two points showing that we can reach for a molecule 10 atoms the area of interest (i.e. more than 2 400 eigenvalues). Moreover, we continue to extend our shared memory parallelization to distributed memory using the message exchange paradigm to speedup the eigensolver time.

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

7.5.2.1. Numerical and parallel scalable hybrid solvers in large scale calculations

We have been working with the NACHOS team on the treatment of the system of three-dimensional frequency-domain (or time-harmonic) Maxwell equations using a high order hybridizable discontinuous Galerkin (HDG) approximation method combined to domain decomposition (DD) based hybrid iterative-direct parallel solution strategies. The proposed HDG method preserves the advantages of classical DG methods previously introduced for the time-domain Maxwell equations, in particular in terms of accuracy and flexibility with regards to the discretization of complex geometrical features, while keeping the computational efficiency at the level of the reference edge element based finite element formulation widely adopted for the considered PDE system. We study in details the computational performances of the resulting DD solvers in particular in terms of scalability metrics by considering both a model test problem and more realistic large-scale simulations performed on high performance computing systems consisting of networked multicore nodes. More information on these results can be found in [2].

In the context of a parallel plasma physics simulation code, we perform a qualitative performance study between two natural candidates for the parallel solution of 3D Poisson problems that are multigrid and domain decomposition. We selected one representative of each of these numerical techniques implemented in state of the art parallel packages and show that depending on the regime used in terms of number of unknowns per computing cores the best alternative in terms of time to solution varies. Those results show the interest of having both types of numerical solvers integrated in a simulation code that can be used in very different configurations in terms of problem sizes and parallel computing platforms. More information on these results will be shortly available in an Inria scientific report.

7.5.2.2. Efficient Parallel Solution of the 3D Stationary Boltzmann Transport Equation for Diffusive Problems

In the context of a collaboration with EDF-Lab with the Phd of Salli Moustafa, we present an efficient parallel method for the deterministic solution of the 3D stationary Boltzmann transport equation applied to diffusive problems such as nuclear core criticality computations. Based on standard MultiGroup-Sn-DD discretization schemes, our approach combines a highly efficient nested parallelization strategy with the PDSA parallel acceleration technique applied for the first time to 3D transport problems. These two key ingredients enable us to solve extremely large neutronic problems involving up to 10^{12} degrees of freedom in less than an hour using 64 super-computer nodes.

These contributions have been published in Journal of Computational Physics (JCP) [7].

7.5.2.3. Bridging the Gap Between $\mathcal{H}$-Matrices and Sparse Direct Methods for the Solution of Large Linear Systems

For the sake of numerical robustness in aeroacoustics simulations, the solution techniques based on the factorization of the matrix associated with the linear system are the methods of choice when affordable. In that respect, hierarchical methods based on low-rank compression have allowed a drastic reduction of the computational requirements for the solution of dense linear systems over the last two decades. For sparse linear systems, their application remains a challenge which has been studied by both the community of hierarchical matrices and the community of sparse matrices. On the one hand, the first step taken by the community of hierarchical matrices most often takes advantage of the sparsity of the problem through the use of nested dissection. While this approach benefits from the hierarchical structure, it is not, however, as efficient as sparse solvers regarding the exploitation of zeros and the structural separation of zeros from non-zeros. On the other hand, sparse factorization is organized so as to lead to a sequence of smaller dense operations, enticing sparse solvers to use this property and exploit compression techniques from hierarchical methods in order to reduce the computational cost of these elementary operations. Nonetheless, the globally hierarchical structure may be lost if the compression of hierarchical methods is used only locally on dense submatrices. In [1], we have reviewed the main techniques that have been employed by both those communities, trying to highlight their common properties and their respective limits with a special emphasis on studies that have aimed to bridge the gap between them. With these observations in mind, we have proposed a class of hierarchical algorithms based on the symbolic analysis of the structure of the factors of a sparse matrix. These algorithms rely on a symbolic information to cluster and construct a hierarchical structure coherent with the non-zero pattern of the matrix. Moreover, the resulting hierarchical matrix relies on low-rank compression for the reduction of the memory consumption of large submatrices as well as the time to solution of the solver. We have also compared multiple ordering techniques based on geometrical or topological properties. Finally, we have opened the discussion to a coupling between the Finite Element Method and the Boundary Element Method in a unified computational framework.

7.5.2.4. Design of a coupled MUMPS - $\mathcal{H}$-Matrix solver for FEM-BEM applications

In that approach, the FEM matrix is eliminated by computing a Schur complement using MUMPS. Given the size of the BEM matrix, this can not be done in one operation, so it is done block by block, and added in the $\mathcal{H}$-matrix, which is then factorized to complete the process. The overall process yields an interesting boost in performance when compared to the previously existing approach that coupled MUMPS with a classical dense solver. However, a full comparison with all the other existing methods must still be performed (full $\mathcal{H}$-matrix solver with [22] or without nested dissection, iterative approaches, etc.).

7.5.2.5. Metabarcoding

Distance Geometry Problem (DGP) and Nonlinear Mapping (NLM) are two well established questions: DGP is about finding a Euclidean realization of an incomplete set of distances in a Euclidean space, whereas Nonlinear Mapping is a weighted Least Square Scaling (LSS) method. We show how all these methods (LSS, NLM, DGP) can be assembled in a common framework, being each identified as an instance of an optimization problem with a choice of a weight matrix. In [6], we studied the continuity between the solutions (which are point clouds) when the weight matrix varies, and the compactness of the set of solutions (after centering). We finally studied a numerical example, showing that solving the optimization problem is far from being simple and that the numerical solution for a given procedure may be trapped in a local minimum.

We are involved in the ADT Gordon ((partners: TADAAM (coordinator), STORM, HIEPACS, PLEIADE). The objectives of this ADT is to scale our slolver stack on a PLEIADE dimensioning metabarcoding application (multidimensional scaling method). Our goal is to be able to handle a problem leading to a distance matrix around 100 million individuals. Our contribution concerns the the scalability of the multidimensional scaling method and more particulary the random projection methods to speed up the SVD solver. Experiments son PlaFRIM and MCIA CURTA plateforms have allowed us to show that the solver stack was able to solve efficiently a large problem up to 300,000 individuals in less than 10 minutes on 25 nodes. This has highlighted that for these problem sizes the management of I/O, inputs and outputs with the disks, becomes critical and dominates calculation times.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. HPC-Ecosystem

Participants: Emmanuel Agullo, Olivier Beaumont, Olivier Coulaud, Aurélien Esnard, Lionel Eyraud-Dubois, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Pierre Ramet, Guillaume Sylvand.

Grant: Regional council
Dates: 2018 – 2020
Partners: EPIs STORM, TADAAM from Inria Bordeaux Sud-Ouest, Airbus, CEA-CESTA, INRA
Overview:

Numerical simulation is today integrated in all cycles of scientific design and studies, whether academic or industrial, to predict or understand the behavior of complex phenomena often coupled or multi-physical. The quality of the prediction requires having precise and adapted models, but also to have computation algorithms efficiently implemented on computers with architectures in permanent evolution. Given the ever increasing size and sophistication of simulations implemented, the use of parallel computing on computers with up to several hundred thousand computing cores and consuming / generating massive volumes of data becomes unavoidable; this domain corresponds to what is now called High Performance Computing (HPC). On the other hand, the digitization of many processes and the proliferation of connected objects of all kinds generate ever-increasing volumes of data that contain multiple valuable information; these can only be highlighted through sophisticated treatments; we are talking about Big Data. The intrinsic complexity of these digital treatments requires a holistic approach with collaborations of multidisciplinary teams capable of mastering all the scientific skills required for each component of this chain of expertise.

To have a real impact on scientific progress and advances, these skills must include the efficient management of the massive number of compute nodes using programming paradigms with a high level of expressiveness, exploiting high-performance communications layers, effective management for intensive I / O, efficient scheduling mechanisms on platforms with a large number of computing units and massive I / O volumes, innovative and powerful numerical methods for analyzing volumes of data produced and efficient algorithms that can be integrated into applications representing recognized scientific challenges with high societal and economic impacts. The project we propose aims to consider each of these links in a consistent, coherent and consolidated way.

For this purpose, we propose to develop a unified Execution Support (SE) for large-scale numerical simulation and the processing of large volumes of data. We identified four Application Challenges (DA) identified by the Nouvelle-Aquitaine region that we propose to carry over this unified support. We will finally develop four Methodological Challenges (CM) to evaluate the impact of the project. This project will make a significant contribution to the emerging synergy on the convergence between two yet relatively distinct domains, namely High Performance Computing (HPC) and the processing, management of large masses of data (Big Data); this project is therefore clearly part of the emerging field of High Performance Data Analytics (HPDA).

8.2. National Initiatives

8.2.1. ANR

8.2.1.1. SASHIMI: Sparse Direct Solver using Hierarchical Matrices

Participants: Aurélien Esnard, Mathieu Faverge, Pierre Ramet.

Grant: ANR-18-CE46-0006
Dates: 2018 – 2022
Overview: Nowadays, the number of computational cores in supercomputers has grown largely to a few millions. However, the amount of memory available has not followed this trend, and the memory per core ratio is decreasing quickly with the advent of accelerators. To face this problem, the SaSHiMi project wants to tackle the memory consumption of linear solver libraries used by many major simulation applications by using low-rank compression techniques. In particular, the direct solvers which offer the most robust solution to strategy but suffer from their memory cost. The project will especially investigate the super-nodal approaches for which low-rank compression techniques have been less studied despite the attraction of their large parallelism and their lower memory cost than for the multi-frontal approaches. The results will be integrated in the PaStiX solver that supports distributed and heterogeneous architectures.

8.2.1.2. SOLHARIS: SOLvers for Heterogeneous Architectures over Runtime systems, Investigating Scalability

Participants: Emmanuel Agullo, Olivier Beaumont, Mathieu Faverge, Lionel Eyraud-Dubois, Abdou Guermouche, Pierre Ramet, Guillaume Sylvand.

Grant: ANR-19-CE46-0009
Dates: 2019 – 2023
Overview: The SOLHARIS project aims at addressing the issues related to the development of fast and scalable linear solvers for large-scale, heterogeneous supercomputers. Because of the complexity and heterogeneity of the targeted algorithms and platforms, this project intends to rely on modern runtime systems to achieve high performance, programmability and portability. By gathering experts in computational linear algebra, scheduling algorithms and runtimes, SOLHARIS intends to tackle these issues through a considerable research effort for the development of numerical algorithms and scheduling methods that are better suited to the characteristics of large scale, heterogeneous systems and for the improvement and extension of runtime systems with novel features that more accurately fulfill the requirements of these methods. This is expected to lead to fundamental research results and software of great interest for researchers of the scientific computing community.

8.2.2. FUI

8.2.2.1. ICARUS: Intensive Calculation for AeRo and automotive engines Unsteady Simulations

Participants: Cyril Bordage, Aurélien Esnard.

Grant: FUI-22
Dates: 2016-2020
Partners: SAFRAN, SIEMENS, IFPEN, ONERA, DISTENE, CENAERO, GDTECH, Inria, CORIA, CERFACS.
Overview: Large Eddy Simulation (LES) is an increasingly attractive unsteady modelling approach for modelling reactive turbulent flows due to the constant development of massively parallel supercomputers. It can provide open and robust design tools that allow access to new concepts (technological breakthroughs) or a global consideration of a structure (currently processed locally). The mastery of this method is therefore a major competitive lever for industry. However, it is currently constrained by its access and implementation costs in an industrial context. The ICARUS project aims to significantly reduce them (costs and deadlines) by bringing together major industrial and research players to work on the entire high-fidelity LES computing process by:

- increasing the performance of existing reference tools (for 3D codes: AVBP, Yales2, ARGO) both in the field of code coupling and code/machine matching;
- developing methodologies and networking tools for the LES;
- adapting the ergonomics of these tools to the industrial world: interfaces, data management, code interoperability and integrated chains;
- validating this work on existing demonstrators, representative of the aeronautics and automotive industries.

8.2.3. Inria Project Labs

8.2.3.1. IPL HPC BigData

The goal of the HPC-BigData IPL is to gather teams from the HPC, Big Data and Machine Learning (ML) areas to work at the intersection between these domains. HPC and Big Data evolved with their own infrastructures (supercomputers versus clouds), applications (scientific simulations versus data analytics) and software tools (MPI and OpenMP versus Map/Reduce or Deep Learning frameworks). But Big Data analytics is becoming more compute-intensive (thanks to deep learning), while data handling is becoming a major concern for scientific computing. Within the IPL, we are in particular involved in a tight collaboration with Zenith Team (Montpellier) on how to parallelize and how to deal with memory issues in the context of the training phase of Pl@ntnet (https://www.plantnet.org). Alexis Joly (Zenith) co supervises with Olivier Beaumont the PhD Thesis of Alena Shilova.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. EoCoE-II

Title: Energy oriented Centre of Excellence for computer applications

Program: H2020

Duration: January 2019 - December 2021

Coordinator: CEA

Partners:

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)

Commissariat A L Energie Atomique et Aux Energies Alternatives (France)

Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique (France)

Consiglio Nazionale Delle Ricerche (Italy)

The Cyprus Institute (Cyprus)

Agenzia Nazionale Per le Nuove Tecnologie, l'energia E Lo Sviluppo Economico Sostenibile (Italy)

Fraunhofer Gesellschaft Zur Forderung Der Angewandten Forschung Ev (Germany)

Instytut Chemii Bioorganicznej Polskiej Akademii Nauk (Poland)

Forschungszentrum Julich (Germany)

Max Planck Gesellschaft Zur Foerderung Der Wissenschaften E.V. (Germany)

University of Bath (United Kingdom)

Universite Libre de Bruxelles (Belgium)

Universita Degli Studi di Trento (Italy)

Inria contact: Bruno Raffin

The Energy-oriented Centre of Excellence (EoCoE) applies cutting-edge computational methods in its mission to accelerate the transition to the production, storage and management of clean, decarbonized energy. EoCoE is anchored in the High Performance Computing (HPC) community and targets research institutes, key commercial players and SMEs who develop and enable energy-relevant numerical models to be run on exascale supercomputers, demonstrating their benefits for low carbon energy technology. The present project will draw on a successful proof-of-principle phase of EoCoE-I, where a large set of diverse computer applications from four such energy domains achieved significant efficiency gains thanks to its multidisciplinary expertise in applied mathematics and supercomputing. During this 2nd round, EoCoE-II will channel its efforts into 5 scientific Exascale challenges in the low-carbon sectors of Energy Meteorology, Materials, Water, Wind and Fusion. This multidisciplinary effort will harness innovations in computer science and mathematical algorithms within a tightly integrated co-design approach to overcome performance bottlenecks and to anticipate future HPC hardware developments. A world-class consortium of 18 complementary partners from 7 countries will form a unique network of expertise in energy science, scientific computing and HPC, including 3 leading European supercomputing centres. New modeling capabilities in selected energy sectors will be created at unprecedented scale, demonstrating the potential benefits to the energy industry, such as accelerated design of storage devices, high-resolution probabilistic wind and solar forecasting for the power grid and quantitative understanding of plasma core-edge interactions in ITER-scale tokamaks. These flagship applications will provide a high-visibility platform for high-performance computational energy science, cross-fertilized through close working connections to the EERA and EUROfusion consortia.

8.3.1.2. PRACE 6IP

Title: PRACE Sixth Implementation Phase (PRACE-6IP) project

Duration: May 2019 - December 2021

Partners: see the following url

Inria contact: Luc Giraud

PRACE, the Partnership for Advanced Computing is the permanent pan-European High Performance Computing service providing world-class systems for world-class science. Systems at the highest performance level (Tier-0) are deployed by Germany, France, Italy, Spain and Switzerland, providing researchers with more than 17 billion core hours of compute time. HPC experts from 25 member states enabled users from academia and industry to ascertain leadership and remain competitive in the Global Race. Currently PRACE is finalizing the transition to PRACE 2, the successor of the initial five year period. The objectives of PRACE-6IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. These include: assisting the development of PRACE 2; strengthening the internationally recognised PRACE brand; continuing and extend advanced training which so far provided more than 36 400 person·training days; preparing strategies and best practices towards Exascale computing, work on forward-looking SW solutions; coordinating and enhancing the operation of the multi-tier HPC systems and services; and supporting users to exploit massively parallel systems and novel architectures. A high level Service Catalogue is provided. The proven project structure will be used to achieve each of the objectives in 7 dedicated work packages. The activities are designed to increase Europe's research and innovation potential especially through: seamless and efficient Tier-0 services and a pan-European HPC ecosystem including national capabilities; promoting take-up by industry and new communities and special offers to SMEs; assistance to PRACE 2 development; proposing strategies for deployment of leadership systems; collaborating with the ETP4HPC, CoEs and other European and international organisations on future architectures, training, application support and policies. This will be monitored through a set of KPIs.

8.3.1.3. EOSC-Pillar

Title: Coordination and Harmonisation of National and Thematic Initiatives to support EOSC

Duration: 2019 - 2023

Partners: see the following url

Inria contact: Stefano Zacchiroli

The project aims to support the coordination and harmonization of national initiatives relevant to EOSC in Europe and investigate the option for them to interfederate at a later stage, help integrating initiatives and data/cloud providers through the development of common policies and tools, and facilitate user communities in adopting and using these services and propose new ones born from their scientific domain. To this end, the project will integrate a bottom-up approach (by voicing the requirements and needs expressed by the different scientific communities operating at the national level) and a top-down one (by harmonising the national strategies and translating them in a viable work plan). In the longer term, this is expected to facilitate the design and adoption of common policies and streamline the process of joining EOSC for service providers and user communities while helping populating the EOSC with useful services of wider European interest, based on the real needs and interests of the European scientific communities. In order to maximise this simplification process, the project will collaborate with related regional and thematic initiatives.

8.3.1.4. EXDCI-2

Title: European Extreme Data & Computing Initiative

Duration: 2010 - 2020

Partners: see the following url

Inria contact: Olivier Beaumont

Through the joint action of PRACE and ETP4HPC, EXDCI-2 mobilises the European HPC stakeholders. The project participates in the support of the European HPC Ecosystem with two main goals. First, the development and advocacy of a competitive European HPC Exascale Strategy by supporting the implementation of a common European HPC strategy, open to synergistic areas including High Performance Data Analytics (HPDA) and Artificial Intelligence (AI). Secondly, the coordination of the stakeholder community for European HPC at the Exascale through joint community structuring and synchronisation, such as (i) the development of relationships with other ecosystems including upstream technologies as Big Data (BDVA) (ii) in the context of the upcoming European Data Infrastructure (EDI) a road mapping activity toward future converged HPC, HPDA and AI needs and new services from PRACE users communities and CoE and (iii) the continuation of BDEC activities, for international participation of European stakeholders on the integration from edge computing to HPC, including Data Analytics and AI.

8.4. International Initiatives

8.4.1. Inria International Labs

There is an ongoing reasearch activity with Argonne National Laboratory in the framework of the JLESC International Lab, through a postdoc funded by the DPI, namely Nick Schenkels, who work on data compression techniques in Krylov methods for the solution of large linear systems. The objective is to use agnostic compressor developped at Argonne to compress the basis involved in Krylov methods that have a large memory footprint. The challange is to design algorithm that reduce the memory consumption, hence the energy, while preserving the numerical convergence of the numerical technique.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events: Organisation

9.1.1.1. Member of the Organizing Committees

SIAM PP'20, Seattle (O. Beaumont).

9.1.1.2. Chair of Conference Program Committees

COMPAS'19 Algorithm Track (E. Agullo) ICPP'19 Algorithm Track vice-chair (E. Agullo)

9.1.1.3. Member of the Conference Program Committees

AlgoCloud'19 (O. Beaumont), COMPAS'19 (O. Beaumont), EuroPar'20 (O. Beaumont), HiPC'19 (L. Giraud), HPML'19 (O. Beaumont), ICPP'19 (A. Guermouche), IPDPS'19 (L. Eyraud-Dubois, O. Beaumont), IPDPS Workshops'19 (O. Beaumont), ISC'20 Workshops (E. Agullo), PDSEC'19 (O. Coulaud, M. Faverge, L. Giraud), IEEE PDP'19 (J. Roman), SC'19 (E. Agullo), SPAA'19 (O. Beaumont).

9.1.2. Journal

9.1.2.1. Member of the Editorial Boards

- O. Beaumont is Associate Editor in Chief for the Journal of Parallel and Distributed Computing (Elsevier).
- L. Giraud is member of the editorial board of the SIAM Journal on Scientific Computing (SISC) and SIAM Journal on Matrix Analysis and Applications (SIMAX).

9.1.2.2. Reviewer - Reviewing Activities

The members of the HiePACS project have performed reviewing for the following list of journals: Computing and Fluid, International Journal of Antennas and Propagation, Parallel Computing, SIAM J. Matrix Analysis and Applications, SIAM J. Scientific Computing, Journal of Parallel and Distributed Computing, IEEE Transactions on Parallel and Distributed Systems, IEEE Access, Concurrency and Computation: Practice and Experience, ACM Transactions on Mathematical Software, ACM Computational and Mathematical Methods, International Journal of High Performance Computing Applications, Journal Of Computational Science.

The members of the HIEPACS project have performed reviewing for the following list of conferences (additionally to PC): Europar'19, IPDPS'19, SC'18, STACS'20, SPAA'19, SC'19.

9.1.3. Invited Talks

- L. Giraud, "Dealing with unreliable computing platforms at extreme scale" invited MOX Seminars (Laboratory for Modeling and Scientific Computing MOX), Politecnico di Milano, January 23, in conjunction with the ESCAPE2 workshop on fault tolerant algorithms and resilient approaches.

9.1.4. Scientific Expertise

- Olivier Beaumont acted as expert for 2019 FET Open Evaluation Committee
- Luc Giraud is member of the board on Modelization, Simulation and data analysis of the Competitiveness Cluster for Aeronautics, Space and Embedded Systems.
- Pierre Ramet is Scientific Advisor at the CEA-DAM CESTA.
- 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 French Working Group for EuroHPC, and of the Technical Group of GENCI.

9.1.5. Research Administration

- Emmanuel Agullo and Luc Giraud are the scientific correspondents of the European and International partnership for Inria Bordeaux Sud-Ouest.
- Olivier Coulaud is the scientific manager of the PLAFRIM platform for Inria Bordeaux Sud-Ouest.
- Jean Roman is a member of the Direction for Science at Inria : he was until the end of December 2019 the Deputy Scientific Director of the Inria research domain entitled *Applied Mathematics, Computation and Simulation* and was in charge at the national level of the Inria activities concerning High Performance Computing.
- Until July 2019, Olivier Beaumont was the vice-head of Inria Evaluation Commission.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Undergraduate level/Licence

- A. Esnard: System programming 36h, Computer architecture 40h, Network 23h, C programming 35h at Bordeaux University. He is also responsible for the second year of the computer science degree (L2 Informatique), which involves managing about 200 students each year.
- M. Faverge: Programming environment 26h, Numerical algorithmic 40h, C projects 25h at Bordeaux INP (ENSEIRB-MatMeca).
- A. Guermouche: System programming 36h at Bordeaux University.
- P. Ramet: System programming 24h, Databases 32h, Object programming 48h, Distributed programming 32h, Cryptography 32h, Introduction to AI Deep Learning and Data Analytics 16h at Bordeaux University.

Post graduate level/Master

- E. Agullo: Operating systems 24h at Bordeaux University ; Dense linear algebra kernels 8h, Numerical algorithms 30h at Bordeaux INP (ENSEIRB-MatMeca).
- O. Coulaud: Paradigms for parallel computing 8h, Introduction to Tensor methods 4h at Bordeaux INP (ENSEIRB-MatMeca).

- A. Esnard: Network management 27h, Network security 27h at Bordeaux University; Programming distributed applications 35h at Bordeaux INP (ENSEIRB-MatMeca).
- L. Eyraud-Dubois and Olivier Beaumont: Approximation and BigData 24h at Bordeaux University.
- M. Faverge: System programming 72h, Linear Algebra for high Performance Computing 13h at Bordeaux INP (ENSEIRB-MatMeca).
  He is also in charge of the master 2 internship for the Computer Science department at Bordeaux INP (ENSEIRB-MatMeca). Starting in September, he is in charge with Raymond Namyst of the High Performance Computing - High Performance Data Analytics option at ENSEIRB-MatMeca. This is a common training curriculum between the Computer Science and MatMeca departments at Bordeaux INP and with Bordeaux University in the context of the Computer Science Research Master.
- Alena Shilova and Olivier Beaumont: Deep Learning Frameworks, at Bordeaux INP (ENSEIRB-MatMeca), 20h.
- Olivier Beaumont, Sketching and Streaming Algorithms, ENS Lyon, 8h
- L. Giraud: Introduction to intensive computing and related programming tools 30h, INSA Toulouse; On mathematical tools for numerical simulations 10h, ENSEEIHT Toulouse.
- A. Guermouche: Network management 92h, Network security 64h, Operating system 24h at Bordeaux University.
- P. Ramet: Load balancing and scheduling 13h and Numerical algorithmic 40h at Bordeaux INP (ENSEIRB-Matmeca).

High School teachers

- A. Esnard, M. Faverge, and A. Guermouche participated to the training of the High School teachers (DIU Enseigner l'Informatique au Lycée) in computer science for the new computer science program starting in September 2019.

9.2.2. Supervision

- PhD Aurélien Falco; Data sparse calculation in Bridging the gap between $\mathcal{H}$-matrices and sparse direct methods for the solution of large linear systems; E. Agullo, L. Girau, G. Sylvand; defended on June 24, 2019; jury members: E. Ng (Lawrence Berkeley National Laboratory), S. Le Borne (Technische Universitat Hamburg), D. LLvadoux (ONERA) F. Alouges (Ecole Polytechnique), G. Pont (Airbus Group).
- PhD in progress: Tobias Castanet; Replication algorithms for multi-player virtual worlds; started Sep. 2019; O. Beaumont, N. Hanusse (LaBRI), C. Travers (Bordeaux INP - LaBRI).
- PhD in progress: Marek Felsoci; Fast solvers for high-frequency aeroacoustics; G. Sylvand, E. Agullo.
- PhD in progress: Martina Iannacito; Linear solvers in tensorial format for high dimensional problems; started Oct 2019; O. Coulaud, L. Giraud.
- PhD in progress: Esragul Korkmaz; Sparse linear solver and hierachical matrices; started Nov. 2018; M. Faverge, P. Ramet.
- PhD in progress: Romain Peressoni; Fast multidimensional scaling method for the study of biodiversity; started Oct 2019; E. Agullo, O. Coulaud, A. Franc (PLEIADE)
- PhD in progress: Alena Shilova; Scheduling for deep learning applications; started Oct. 2018; L. Eyraud-Dubois, O. Beaumont.
- PhD in progress: Nicolas Venkovic; Domain decomposition techniques for the solution of stochastics elliptic PDEs; started Nov. 2018; L. Giraud, P. Mycek (CERFACS).
- PhD in progress: Mathieu Vérité; Static allocation algorithms for scheduling High-Performance applications; started Sept. 2019; L. Eyraud-Dubois, O. Beaumont.

- PhD in progress: Yanfei Xiang; Solution of large linear systems with massive numbers of right-hand sides. Started Nov. 2019; L. Giraud, P. Mycek (CERFACS).

9.2.3. Juries

- Mohammad Issa, “Modélisation asymptotique et discrétisation des composants magnétiques dans les problèmes de courant de Foucault.", referees: R. V. Sabariego, S. Clénet, members: O. Coulaud, Y. Kefevren, R. Perrussel, J-R. Poirier, L. Krähenbül. Université Toulouse 3 Paul Sabatier, spécialité: électromagnétisme et Systèmes Haute Fréquence, 30 November 2019.
- Raphaël Prat, “Equilibrage dynamique de charge sur supercalculateur exaflopique appliqué à la dynamique moléculaire", referees: C. Calvin, J.F. Mehaut, reviewers: M. Baader, L. Colombet, P. Fortin, R. Namyst, J. Roman, CEA - Maison de la Simulation et Université de Bordeaux, spécialité: informatique, 9 October 2019.
- Mohamad El Sayah, "Random Generation for the Performance Evaluation of Scheduling Algorithms," referees: Olivier Beaumont and Arnaud Legrand, reviewers: Jean-Marc Nicod, Fany Dufosse, Pierre-Cyrille Heam, University of Besancon, 20 November 2019.

9.3. Popularization

9.3.1. Interventions

- Olivier Beaumont spoke to a class of high school students on algorithms (routing algorithms in particular) as part of the digital week organized by the BIJ (Bureau Information Jeunesse) of the City of La Teste de Buch.

10. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] A. FALCO. *Combler l’écart entre H-Matrices et méthodes directes creuses pour la résolution de systèmes linéaires de grandes tailles*, Université de Bordeaux, June 2019, https://tel.archives-ouvertes.fr/tel-02183902

Articles in International Peer-Reviewed Journals

[2] E. AGULLO, L. GIRAUD, A. GOBÉ, M. KUHN, S. LANTERI, L. MOYA. *High order HDG method and domain decomposition solvers for frequency-domain electromagnetics*, in "International Journal of Numerical Modelling: Electronic Networks, Devices and Fields", October 2019 [*DOI :* 10.1002/JNM.2678], https://hal.inria.fr/hal-02327982

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[8] E. Agullo, L. Giraud, S. Lanteri, G. Marait, A.-C. Orgerie, L. Poirel. *Energy Analysis of a Solver Stack for Frequency-Domain Electromagnetics*, in "PDP 2019 - 27th Euromicro International Conference on Parallel, Distributed and Network-Based Processing", Pavia, Italy, 2019 27th Euromicro International Conference on Parallel, Distributed and Network-Based Processing (PDP), IEEE, February 2019, pp. 385-391 [*DOI :* 10.1109/EMPDP.2019.8671555], https://hal.archives-ouvertes.fr/hal-02191331

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[11] S. Kumar, L. Eyraud-Dubois, S. Krishnamoorthy. *Performance Models for Data Transfers: A Case Study with Molecular Chemistry Kernels*, in "ICPP 2019 - 48th International Conference on Parallel Processing", Kyoto, Japan, August 2019 [*DOI :* 10.1145/3337821.3337921], https://hal.inria.fr/hal-02431877

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