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Sorbonne Université (UPMC)

Activity Report 2019

Project-Team ALPINES

Algorithms and parallel tools for integrated
numerical simulations

IN COLLABORATION WITH: Laboratoire Jacques-Louis Lions (LJLL)

RESEARCH CENTER
Paris

THEME
**Distributed and High Performance
Computing**

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Project-Team ALPINES

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Computer Science and Digital Science:

- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.4. - Multiscale modeling
- A6.1.5. - Multiphysics modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.2.5. - Numerical Linear Algebra
- A6.2.7. - High performance computing
- A6.3. - Computation-data interaction
- A6.3.1. - Inverse problems
- A7.1. - Algorithms

Other Research Topics and Application Domains:

- B3.3.1. - Earth and subsoil
- B9.5.2. - Mathematics
- B9.5.3. - Physics

1. Team, Visitors, External Collaborators

Research Scientists

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- Frédéric Nataf [CNRS, Senior Researcher, HDR]

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2. Overall Objectives

2.1. Introduction

The focus of our research is on the development of novel parallel numerical algorithms and tools appropriate for state-of-the-art mathematical models used in complex scientific applications, and in particular numerical simulations. The proposed research program is by nature multi-disciplinary, interweaving aspects of applied mathematics, computer science, as well as those of several specific applications, as porous media flows, elasticity, wave propagation in multi-scale media and inverse problems.

Our first objective is to develop numerical methods and tools for complex scientific and industrial applications, that will enhance their scalable execution on the emergent heterogeneous hierarchical models of massively parallel machines. Our second objective is to integrate the novel numerical algorithms into a middle-layer that will hide as much as possible the complexity of massively parallel machines from the users of these machines.

3. Research Program

3.1. Overview

The research described here is directly relevant to several steps of the numerical simulation chain. Given a numerical simulation that was expressed as a set of differential equations, our research focuses on mesh generation methods for parallel computation, novel numerical algorithms for linear algebra, as well as algorithms and tools for their efficient and scalable implementation on high performance computers. The validation and the exploitation of the results is performed with collaborators from applications and is based on the usage of existing tools. In summary, the topics studied in our group are the following:

- Numerical methods and algorithms
 - Mesh generation for parallel computation
 - Solvers for numerical linear algebra
 - * Domain decomposition methods
 - * Preconditioning for iterative methods
 - Computational kernels for numerical linear algebra
 - Tensor computations
- Validation on numerical simulations and other numerical applications

3.2. Domain specific language - parallel FreeFem++

In the engineering, researchers, and teachers communities, there is a strong demand for simulation frameworks that are simple to install and use, efficient, sustainable, and that solve efficiently and accurately complex problems for which there are no dedicated tools or codes available. In our group we develop FreeFem++ (see <https://www.freefem.org/>), a user dedicated language for solving PDEs. The goal of FreeFem++ is not to be a substitute for complex numerical codes, but rather to provide an efficient and relatively generic tool for:

- getting a quick answer to a specific problem,
- prototyping the resolution of a new complex problem.

The current users of FreeFem++ are mathematicians, engineers, university professors, and students. In general for these users the installation of public libraries as MPI, MUMPS, Ipopt, Blas, lapack, OpenGL, fftw, scotch, PETSc, SLEPc is a very difficult problem. For this reason, the authors of FreeFem++ have created a user friendly language, and over years have enriched its capabilities and provided tools for compiling FreeFem++ such that the users do not need to have special knowledge of computer science. This leads to an important work on porting the software on different emerging architectures.

Today, the main components of parallel FreeFem++ are:

1. definition of a coarse grid,
2. splitting of the coarse grid,
3. mesh generation of all subdomains of the coarse grid, and construction of parallel data structures for vectors and sparse matrices from the mesh of the subdomain,
4. call to a linear solver,
5. analysis of the result.

All these components are parallel, except for point (5) which is not in the focus of our research. However for the moment, the parallel mesh generation algorithm is very simple and not sufficient, for example it addresses only polygonal geometries. Having a better parallel mesh generation algorithm is one of the goals of our project. In addition, in the current version of FreeFem++, the parallelism is not hidden from the user, it is done through direct calls to MPI. Our goal is also to hide all the MPI calls in the specific language part of FreeFem++. In addition to these in-house domain decomposition methods, FreeFem++ is also linked to PETSc solvers which enables an easy use of third parties parallel multigrid methods.

3.3. Solvers for numerical linear algebra

Iterative methods are widely used in industrial applications, and preconditioning is the most important research subject here. Our research considers domain decomposition methods and iterative methods and its goal is to develop solvers that are suitable for parallelism and that exploit the fact that the matrices are arising from the discretization of a system of PDEs on unstructured grids.

One of the main challenges that we address is the lack of robustness and scalability of existing methods as incomplete LU factorizations or Schwarz-based approaches, for which the number of iterations increases significantly with the problem size or with the number of processors. This is often due to the presence of several low frequency modes that hinder the convergence of the iterative method. To address this problem, we study different approaches for dealing with the low frequency modes as coarse space correction in domain decomposition or deflation techniques.

We also focus on developing boundary integral equation methods that would be adapted to the simulation of wave propagation in complex physical situations, and that would lend themselves to the use of parallel architectures. The final objective is to bring the state of the art on boundary integral equations closer to contemporary industrial needs. From this perspective, we investigate domain decomposition strategies in conjunction with boundary element method as well as acceleration techniques (H-matrices, FMM and the like) that would appear relevant in multi-material and/or multi-domain configurations. Our work on this topic also includes numerical implementation on large scale problems, which appears as a challenge due to the peculiarities of boundary integral equations.

3.4. Computational kernels for numerical linear and multilinear algebra

The design of new numerical methods that are robust and that have well proven convergence properties is one of the challenges addressed in Alpines. Another important challenge is the design of parallel algorithms for the novel numerical methods and the underlying building blocks from numerical linear algebra. The goal is to enable their efficient execution on a diverse set of node architectures and their scaling to emerging high-performance clusters with an increasing number of nodes.

Increased communication cost is one of the main challenges in high performance computing that we address in our research by investigating algorithms that minimize communication, as communication avoiding algorithms. We propose to integrate the minimization of communication into the algorithmic design of numerical linear algebra problems. This is different from previous approaches where the communication problem was addressed as a scheduling or as a tuning problem. The communication avoiding algorithmic design is an approach originally developed in our group since 2007 (initially in collaboration with researchers from UC Berkeley and CU Denver). While at mid term we focus on reducing communication in numerical linear algebra, at long term we aim at considering the communication problem one level higher, during the parallel mesh generation tool described earlier.

Our research also focuses on solving problems of large size that feature high dimensions as in molecular simulations. The data in this case is represented by objects called tensors, or multilinear arrays. The goal is to design novel tensor techniques to allow their effective compression, i.e. their representation by simpler objects in small dimensions, while controlling the loss of information. The algorithms are aiming to being highly parallel to allow to deal with the large number of dimensions and large data sets, while preserving the required information for obtaining the solution of the problem.

4. Application Domains

4.1. Compositional multiphase Darcy flow in heterogeneous porous media

We study the simulation of compositional multiphase flow in porous media with different types of applications, and we focus in particular on reservoir/bassin modeling, and geological CO₂ underground storage. All these simulations are linearized using Newton approach, and at each time step and each Newton step, a linear system needs to be solved, which is the most expensive part of the simulation. This application leads to some of the difficult problems to be solved by iterative methods. This is because the linear systems arising in multiphase porous media flow simulations cumulate many difficulties. These systems are non-symmetric, involve several unknowns of different nature per grid cell, display strong or very strong heterogeneities and anisotropies, and change during the simulation. Many researchers focus on these simulations, and many innovative techniques for solving linear systems have been introduced while studying these simulations, as for example the nested factorization [Appleyard and Cheshire, 1983, SPE Symposium on Reservoir Simulation].

4.2. Inverse problems

We focus on methods related to the blend of time reversal techniques and absorbing boundary conditions (ABC) used in a non standard way. Since the seminal paper by [M. Fink et al., Imaging through inhomogeneous media using time reversal mirrors. *Ultrasonic Imaging*, 13(2):199, 1991.], time reversal is a subject of very active research. The principle is to back-propagate signals to the sources that emitted them. The initial experiment was to refocus, very precisely, a recorded signal after passing through a barrier consisting of randomly distributed metal rods. In [de Rosny and Fink. Overcoming the diffraction limit in wave physics using a time-reversal mirror and a novel acoustic sink. *Phys. Rev. Lett.*, 89 (12), 2002], the source that created the signal is time reversed in order to have a perfect time reversal experiment. In [39], we improve this result from a numerical point of view by showing that it can be done numerically without knowing the source. This is done at the expense of not being able to recover the signal in the vicinity of the source. In [40], time dependent wave splitting is performed using ABC and time reversal techniques. We now work on extending these methods to non uniform media.

All our numerical simulations are performed in FreeFem++ which is very flexible. As a byproduct, it enables us to have an end user point of view with respect to FreeFem++ which is very useful for improving it.

4.3. Numerical methods for wave propagation in multi-scale media

We are interested in the development of fast numerical methods for the simulation of electromagnetic waves in multi-scale situations where the geometry of the medium of propagation may be described through characteristic lengths that are, in some places, much smaller than the average wavelength. In this context, we propose to develop numerical algorithms that rely on simplified models obtained by means of asymptotic analysis applied to the problem under consideration.

Here we focus on situations involving boundary layers and *localized* singular perturbation problems where wave propagation takes place in media whose geometry or material characteristics are submitted to a small scale perturbation localized around a point, or a surface, or a line, but not distributed over a volumic sub-region of the propagation medium. Although a huge literature is already available for the study of localized singular perturbations and boundary layer phenomena, very few works have proposed efficient numerical methods that rely on asymptotic modeling. This is due to their functional framework that naturally involves singular functions, which are difficult to handle numerically. The aim of this part of our research is to develop and analyze numerical methods for singular perturbation methods that are prone to high order numerical approximation, and robust with respect to the small parameter characterizing the singular perturbation.

4.4. Data analysis in astrophysics

We focus on computationally intensive numerical algorithms arising in the data analysis of current and forthcoming Cosmic Microwave Background (CMB) experiments in astrophysics. This application is studied in collaboration with researchers from University Paris Diderot, and the objective is to make available the algorithms to the astrophysics community, so that they can be used in large experiments.

In CMB data analysis, astrophysicists produce and analyze multi-frequency 2D images of the universe when it was 5% of its current age. The new generation of the CMB experiments observes the sky with thousands of detectors over many years, producing overwhelmingly large and complex data sets, which nearly double every year therefore following Moore's Law. Planck (<http://planck.esa.int/>) is a keystone satellite mission which has been developed under auspices of the European Space Agency (ESA). Planck has been surveying the sky since 2010, produces terabytes of data and requires 100 Petaflops per image analysis of the universe. It is predicted that future experiments will collect on the order of petabyte of data around 2025. This shows that data analysis in this area, as many other applications, will keep pushing the limit of available supercomputing power for the years to come.

4.5. Molecular simulations

Molecular simulation is one of the most dynamic areas of scientific computing. Its field of application is very broad, ranging from theoretical chemistry and drug design to materials science and nanotechnology. It provides many challenging problems to mathematicians and computer scientists.

In the context of the ERC Synergy Grant EMC2 we address several important limitations of state of the art molecular simulation. In particular, the simulation of very large molecular systems, or smaller systems in which electrons interact strongly with each other, remains out of reach today. In an interdisciplinary collaboration between chemists, mathematicians and computer scientists, we focus on developing a new generation of reliable molecular simulation algorithms and software.

5. Highlights of the Year

5.1. Highlights of the Year

- HPDDM software is now available through PETSc PCHPDDM routine, for details see [the routine](#). Both Geno and its multilevel extension presented in [32] are available.
- ERC Synergy EMC2 project [kick off meeting](#) took place in September 2019, at Sorbonne University.

6. New Software and Platforms

6.1. FreeFem++

FreeFem++

SCIENTIFIC DESCRIPTION: FreeFem++ is a partial differential equation solver. It has its own language. freefem scripts can solve multiphysics non linear systems in 2D and 3D.

Problems involving PDE (2d, 3d) from several branches of physics such as fluid-structure interactions require interpolations of data on several meshes and their manipulation within one program. FreeFem++ includes a fast 2d-tree-based interpolation algorithm and a language for the manipulation of data on multiple meshes (as a follow up of bang (now a part of FreeFem++)).

FreeFem++ is written in C++ and the FreeFem++ language is a C++ idiom. It runs on Macs, Windows, Unix machines. FreeFem++ replaces the older freefem and freefem+.

FUNCTIONAL DESCRIPTION: FreeFem++ is a PDE (partial differential equation) solver based on a flexible language that allows a large number of problems to be expressed (elasticity, fluids, etc) with different finite element approximations on different meshes.

- Partner: UPMC
- Contact: Frederic Hecht
- URL: <http://www.freefem.org/ff++/>

6.2. HPDDM

SCIENTIFIC DESCRIPTION: HPDDM is an efficient implementation of various domain decomposition methods (DDM) such as one- and two-level Restricted Additive Schwarz methods, the Finite Element Tearing and Interconnecting (FETI) method, and the Balancing Domain Decomposition (BDD) method. This code has been proven to be efficient for solving various elliptic problems such as scalar diffusion equations, the system of linear elasticity, but also frequency domain problems like the Helmholtz equation. A comparison with modern multigrid methods can be found in the thesis of Pierre Jolivet.

FUNCTIONAL DESCRIPTION: HPDDM is an efficient implementation of various domain decomposition methods (DDM) such as one- and two-level Restricted Additive Schwarz methods, the Finite Element Tearing and Interconnecting (FETI) method, and the Balancing Domain Decomposition (BDD) method.

- Participants: Frédéric Nataf and Pierre Jolivet
- Contact: Pierre Jolivet
- URL: <https://github.com/hpddm>

6.3. LORASC

LORASC preconditioner

KEYWORD: Preconditioner

- Participants: Laura Grigori and Rémi Lacroix
- Contact: Laura Grigori

6.4. Platforms

6.4.1. preAlps

KEYWORD: Preconditioned enlarged Krylov subspace methods

FUNCTIONAL DESCRIPTION: Contains enlarged Conjugate Gradient Krylov subspace method and Lorasc preconditioner.

- Partners: Inria
- Contact: Simplice Donfack, Laura Grigori, Olivier Tissot
- URL: <https://github.com/NLAFET/preAlps>

6.4.2. BemTool

KEYWORD: Boundary Element Method

FUNCTIONAL DESCRIPTION: BemTool is a C++ header-only library implementing the boundary element method for the discretisation of the Laplace, Helmholtz and Maxwell equations, in 2D and 3D. Its main purpose is the assembly of classic boundary element matrices, which can be compressed and inverted through its interface with HTOOL.

- Partners: UPMC - ANR NonlocalDD
- Contact: Xavier Claeys
- URL: <https://github.com/xclaeys/BemTool>

6.4.3. HTool

KEYWORD: Hierarchical Matrices

FUNCTIONAL DESCRIPTION: HTOOL is a C++ header-only library implementing compression techniques (e.g. Adaptive Cross Approximation) using hierarchical matrices. The library uses MPI and OpenMP for parallelism, and is interfaced with HPDDM for the solution of linear systems.

- Partners: CNRS - UPMC - ANR NonlocalDD
- Contact: Pierre Marchand
- URL: <https://github.com/PierreMarchand20/htool>

7. New Results

7.1. Adaptive Domain Decomposition Method for Saddle Point Problem

In [37], we introduce an adaptive domain decomposition (DD) method for solving saddle point problems defined as a block two by two matrix. The algorithm does not require any knowledge of the constrained space. We assume that all sub matrices are sparse and that the diagonal blocks are the sum of positive semi definite matrices. The latter assumption enables the design of adaptive coarse space for DD methods.

7.2. A Class of Efficient Locally Constructed Preconditioners Based on Coarse Spaces

In [24] we present a class of robust and fully algebraic two-level preconditioners for SPD matrices. We introduce the notion of algebraic local SPSD splitting of an SPD matrix and we give a characterization of this splitting. It helps construct *algebraically and locally* a class of efficient coarse subspaces which bound the spectral condition number of the preconditioned system by a number defined a priori. Some PDEs-dependant preconditioners correspond to a special case of the splitting. The examples of the algebraic coarse subspaces in this paper are not practical due to expensive construction. We propose an heuristic approximation that is not costly. Numerical experiments illustrate the efficiency of the proposed method.

7.3. A Multilevel Schwarz Preconditioner Based on a Hierarchy of Robust Coarse Spaces

In [32] we present a multilevel preconditioner for SPD matrices. Robust two-level additive Schwarz preconditioners guarantee a fast convergence of the Krylov method. To maintain the robustness each subdomain contributes a small number of vectors to construct a basis for the second level (the coarse space). As long as the dimension of the coarse space is reasonable i.e., direct solvers can be used efficiently, the two-level method scales well. However, the bottleneck arises when factoring the coarse space matrix becomes costly. Using an iterative Krylov method on the second level might be the right choice. Nevertheless, the condition number of the coarse space matrix is typically larger than the one of the first level. One of the difficulties of using two-level methods to solve the coarse problem is that the matrix does not arise from a PDE anymore. We introduce in this paper a practical method of applying a multilevel additive Schwarz preconditioner efficiently. This multilevel preconditioner is implemented in HPDDM and the code for reproducing the results from the paper is available [here](#).

7.4. Inverse scattering problems without knowing the source term

The solution of inverse scattering problems always presupposed knowledge of the incident wave-field and require repeated computations of the forward problem, for which knowing the source term is crucial. In [26], we present a three-step strategy to solve inverse scattering problems when the time signature of the source is unknown. The proposed strategy combines three recent techniques: (i) wave splitting to retrieve the incident and the scattered wavefields, (ii) time-reversed absorbing conditions (TRAC) for redatuming the data inside the computational domain, (iii) adaptive eigenspace inversion (AEI) to solve the inverse problem. Numerical results illustrate step-by-step the feasibility of the proposed strategy.

7.5. Envelope following methods

One difficulty when solving problems in plasma physics is the behaviour at several scales in time and space of the solutions of equations. For example, central equations in this domain of application are highly oscillatory in time. The multiscale aspect makes the models difficult to tackle when we aim at avoiding a high computational cost. A solution to this problem is to solve the models by designing adapted numerical methods with a low computational cost and which are able to deal efficiently with rapid and slow scales in time. In this direction, we worked on envelope following methods, which have been efficiently applied in the community of oscillators in RF circuits. The method has (at least) two variants: in a first place, it is based on the concept of using extra variables to represent the changing rapid period and the cumulative effect of changing periods and then, use of Newton iterations allows to find these unknowns. In a second place, we adopt a similar strategy except that the rapid period is not an extra variable but a direct outcome of the numerical integration by the use of the Poincaré map. We implemented and tested both approaches for equations of interest in plasma physics and we observed that these methods didn't perform accurate results.

7.6. Domain decomposition preconditioning for high frequency wave propagation problems

The work about domain decomposition preconditioning for Maxwell equations has been published in [21]. It studies two-level preconditioners where the coarse space is based on the discretisation of the PDE on a coarse mesh. The PDE is discretised using finite-element methods of fixed, arbitrary order. The theoretical part of this work is the Maxwell analogue of a previous work for Helmholtz equation, and shows that for Maxwell problems with absorption, if the absorption is large enough and if the subdomain and coarse mesh diameters are chosen appropriately, then classical two-level overlapping Additive Schwarz Domain Decomposition preconditioning performs optimally – in the sense that GMRES converges in a wavenumber-independent number of iterations. The theory is also illustrated by various numerical experiments.

Ongoing studies are being conducted on recursive one-level optimized Schwarz methods for the high frequency Helmholtz and Maxwell equations. The method consists in solving the subdomain problems in a one-level optimized Schwarz preconditioner only approximately, using inner GMRES iterations preconditioned again by a one-level method, with smaller subdomains. The asymptotic behaviour and parallel scalability of the method are being investigated. Exhaustive numerical experiments are being conducted to compare the efficiency of this method with two-level preconditioners, including cavity problems and benchmarks in seismic imaging.

7.7. The boundary element method in FreeFEM

The BemTool and HTOOL libraries developed by the team, implementing respectively the Boundary Element Method and Hierarchical Matrices, have been interfaced with FreeFEM to allow FreeFEM users to use the Boundary Element Method (BEM) in their FreeFEM scripts. New additions to the Domain Specific Language (DSL) of FreeFEM allows the user to define and manipulate curved (1D) and surface (2D) meshes, as well as define and solve BEM variational problems in a high-level manner, similarly to FEM problems. The parallelization of the HTOOL library allows the user to assemble and solve their BEM problems in parallel in a transparent way.

Ongoing work consists in finalizing the BEM DSL to propose complete and documented features to the FreeFEM user in the next release, as well as investigating FEM-BEM coupling.

7.8. New Optimised Schwarz Method for dealing with cross-points

We consider a scalar wave propagation in harmonic regime modelled by Helmholtz equation with heterogeneous coefficients. Using the Multi-Trace Formalism (MTF), we propose a new variant of the Optimized Schwarz Method (OSM) that can accommodate the presence of cross-points in the subdomain partition. This leads to the derivation of a strongly coercive formulation of our Helmholtz problem posed on the union of all interfaces. The corresponding operator takes the form "identity + contraction".

7.9. Two-level preconditioning for h-version boundary element approximation of hypersingular operator with GenEO

We consider symmetric positive definite operators stemming from boundary integral equation (BIE), and we analysed a two-level preconditioner where the coarse space is built using local generalized eigenproblems in the overlap. We will refer to this coarse space as the GenEO coarse space. We obtained bounds on the condition number of the preconditioned system. In this work package, we also performed large scale numerical experiments for testing the scalability of our approach. We relied on parallel implementation of our algorithm.

7.10. Adaptive resolution of linear systems based on a posteriori error estimators

In [18] we discuss a new adaptive approach for iterative solution of sparse linear systems arising from partial differential equations (PDEs) with self-adjoint operators. The idea is to use the a posteriori estimated local distribution of the algebraic error in order to steer and guide the solve process in such way that the algebraic error is reduced more efficiently in the consecutive iterations. We first explain the motivation behind the proposed procedure and show that it can be equivalently formulated as constructing a special combination of preconditioner and initial guess for the original system. We present several numerical experiments in order to identify when the adaptive procedure can be of practical use.

7.11. Adaptive hierarchical subtensor partitioning for tensor compression

In [33] a numerical method is proposed to compress a tensor by constructing a piece-wise tensor approximation. This is defined by partitioning a tensor into sub-tensors and by computing a low-rank tensor approximation (in a given format) in each sub-tensor. Neither the partition nor the ranks are fixed a priori, but, instead, are obtained in order to fulfill a prescribed accuracy and optimize, to some extent, the storage. The different steps of the method are detailed and some numerical experiments are proposed to assess its performances.

7.12. Frictionless contact problem for hyper-elastic materials with interior point optimizer

In [35] we present a method to solve the mechanical problems undergoing finite deformations and the unilateral contact problems without friction for hyperelastic materials. We apply it to an industrial application: contact between a mechanical gasket and an obstacle. The main idea is to formulate the contact problem into an optimization one, in order to use the Interior Point OPTimizer (IPOPT) to solve it. Finally, the FreeFEM software is used to compute and solve the contact problem. Our method is validated against several benchmarks and used on an industrial application example.

7.13. A posteriori error estimates for Darcy's problem coupled with the heat equation

In [25] we derive a posteriori error estimates, in two and three dimensions, for the heat equation coupled with Darcy's law by a nonlinear viscosity depending on the temperature. We introduce two variational formulations and discretize them by finite element methods. We prove optimal a posteriori errors with two types of computable error indicators. The first one is linked to the linearization and the second one to the discretization. Then we prove upper and lower error bounds under regularity assumptions on the solutions. Finally, numerical computations are performed to show the effectiveness of the error indicators.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Contract with IFPEN, February 2016 - April 2019, that funds the Phd thesis of Zakariae Jorti on adaptive preconditioners using a posteriori error estimators. Supervisor L. Grigori.
- Contract with IFPEN, October 2016 - October 2019, that funds the Phd thesis of Julien Coulet on the virtual element method (VEM). Supervisor F. Nataf and V. Girault.

9. Partnerships and Cooperations

9.1. Regional Initiatives

GIS, Géosciences franciliennes: scientific collaboration network between ten public institutions from the Paris (Ile-de-France) region, focused on natural resources and environment. The project-team Alpines is a member.

9.2. National Initiatives

9.2.1. ANR

9.2.1.1. B3DCMB

ANR Decembre 2017 - Novembre 2021 This project is in the area of data analysis of cosmological data sets as collected by contemporary and forthcoming observatories. This is one of the most dynamic areas of modern cosmology. Our special target are data sets of Cosmic Microwave Background (CMB) anisotropies, measurements of which have been one of the most fruitful of cosmological probes. CMB photons are remnants of the very early evolution of the Universe and carry information about its physical state at the time when the Universe was much younger, hotter and denser, and simpler to model mathematically. The CMB has been, and continue to be, a unique source of information for modern cosmology and fundamental physics. The main objective of this project is to empower the CMB data analysis with novel high performance tools and algorithms superior to those available today and which are capable of overcoming the existing performance gap. Partners: AstroParticules et Cosmologie Paris 7 (PI R. Stompor), ENSAE Paris Saclay.

9.2.1.2. ANR Cine-Para

October 2015 - September 2019, Laura Grigori is Principal Coordinator for Inria Paris. Funding for Inria Paris is 145 Keuros. The funding for Inria is to combine Krylov subspace methods with parallel in time methods. Partners: University Pierre and Marie Curie, J. L. Lions Laboratory (PI Y. Maday), CEA, Paris Dauphine University, Paris 13 University.

9.2.1.3. Non-local DD

ANR appel à projet générique October 2015 - September 2020

This project in scientific computing aims at developing new domain decomposition methods for massively parallel simulation of electromagnetic waves in harmonic regime. The specificity of the approach that we propose lies in the use of integral operators not only for solutions local to each subdomain, but for coupling subdomains as well. The novelty of this project consists, on the one hand, in exploiting multi-trace formalism for domain decomposition and, on the other hand, considering optimized Schwarz methods relying on Robin type transmission conditions involving quasi-local integral operators.

9.2.1.4. Soil μ -3D

ANR appel à projet générique October 2015 - april 2019

In spite of decades of work on the modeling of greenhouse gas emission such as CO₂ and N₂O and on the feedback effects of temperature and water content on soil carbon and nitrogen transformations, there is no agreement on how these processes should be described, and models are widely conflicting in their predictions. Models need improvements to obtain more accurate and robust predictions, especially in the context of climate change, which will affect soil moisture regime.

The goal of this new project is now to go further using the models developed in MEPSOM to upscale heterogeneities identified at the scale of microbial habitats and to produce macroscopic factors for biogeochemical models running at the field scale.

To achieve this aim, it will be necessary to work at different scales: the micro-scale of pores (μm) where the microbial habitats are localized, the meso-scale of cores at which laboratory measurements on CO₂ and N₂O fluxes can be performed, and the macro-scale of the soil profile at which outputs are expected to predict greenhouse gas emission. The aims of the project are to (i) develop new descriptors of the micro-scale 3D soil architecture that explain the fluxes measured at the macro-scale, (ii) Improve the performance of our 3D pore scale models to simulate both micro-and meso- scales at the same time. Upscaling methods like "homogeneization" would help to simulate centimeter samples which cannot be achieved now. The reduction of the computational time used to solve the diffusion equations and increase the number of computational units, (iii) develop new macro-functions describing the soil micro-heterogeneity and integrate these features into the field scale models.

9.2.1.5. Muffin

ANR appel à projet générique 2019.

S. Hirstoaga and P.-H. Tournier are members of the project MUFFIN, whose objective is to explore and optimize original computational scenarios for multi-scale and high dimensional transport codes, with priority applications in plasma physics. Several approximation methods are planned to be developed. It is at the frontier of computing and numerical analysis and intends to reduce the computational burden in the context of intensive calculation. Principal Investigator: B. Després (Sorbonne University).

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. NLAFFET (197)

Title: Parallel Numerical Linear Algebra for Future Extreme-Scale Systems

Programm: H2020

Duration: November 2015 - April 2019

Coordinator: UMEÅ Universitet

Partners:

Science and Technology Facilities Council (United Kingdom)

Computer Science Department, UmeåUniversitet (Sweden)

Mathematics Department, The University of Manchester (United Kingdom)

Inria, Alpines group

Inria contact: Laura Grigori

The NLAFFET proposal is a direct response to the demands for new mathematical and algorithmic approaches for applications on extreme scale systems, as identified in the FETHPC work programme and call. This project will enable a radical improvement in the performance and scalability of a wide range of real-world applications relying on linear algebra software, by developing novel architecture-aware algorithms and software libraries, and the supporting runtime capabilities to achieve scalable performance and resilience on heterogeneous architectures. The focus is on a critical set of fundamental linear algebra operations including direct and iterative solvers for dense and sparse linear systems of equations and eigenvalue problems. Achieving this requires a co-design effort due to the characteristics and overwhelming complexity and immense scale of such systems. Recognized experts in algorithm design and theory, parallelism, and auto-tuning will work together to explore and negotiate the necessary tradeoffs. The main research objectives are: (i) development of novel algorithms that expose as much parallelism as possible, exploit heterogeneity, avoid communication bottlenecks, respond to escalating fault rates, and help meet emerging power constraints; (ii) exploration of advanced scheduling strategies and runtime systems focusing on the extreme scale and strong scalability in multi/many-core and hybrid environments; (iii) design and evaluation of novel strategies and software support for both offline and online auto-tuning. The validation and dissemination of results will be done by integrating new software solutions into challenging scientific applications in materials science, power systems, study of energy solutions, and data analysis in astrophysics. The deliverables also include a sustainable set of methods and tools for cross-cutting issues such as scheduling, auto-tuning, and algorithm-based fault tolerance packaged into open-source library modules.

9.3.1.2. ERC Synergy grant EMC2

Title: Extreme-scale Mathematically-based Computational Chemistry (EMC2)

Programm: ERC

Duration: September 2019 - August 2025

PIs: E. Cancès (ENPC), L. Grigori (Inria), Y. Maday (Sorbonne University), J. P. Piquemal (Sorbonne University)

Molecular simulation is one of the most dynamic areas of scientific computing. Its field of application is very broad, ranging from theoretical chemistry and drug design to materials science and nanotechnology. Its importance in modern science has been acknowledged by two Nobel Prizes (Kohn & Pople in 1998; Karplus, Levitt & Warshel in 2013). It is also a gold mine of exciting problems for mathematicians and computer scientists.

Molecular simulation can be used as a virtual microscope to study more or less complex molecules with atomic-scale space-time resolution. It can also be used as a tool for computer-aided design (CAD) and the engineering of new molecules, materials and nano-devices.

However, molecular simulation still has important limitations. In particular, the simulation of very large molecular systems, or smaller systems in which electrons interact strongly with each other, remains out of reach today. Overcoming these limitations is extremely difficult. This requires joint breakthroughs in several disciplines, and can, in our opinion, only be achieved through an intensive multidisciplinary effort such as those made possible by ERC-Synergy-type funding.

Our objective is to overcome some of the current limitations in this field and to provide academic communities and industrial companies with new generation, dramatically faster and quantitatively reliable molecular simulation software, to enable those communities to address major technological and societal challenges of the 21st century (in health, energy, and the environment, for example).

9.4. International Initiatives

9.4.1. Inria International Partners

9.4.1.1. Informal International Partners

- J. Demmel, UC Berkeley, USA
- M. Grote, Université de Bâle, Suisse
- F. Assous, Israel
- K.-M. Perfekt, Reading, UK
- T. Chacon, Seville, Spain

9.5. International Research Visitors

9.5.1. Visits to International Teams

9.5.1.1. Research Stays Abroad

- Visit of Laura Grigori to the group of J. Demmel at U.C. Berkeley, july-august 2019.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. General Chair, Scientific Chair

- Organization of the kick-off meeting of ERC Synergy project EMC2 by E. Cancès, L. Grigori, Y. Maday, and J. P. Piquemal. For more details see the [website](#).
- Organization of Horizon Maths 2019 day on Mathematics and Chemistry by E. Cancès, L. Grigori, Y. Maday, and J. P. Piquemal, december 3 2019. For more details see the [website](#).

10.1.2. Scientific Events: Selection

- Gene Golub Summer school on **High Performance Data Analytics**, June 17-28, 2019 in Aussois, France. Co-organized by L. Grigori with M. Knepley, O. Schenk, R. Vuduc. Sponsored by SIAM through an endowment from the estate of Gene Golub.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Laura Grigori, March 2014 – current. Member of the editorial board for the SIAM book series Software, Environments and Tools. See <http://bookstore.siam.org/software-environments-and-tools/>.
- Laura Grigori, January 2016 – current. Associate Editor, SIAM Journal on Scientific Computing.
- Laura Grigori, January 2017 – current. Associate Editor, SIAM Journal on Matrix Analysis and Applications.
- Laura Grigori, January 2016 – current. Editorial board, Numerical linear algebra with applications Journal, Wiley.
- Laura Grigori, October 2019 – current. Editorial board, Calcolo Journal, Springer.
- Frédéric Nataf, January 2015 – current, Editorial board, Journal of Numerical Mathematics, de Gruyter.

10.1.4. Invited Talks

- Laura Grigori was
 - Invited speaker, Advanced Solvers for modern Architectures Symposium, November 2019, Munster Germany.
 - Keynote speaker, workshop *Parallel solution methods for systems arising from PDEs*, September 2019, CIRM France.
 - Invited plenary speaker, SIAM Conference on Computational Science and Engineering (CSE19), February 2019, Washington USA, <http://www.siam.org/meetings/cse19/>.
- S. Hirstoaga gave a talk at the seminar of Laboratoire Jacques-Louis Lions, March 2019, Paris.
- Frédéric Nataf was invited speaker at RMR 2019: Rencontres Mathématiques de Rouen 2019, juin 2019, Rouen, France.
- Frédéric Hecht was
 - invited speaker at HPCSE 2019: HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING, University of Ostrava, Czech.
 - invited speaker at RMR 2019: Rencontres Mathématiques de Rouen 2019, juin 2019, Rouen, France.
 - invited speaker at COUPLED 2019: june 2019, Sigtes, Spain.
 - invited speaker, workshop *Parallel solution methods for systems arising from PDEs*, September 2019, CIRM France.

10.1.5. Leadership within the Scientific Community

- Laura Grigori, member elected of SIAM Council, January 2018 - December 2020, the committee supervising the scientific activities of SIAM. Nominated by a Committee and elected by the members of SIAM.
- Laura Grigori, member of the **PRACE** (Partnership for Advanced Computing in Europe) Scientific Steering Committee, September 2016 - current.
- Laura Grigori and Frédéric Hecht are coordinators of the High Performance in Scientific Computing Major of second year of Mathematics and Applications Master, Sorbonne University.

10.1.6. Scientific Expertise

- Laura Grigori: November 2015 - current, expert to the Scientific Commission of IFPEN (French Petroleum Institute). Evaluation of research programs, PhD theses, work representing a total of 5 days per year.

10.1.7. Research Administration

- Laura Grigori was vice-president of the committee CE46 of ANR, September 2017 - July 2019.
- Frédéric Nataf was president of the committee "Mathématiques et leurs interactions" (CE40) at ANR, September 2016 - August 2019.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master 1: Xavier Claeys, Initiation to C++, 36 hrs of programming tutorials in C++, SU.

Master 1: Xavier Claeys, Computational Linear Algebra, 32 hrs of lectures, SU.

Master 1: Xavier Claeys, Approximation of PDEs, 24 hrs of programming tutorials in Python, SU.

Master 2: Laura Grigori, Winter 2019, Participation in the course on High Performance Computing given at Sorbonne University, Computer Science, intervention for 8 hours per year.

Master 2: Laura Grigori, Course on *High performance computing for numerical methods and data analysis*, https://who.rocq.inria.fr/Laura.Grigori/TeachingDocs/UPMC_Master2/HPC_MN_DA.html, Master 2nd year, Mathematics & Applications, Sorbonne University, 24 hours per year.

Licence 1: S. Hirstoaga, analysis and matrix calculus, 24 HETD, INSEP, Sorbonne University.

Master 1: Frédéric Hecht, Initiation au C++, 24hrs, SU, France

Master 2: Frédéric Hecht, Des EDP à leur résolution par la méthode des éléments finis (MEF), 36hrs, M2, SU, France

Master 2: Frédéric Hecht, Numerical methods for fluid mechanics, 10hrs, SU, France

Master 2: Frédéric Hecht, Calcul scientifique 3 / projet industriel FreeFem++, 28hrs, M2, SU, France

Master 2: Frédéric Hecht, Ingénierie 1 / Logiciel pour la simulation (FreeFem++), 21hrs, SU, France

Master 2: Frédéric Hecht, Ingénierie 2 / Projet collaboratif, 21hrs, SU, France

Cours CIMPA: Frédéric Hecht, Modélisation, Analyse mathématique et calcul scientifique dans la gestion des déchets ménagers, 12h, Kenitra, Maroc

Master 2: Frédéric Nataf, Course on Domain Decomposition Methods, Sorbonne University.

10.2.2. Supervision

PhD: Sebastien Cayrols, Minimizing communication for incomplete factorizations and low-rank approximations on large scale computers, Sorbonne Université, February 2019, advisor Laura Grigori.

PhD: Zakariae Jorti, Fast solution of sparse linear systems with adaptive choice of preconditioners, Sorbonne University, September 2019, advisor Laura Grigori.

PhD: Olivier Tissot, Solving linear systems on massively parallel architectures, Sorbonne University, January 2019, advisor Laura Grigori.

PhD: Julien Coulet, Sorbonne University, Méthode des Eléments Virtuels pour le calcul de la déformation mécanique couplée aux écoulements en milieux poreux, October 2019, advisors Frédéric Nataf, Vivette Girault (SU), Isabelle Faille (IFPEN) and Nicolas Guy (IFPEN).

PhD: Rim El Dbaissy, Sorbonne University, Discrétisation du problème de couplage instationnaire des équations de Navier- Stokes avec l'équation de la chaleur, Mars 2019, advisors Tony Sayah, Frédéric Hecht.

PhD in progress: Matthias Beaupere, since October 2019 (funded by ERC Synergy EMC2), advisor Laura Grigori.

PhD in progress: Igor Chollet, since October 2017 (funded by ICSD), advisors Xavier Claeys, Pierre Fortin, Laura Grigori.

PhD in progress: Thibault Cimic, since October 2017 (funded by ANR B3DCMB), advisor Laura Grigori.

PhD in progress: Pierre Marchand, since October 2016 (funded by ANR NonLocalDD project), advisors Xavier Claeys and Frédéric Nataf.

PhD in progress: Thanh Van Nguyen, since November 2017 (funded by ANR CinePara), advisor Laura Grigori.

PhD in progress: Jeremy Weisman, since October 2019 (funded by ERC Synergy EMC2), advisors Laura Grigori and J. P. Piquemal.

PhD in progress: Houssam Houssein, since January 2018 (CIFRE, funded by Airthium), advisor Frédéric Hecht.

10.2.3. *Juries*

- Xavier Claeys was reviewer and member of the jury for the PhD thesis of Federica CAFORIO, defended at Université Paris-Saclay, on January the 24th 2019.
- Xavier Claeys was member of the jury for the PhD thesis of Yohannes Tjandrawidjaja, defended at Université Paris-Saclay on December the 17th 2019.
- Laura Grigori was a member of the jury of Phd defense of Oleg Balabanov, September 2019.
- Laura Grigori was president of the jury of the HDR habilitation of Sever Hirstoaga, Université de Strasbourg, April 2019.
- Laura Grigori was a member of the jury of HDR habilitation of Stéphanie Chaillat, Examineur, ENSTA, March 2019.
- Laura Grigori was a member of the jury of Phd defense of Fabio Verbosio, USI Lugano, February 2019.
- Frédéric Hecht was president of the HDR defense of Mourad Ismail, 2019, LIPhy, Université Grenoble Alpes.
- Frédéric Hecht was president of the PhD defense of Alexandre This, 2019, Sorbonne University.
- Frédéric Hecht was president of the PhD defense of Zakariae Jorti, 2019, Sorbonne University.
- Frédéric Hecht was president of the PhD defense of Sebastien Cayrols, 2019, Sorbonne University.
- Frédéric Nataf was president of the PhD defense of Rim ALDBAISSY, 2019, Sorbonne University.

10.3. Popularization

10.3.1. *Internal or external Inria responsibilities*

- Laura Grigori was vice-president of the Evaluation Commission of Inria, March 2018 - August 2019.

11. Bibliography

Major publications by the team in recent years

- [1] X. CLAEYS. *Essential spectrum of local multi-trace boundary integral operators*, in "IMA J. Appl. Math.", 2016, vol. 81, n^o 6, pp. 961–983, <https://doi-org.accesdistant.sorbonne-universite.fr/10.1093/imamat/hxw019>

- [2] X. CLAEYS, R. HIPTMAIR. *Integral equations for electromagnetic scattering at multi-screens*, in "Integral Equations Operator Theory", 2016, vol. 84, n^o 1, pp. 33–68, <https://doi-org.accesdistant.sorbonne-universite.fr/10.1007/s00020-015-2242-5>
- [3] X. CLAEYS, R. HIPTMAIR, E. SPINDLER. *Second kind boundary integral equation for multi-subdomain diffusion problems*, in "Adv. Comput. Math.", 2017, vol. 43, n^o 5, pp. 1075–1101, <https://doi-org.accesdistant.sorbonne-universite.fr/10.1007/s10444-017-9517-0>
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- [6] L. GRIGORI, J. W. DEMMEL, H. XIANG. *CALU: a communication optimal LU factorization algorithm*, in "SIAM Journal on Matrix Analysis and Applications", 2011, vol. 32, pp. 1317-1350
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- [8] R. HAFERSSAS, P. JOLIVET, F. NATAF. *An Additive Schwarz Method Type Theory for Lions's Algorithm and a Symmetrized Optimized Restricted Additive Schwarz Method*, in "SIAM J. Sci. Comput.", 2017, vol. 39, n^o 4, pp. A1345–A1365, <http://dx.doi.org/10.1137/16M1060066>
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- [10] P. JOLIVET, F. NATAF. *HPDDM: High-Performance Unified framework for Domain Decomposition methods, MPI-C++ library*, 2014, <https://github.com/hpddm/hpddm>
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Doctoral Dissertations and Habilitation Theses

- [12] R. ALDBAISSY. *Scalable domain decomposition preconditioner for Navier-Stokes equations coupled with the heat equation*, Sorbonne Université / Université Pierre et Marie Curie - Paris VI ; Université Saint-Joseph (Beyrouth), March 2019, <https://hal.archives-ouvertes.fr/tel-02458872>
- [13] S. CAYROLS. *Minimizing communication for incomplete factorizations and low-rank approximations on large scale computers*, Sorbonne Universites, UPMC University of Paris 6, February 2019, <https://tel.archives-ouvertes.fr/tel-02437769>
- [14] J. COULET. *Coupling Virtual Element Methods and finite volume schemes for computational geomechanics*, Sorbonne-Université, November 2019, <https://tel.archives-ouvertes.fr/tel-02416511>

- [15] S. A. HIRSTOAGA. *Design and performant implementation of numerical methods for multiscale problems in plasma physics*, Université de Strasbourg, IRMA UMR 7501, April 2019, Habilitation à diriger des recherches, <https://tel.archives-ouvertes.fr/tel-02081304>
- [16] Z. JORTI. *Fast solution of sparse linear systems with adaptive choice of preconditioners*, Sorbonne Université / Université Pierre et Marie Curie - Paris VI, October 2019, <https://tel.archives-ouvertes.fr/tel-02425679>
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- [18] A. ANCIAUX-SEDRAKIAN, L. GRIGORI, Z. JORTI, J. PAPEŽ, S. YOUSEF. *Adaptive solution of linear systems of equations based on a posteriori error estimators*, in "Numerical Algorithms", May 2019 [DOI : 10.1007/s11075-019-00757-z], <https://hal.inria.fr/hal-02425391>
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- [25] S. DIB, V. GIRAULT, F. HECHT, T. SAYAH. *A posteriori error estimates for Darcy's problem coupled with the heat equation*, in "ESAIM: Mathematical Modelling and Numerical Analysis", June 2019, vol. 53, n^o 6, pp. 2121 - 2159 [DOI : 10.1051/M2AN/2019049], <https://hal.archives-ouvertes.fr/hal-02427095>
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- [31] L. EYRAUD-DUBOIS, S. KUMAR. *Analysis of a List Scheduling Algorithm for Task Graphs on Two Types of Resources*, in "IPDPS 2020 - 34th IEEE International Parallel and Distributed Processing Symposium", New Orleans, United States, May 2020, <https://hal.inria.fr/hal-02431810>

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- [32] H. AL DAAS, L. GRIGORI, P. JOLIVET, P.-H. TOURNIER. *A Multilevel Schwarz Preconditioner Based on a Hierarchy of Robust Coarse Spaces*, June 2019, working paper or preprint, <https://hal.archives-ouvertes.fr/hal-02151184>
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