Activity Report 2015

Project-Team ALPINENES

Algorithms and parallel tools for integrated numerical simulations

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

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6.2.1. - Numerical analysis of PDE and ODE
6.2.5. - Numerical Linear Algebra
6.2.7. - High performance computing
7.1. - Parallel and distributed algorithms

Other Research Topics and Application Domains:
3.3.1. - Earth and subsoil
9.4.2. - Mathematics
9.4.3. - Physics

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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.

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 will be performed with collaborators from applications and it will be 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
  - Computational kernels for numerical linear algebra
- Validation on numerical simulations

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 http://www.freefem.org/ff++), 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, 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++.

### 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 direction preserving solvers in the context of multilevel domain decomposition methods with adaptive coarse spaces and multilevel incomplete decompositions. A judicious choice for the directions to be preserved through filtering or low rank approximations allows us to alleviate the effect of low frequency modes on the convergence.

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, which includes devising adapted domain decomposition approaches. The final objective is to bring the state of the art on boundary integral equations closer to contemporary industrial needs.

### 3.4. Computational kernels for numerical linear 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.
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

The research of F. Nataf on inverse problems is rather new since this activity was started from scratch in 2007. Since then, several papers were published in international journals and conference proceedings. All our numerical simulations were performed in FreeFem++. We focus on methods related to time reversal techniques. 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 main idea is to take advantage of the reversibility of wave propagation phenomena such as it occurs in acoustics, elasticity or electromagnetism in a non-dissipative unknown medium to back-propagate signals to the sources that emitted them. Number of industrial applications have already been developed: touchscreen, medical imaging, non-destructive testing and underwater communications. 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. Since then, numerous applications of this physical principle have been designed, see [Fink, Renversement du temps, ondes et innovation. Ed. Fayard, 2009] or for numerical experiments [Larmat et al., Time-reversal imaging of seismic sources and application to the great sumatra earthquake. Geophys. Res. Lett., 33, 2006] and references therein.

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 natural functional framework that naturally involves singular functions, which are difficult 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 half petabyte of data, and will require 100 Exaflops per analysis as early as in 2020. 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.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. FreeFem++

We have released a version of FreeFem++ (v 3.42) which introduces new and important features related to high performance computing:

- improved interface,
- improved interface with PETSc library,
- improved interface with HPDDM (see above).

This release enables, for the first time, end-users to run the very same code on computers ranging from laptops to clusters and even large scale computers with thousands of computing nodes.

5.1.2. Invited talk Supercomputing 2015

Laura Grigori was an Invited speaker at the ACM/IEEE Supercomputing’15, International Conference for High Performance Computing, Networking, Storage, and Analysis, Austin, November 2015, http://sc15.supercalculing.org/schedule/event_detail?evid=inv103. This is the major conference of high performance computing, attended by 12,000 people. A blog can be found at http://sc15blog.blogspot.com/2015/10/sc15-invited-talk-dr-laura-grigori.html.

5.1.3. SIAM Lecture Note book

Frédéric Nataf, with V. Dolean and P. Jolivet, published a SIAM lecture note book on domain decomposition methods. The four draft versions on HAL https://hal.archives-ouvertes.fr/cel-01100932 were downloaded more than 2 300 times.

5.1.4. SIAM SIAG on Supercomputing

Laura Grigori was elected the Chair of the SIAM SIAG on Supercomputing (SIAM special interest group on supercomputing) for the period of January 2016 - December 2017. She was nominated by a Committee and elected by the members of this SIAG.

6. New Software and Platforms

6.1. FreeFem++

FeeFrem++
**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 bamg (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. HPDDDM

**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: Pierre Jolivet and Frédéric Nataf
- Contact: Pierre Jolivet and Frédéric Nataf
- URL: https://github.com/hpddm

### 6.3. DPREPack

**Keyword:** Large scale

**Functional Description**

This library solves linear systems on parallel computers from PCs based on multicore processors to large scale computers. It implements recent parallel algorithms issued from domain decomposition methods and parallel approximate factorizations.

- Partners: CNRS - UPMC
- Contact: Laura Grigori
- URL: https://team.inria.fr/alpines/

Submodules:

- Sparse Toolbox
**KEYWORDS:** Preconditioner - Interactive method - Linear system
- Participants: Laura Grigori and Rémi Lacroix
- Contact: Laura Grigori
- not yet publicly available

- **Block Filtering Decomposition preconditioner**
  **KEYWORDS:** Preconditioner - Linear system

**FUNCTIONAL DESCRIPTION**
Iterative methods are used in many industrial and academic applications to solve large sparse linear systems of equations, and preconditioning these methods is often necessary to accelerate their convergence. Several highly used preconditioners as incomplete LU factorizations are known to have scalability problems, often due to the presence of several low frequency modes that hinder the convergence of the iterative method. To address this problem, we work on filtering preconditioners. A judicious choice of the filtering vector allows to alleviate the effect of low frequency modes, and can accelerate significantly the convergence of the iterative method.
- Participants: Laura Grigori, Rémi Lacroix and Frédéric Nataf
- Partners: CNRS - UPMC
- Contact: Laura Grigori
- not yet publicly available

- **LORASC preconditioner**
  **KEYWORD:** Preconditioner

- Participants: Laura Grigori and Rémi Lacroix
- Contact: Laura Grigori
- URL: not yet publicly available

- **NFF Nested Filtering Factorization**
  **KEYWORDS:** Preconditioner - Interactive method - Linear system

- Participants: Laura Grigori, Frédéric Nataf and Long Qu
- Partners: UPMC - Université Paris-Sud
- Contact: Laura Grigori
- not yet publicly available

7. New Results

7.1. Communication avoiding algorithms for dense linear algebra

Our group continues to work on algorithms for dense linear algebra operations that minimize communication. During this year we focused on improving the performance of communication avoiding QR factorization as well as designing algorithms for computing rank revealing and low rank approximations of dense and sparse matrices.

In [2] we discuss the communication avoiding QR factorization of a dense matrix. The standard algorithm for computing the QR decomposition of a tall and skinny matrix (one with many more rows than columns) is often bottlenecked by communication costs. The algorithm which is implemented in LAPACK, ScaLAPACK, and Elemental is known as Householder QR. For tall and skinny matrices, the algorithm works column-by-column, computing a Householder vector and applying the corresponding transformation for each column in the matrix. When the matrix is distributed across a parallel machine, this requires one parallel reduction per column. The TSQR algorithm, on the other hand, performs only one reduction during the entire computation. Therefore, TSQR requires asymptotically less inter-processor synchronization than Householder QR on parallel machines (TSQR also achieves asymptotically higher cache reuse on sequential machines). However, TSQR produces a different representation of the orthogonal factor and therefore requires more software development to support the new representation. Further, implicitly applying the orthogonal factor to the trailing matrix in the context of factoring a square matrix is more complicated and costly than with the Householder representation.
We show how to perform TSQR and then reconstruct the Householder vector representation with the same asymptotic communication efficiency and little extra computational cost. We demonstrate the high performance and numerical stability of this algorithm both theoretically and empirically. The new Householder reconstruction algorithm allows us to design more efficient parallel QR algorithms, with significantly lower latency cost compared to Householder QR and lower bandwidth and latency costs compared with Communication-Avoiding QR (CAQR) algorithm. Experiments on supercomputers demonstrate the benefits of the communication cost improvements: in particular, our experiments show substantial improvements over tuned library implementations for tall-and-skinny matrices. We also provide algorithmic improvements to the Householder QR and CAQR algorithms, and we investigate several alternatives to the Householder reconstruction algorithm that sacrifice guarantees on numerical stability in some cases in order to obtain higher performance.

In [4] we introduce CARRQR, a communication avoiding rank revealing QR factorization with tournament pivoting. Revealing the rank of a matrix is an operation that appears in many important problems as least squares problems, low rank approximations, regularization, nonsymmetric eigenproblems. In practice the QR factorization with column pivoting often works well, and it is widely used even if it is known to fail, for example on the so-called Kahan matrix. However in terms of communication, the QR factorization with column pivoting is sub-optimal with respect to lower bounds on communication. If the algorithm is performed in parallel, then typically the matrix is distributed over \(P\) processors by using a two-dimensional block cyclic partitioning. This is indeed the approach used in the \texttt{psgeqpf} routine from ScaLAPACK. At each step of the decomposition, the QR factorization with column pivoting finds the column of maximum norm and permutes it to the leading position, and this requires exchanging \(O(n)\) messages, where \(n\) is the number of columns of the input matrix. For square matrices, when the memory per processor used is on the order of \(O(n^2/P)\), the lower bound on the number of messages to be exchanged is \(\Omega(\sqrt{P})\). The number of messages exchanged during the QR factorization with column pivoting is larger by at least a factor of \(n/\sqrt{P}\) than the lower bound.

In this paper we introduce CARRQR, a communication optimal (modulo polylogarithmic factors) rank revealing QR factorization based on tournament pivoting. The factorization is based on an algorithm that computes the decomposition by blocks of \(b\) columns (panels). For each panel, tournament pivoting proceeds in two steps. The first step aims at identifying a set of \(b\) candidate pivot columns that are as well-conditioned as possible. These columns are permuted to the leading positions, and they are used as pivots for the next \(b\) steps of the QR factorization. To identify the set of \(b\) candidate pivot columns, a tournament is performed based on a reduction operation, where at each node of the reduction tree \(b\) candidate columns are selected by using the strong rank revealing QR factorization. The idea of tournament pivoting has been first used to reduce communication in Gaussian elimination, an algorithm referred to as CALU.

We show that CARRQR reveals the numerical rank of a matrix in an analogous way to QR factorization with column pivoting (QRCP). Although the upper bound of a quantity involved in the characterization of a rank revealing factorization is worse for CARRQR than for QRCP, our numerical experiments on a set of challenging matrices show that this upper bound is very pessimistic, and CARRQR is an effective tool in revealing the rank in practical problems.

Our main motivation for introducing CARRQR is that it minimizes data transfer, modulo polylogarithmic factors, on both sequential and parallel machines, while previous factorizations as QRCP are communication sub-optimal and require asymptotically more communication than CARRQR. Hence CARRQR is expected to have a better performance on current and future computers, where communication is a major bottleneck that highly impacts the performance of an algorithm.

7.2. Algebraic preconditioners

Our work focused on the design of robust algebraic preconditioners and domain decomposition methods to accelerate the convergence of iterative methods.

In [5] we present a communication avoiding ILU0 preconditioner for solving large linear systems of equations by using iterative Krylov subspace methods. Recent research has focused on communication avoiding
Krylov subspace methods based on so called s-step methods. However there is no communication avoiding preconditioner yet, and this represents a serious limitation of these methods. Our preconditioner allows to perform \( s \) iterations of the iterative method with no communication, through ghosting some of the input data and performing redundant computation. It thus reduces data movement by a factor of \( 3s \) between different levels of the memory hierarchy in a serial computation and between different processors in a parallel computation. To avoid communication, an alternating reordering algorithm is introduced for structured and unstructured matrices, that requires the input matrix to be ordered by using a graph partitioning technique such as kway or nested dissection. We show that the reordering does not affect the convergence rate of the ILU0 preconditioned system as compared to kway or nested dissection ordering, while it reduces data movement and should improve the expected time needed for convergence. In addition to communication avoiding Krylov subspace methods, our preconditioner can be used with classical methods such as GMRES or s-step methods to reduce communication.

7.3. A robust coarse space for Optimized Schwarz methods SORAS-GenEO-2

Optimized Schwarz methods (OSM) are very popular methods which were introduced by P.L. Lions for elliptic problems and Després for propagative wave phenomena. In [18], we have built a coarse space for which the convergence rate of the two-level method is guaranteed regardless of the regularity of the coefficients. We do this by introducing a symmetrized variant of the ORAS (Optimized Restricted Additive Schwarz) algorithm and by identifying the problematic modes using two different generalized eigenvalue problems instead of only one as for the ASM (Additive Schwarz method), BDD (balancing domain decomposition) or FETI (finite element tearing and interconnection) methods.

7.4. Time-dependent wave splitting and source separation

Starting from classical absorbing boundary conditions, we propose, in [17], a method for the separation of time-dependent scattered wave fields due to multiple sources or obstacles. In contrast to previous techniques, our method is local in space and time, deterministic, and also avoids a priori assumptions on the frequency spectrum of the signal. Numerical examples in two space dimensions illustrate the usefulness of wave splitting for time-dependent scattering problems.

7.5. Boundary integral formulations of wave scattering

We have continued to develop and further analyze new boundary integral formulation for wave scattering by complex objects.

In [13] we considered acoustic scattering of time-harmonic waves at objects composed of several homogeneous parts. Some of those may be impenetrable, giving rise to Dirichlet boundary conditions on their surfaces. We started from the second-kind boundary integral approach of [X. Claeys, and R. Hiptmair, and E. Spindler. A second-kind Galerkin boundary element method for scattering at composite objects. BIT Numerical Mathematics, 55(1):33-57, 2015] and extended it to this new setting. Based on so-called global multi-potentials, we derived variational second-kind boundary integral equations posed in \( L^2(\Sigma) \), where \( \Sigma \) denotes the union of material interfaces. To suppress spurious resonances, we introduced a combined-field version (CFIE) of our new method. We conducted thorough numerical tests that highlighted the low and mesh-independent condition numbers of Galerkin matrices obtained with discontinuous piecewise polynomial boundary element spaces. They also confirmed competitive accuracy of the numerical solution in comparison with the widely used first-kind single-trace approach.

We spent much effort investigating the potentialities of multi-trace formulations in terms of domain decomposition. We considered multi-trace formulations in this perspective. Indeed Multi-Trace Formulations are based on a decomposition of the problem domain into subdomains, and thus domain decomposition solvers are of interest. The fully rigorous mathematical MTF can however be daunting for the non-specialist. In [12], we introduced MTFs on simple model problems using concepts familiar to researchers in domain decomposition. This allowed us to get a new understanding of MTFs and a natural block Jacobi iteration, for which we
determined optimal relaxation parameters. We then showed how iterative multitrace formulation solvers are related to a well known domain decomposition method called optimal Schwarz method: a method which used Dirichlet to Neumann maps in the transmission condition. We finally showed that the insight gained from the simple model problem leads to remarkable identities for Calderón projectors and related operators, and the convergence results and optimal choice of the relaxation parameter we obtained is independent of the geometry, the space dimension of the problem, and the precise form of the spatial elliptic operator, like for optimal Schwarz methods. We confirmed this analysis with numerical experiments.

This work was extended in [10]. Considering pure transmission scattering problems in piecewise constant media, we derived an exact analytic formula for the spectrum of the corresponding local multi-trace boundary integral operators in the case where the geometrical configuration does not involve any junction point and all wave numbers equal. We deduced from this the essential spectrum in the case where wave numbers vary. Numerical evidences of these theoretical results were obtained in 2D.

Finally, in connection with boundary integral formulations, we extended the past work of [X. Claeys and R. Hiptmair, Integral equations on multi-screens. Integral Equations and Operator Theory, 77(2):167–197, 2013] where we had developed a framework for the analysis of boundary integral equations for acoustic scattering at so-called multi-screens, which are arbitrary arrangements of thin panels made of impenetrable material. In [3] we extended these considerations to boundary integral equations for electromagnetic scattering.

Viewing tangential multi-traces of vector fields from the perspective of quotient spaces we introduced the notion of single-traces and spaces of jumps. We also derived representation formulas and established key properties of the involved potentials and related boundary operators. Their coercivity were proved using a splitting of jump fields. Another new aspect emerged in the form of surface differential operators linking various trace spaces.

7.6. Asymptotic models for time harmonic wave propagation

Asymptotic models oriented toward more efficient numerical simulation methods have been investigated in three different directions.

In [8] we considered the Poisson equation in a domain with a small hole of size $\delta$, and presented a simple numerical method, based on an asymptotic analysis, which allows to approximate robustly the far field of the solution as $\delta$ goes to zero without meshing the small hole. We proved the stability of the scheme and provide error estimates. This was confirmed with numerous numerical experiments illustrating the efficiency of the technique.

In [11] we considered a Laplace problem with Dirichlet boundary condition in a three dimensional domain containing an inclusion taking the form of a thin tube with small thickness. We proved convergence in operator norm of the resolvent of this problem as the thickness goes to 0, establishing that the perturbation on the resolvent induced by the inclusion is not greater than some (negative) power of the logarithm of the thickness. From this we deduced convergence of the eigenvalues of the perturbed operator toward the limit operator.

In [9] we investigated the eigenvalue problem $-\text{div}(\sigma \nabla u) = \lambda u$ (P) in a 2D domain $\Omega$ divided into two regions $\Omega_\pm$. We were interested in situations where $\sigma$ takes positive values on $\Omega_+$ and negative ones on $\Omega_-$. Such problems appear in time harmonic electromagnetics in the modeling of plasmonic technologies. In a recent work [L. Chesnel, X. Claeys, and S.A. Nazarov. A curious instability phenomenon for a rounded corner in presence of a negative material. Asymp. Anal., 88(1):43–74, 2014], we had highlighted an unusual instability phenomenon for the source term problem associated with (P): for certain configurations, when the interface between the subdomains $\Omega_\pm$ presents a rounded corner, the solution may depend critically on the value of the rounding parameter. In [9] we explained this property studying the eigenvalue problem (P). We provided an asymptotic expansion of the eigenvalues and prove error estimates. We established an oscillatory behaviour of the eigenvalues as the rounding parameter of the corner tends to zero. This work was ended with numerical illustrations.
7.7. **New results related to FreeFem++**

In [6], we consider a model of soil water and nutrient transport with plant root uptake. The geometry of the plant root system is explicitly taken into account in the soil model. We first describe our modeling approach. Then, we introduce an adaptive mesh refinement procedure enabling us to accurately capture the geometry of the root system and small-scale phenomena in the rhizosphere. Finally, we present a domain decomposition technique for solving the problems arising from the soil model as well as some numerical results.

In [15], we study an interface transport scheme of a two-phase flow of an incompressible viscous immiscible fluid. The problem is discretized by the characteristics method in time and finite elements in space. The interface is captured by the Level-Set function. Appropriate boundary conditions for the problem of mould filling are investigated, a new natural boundary condition under pressure effect for the transport equation is proposed and an algorithm for computing the solution is presented. Finally, numerical experiments show and validate the effectiveness of the proposed scheme.

8. **Bilateral Contracts and Grants with Industry**

8.1. **Bilateral Contracts with Industry**

- Contract with Total, February 2015 - February 2018, that funds the PhD of Hussam Al Daas on enlarged Krylov subspace methods for oil reservoir and seismic imaging applications. Supervisor, L. Grigori.

9. **Partnerships and Cooperations**

9.1. **National Initiatives**

9.1.1. **ANR**

9.1.1.1. **Medimax**

ANR-MN (Modèles Numériques) October 2013 - September 2017

The main goal is the methodological and numerical development of a new robust inversion tool, associated with the numerical solution of the electromagnetic forward problem, including the benchmarking of different other existing approaches (Time Reverse Absorbing Condition, Method of Small-Volume Expansions, Level Set Method). This project involves the development of a general parallel open source simulation code, based on the high-level integrated development environment of FreeFem++, for modeling an electromagnetic direct problem, the scattering of arbitrary electromagnetic waves in highly heterogeneous media, over a wide frequency range in the microwave domain. The first applications considered here will be medical applications: microwave tomographic images of brain stroke, brain injuries, from both synthetic and experimental data in collaboration with EMTensor GmbH, Vienna (Austria), an Electromagnetic Medical Imaging company.

9.1.1.2. **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.

9.1.1.3. **Soilµ-3D**

ANR appel à projet générique October 2015 - September 2020
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 “homogenization” 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. European Initiatives

9.2.1. FP7 & H2020 Projects

9.2.1.1. NLAFET

Title: Parallel Numerical Linear Algebra for Future Extreme-Scale Systems
Programm: H2020
Duration: November 2015 - November 2018
Coordinator: UMEÅUniversitet
Partners:
Science and Technology Facilities Council (United Kingdom)
Computer Science Department, UmeåUniversity (Sweden)
Mathematics Department, The University of Manchester (United Kingdom)
Inria contact: Laura Grigori

The NLAFET 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.

**9.2.1.2. EXA2CT**

**Title:** EXascale Algorithms and Advanced Computational Techniques  
**Programm:** FP7  
**Duration:** September 2013 - August 2016  
**Coordinator:** IMEC

**Partners:**

- Fraunhofer-Gesellschaft Zur Foerderung Der Angewandten Forschung E.V (Germany)
- Interuniversitair Micro-Electronica Centrum Vzw (Belgium)
- Intel Corporations (France)
- Numerical Algorithms Group Ltd (United Kingdom)
- T-Systems Solutions for Research (Germany)
- Universiteit Antwerpen (Belgium)
- Universita della Svizzera italiana (Switzerland)
- Université de Versailles Saint-Quentin-En-Yvelines. (France)
- Vysoka Skola Banska - Technicka Univerzita Ostrava (Czech Republic)

**Inria contact:** Luc Giraud

Numerical simulation is a crucial part of science and industry in Europe. The advancement of simulation as a discipline relies on increasingly compute intensive models that require more computational resources to run. This is the driver for the evolution to exascale. Due to limits in the increase in single processor performance, exascale machines will rely on massive parallelism on and off chip, with a complex hierarchy of resources. The large number of components and the machine complexity introduce severe problems for reliability and programmability. The former of these will require novel fault-aware algorithms and support software. In addition, the scale of the numerical models exacerbates the difficulties by making the use of more complex simulation algorithms necessary, for numerical stability reasons. A key example of this is increased reliance on solvers. Such solvers require global communication, which impacts scalability, and are often used with preconditioners, increasing complexity again. Unless there is a major rethink of the design of solver algorithms, their components and software structure, a large class of important numerical simulations will not scale beyond petascale. This in turn will hold back the development of European science and industry which will fail to reap the benefits from exascale. The EXA2CT project brings together experts at the cutting edge of the development of solvers, related algorithmic techniques, and HPC software architects for programming models and communication. It will take a revolutionary approach to exascale solvers and programming models, rather than the incremental approach of other projects. We will produce modular open source proto-applications that demonstrate the algorithms and programming techniques developed in the project, to help boot-strap the creation of genuine exascale codes.

**9.3. International Initiatives**

**9.3.1. Inria International Labs**

**Inria@SiliconValley**

Associate Team involved in the International Lab:
9.3.1.1. COALA
Title: Communication Optimal Algorithms for Linear Algebra
International Partner (Institution - Laboratory - Researcher):
University of California Berkeley (United States) - Electrical Engineering and Computer Science (EECS) - James Demmel
Start year: 2010
See also: https://who.rocq.inria.fr/Laura.Grigori/COALA2010/coala.html

Our goal is to continue COALA associated team that focuses on the design and implementation of numerical algorithms for today’s large supercomputers formed by thousands of multicore processors, possibly with accelerators. We focus on operations that are at the heart of many scientific applications as solving linear systems of equations or least squares problems. The algorithms belong to a new class referred to as communication avoiding that provably minimize communication, where communication means the data transferred between levels of memory hierarchy or between processors in a parallel computer. This research is motivated by studies showing that communication costs can already exceed arithmetic costs by orders of magnitude, and the gap is growing exponentially over time. An important aspect that we consider here is the validation of the algorithms in real applications through our collaborations. COALA is an Inria associate team that focuses on the design and implementation of numerical algorithms for today’s large supercomputers formed by thousands of multicore processors, possibly with accelerators. We focus on operations that are at the heart of many scientific applications as solving linear systems of equations or least squares problems. The algorithms belong to a new class referred to as communication avoiding that provably minimize communication, where communication means the data transferred between levels of memory hierarchy or between processors in a parallel computer. This research is motivated by studies showing that communication costs can already exceed arithmetic costs by orders of magnitude, and the gap is growing exponentially over time. An important aspect that we consider here is the validation of the algorithms in real applications through our collaborations.

9.4. International Research Visitors
9.4.1. Visits to International Teams
9.4.1.1. Sabbatical programme
Grigori Laura
Date: Aug 2014 - June 2015
Institution: University of California Berkeley (United States)
9.4.1.2. Research stays abroad
- Laura Grigori: long term mission at UC Berkeley, Computer Science Department, from September 2015 to June 2016.

10. Dissemination
10.1. Promoting Scientific Activities
10.1.1. Scientific events organisation
10.1.1.1. General chair, scientific chair
• Frédéric Hecht: Organizing the 7th FreeFem++ days (December 2015, Paris)
• Frédéric Hecht: Organizing Contributions to PDE for Applications, September 2015, Paris

10.1.1.2. Member of the organizing committees
• Laura Grigori: Member of Scientific Committee of Ecole CEA-EDF-Inria on Efficacité Énergétique dans le Calcul Haute Performance / Green HPC, 2015.

10.1.2. Scientific events selection
10.1.2.1. Member of the conference program committees
• Laura Grigori: Member of Program Committee of IEEE International Parallel and Distributed Processing Symposium, IPDPS 2015.
• Laura Grigori: Member of Program Committee of IEEE/ACM SuperComputing SC15 Conference, November 2015.
• Laura Grigori: Member of Program Committee of HiPC 2015, IEEE Int’l Conference on High Performance Computing.
• Laura Grigori: Member of Program Committee of International Conference on Parallel Processing and Applied Mathematics PPAM15, 2015.
• Laura Grigori: Member of Program Committee of Workshop on Parallel Symbolic Computation (PASCO 2015), University of Bath, UK, 2015.

10.1.3. Journal
10.1.3.1. Member of the editorial boards
• Laura Grigori: Area editor for Parallel Computing Journal, Elsevier, since June 2013.
• Frédéric Nataf: Member of the editorial board of Journal of Numerical Mathematics

10.1.4. Invited talks
• Laura Grigori: Invited speaker (plenary), ACM/IEEE Supercomputing’15, International Conference for High Performance Computing, Networking, Storage, and Analysis, Austin, November 2015, http://sc15.supercomputing.org/schedule/event_detail?evid=inv103. This is the major conference of high performance computing, attended by 12,000 people.
• Laura Grigori: Invited plenary speaker, Emerging Technology Conference, June 2015, University of Manchester, http://emit.manchester.ac.uk/.
• Frédéric Nataf: Invited plenary speaker, XXIII International Conference on Domain Decomposition Methods, 6-10 July 2015, South Korea.

10.1.5. Leadership within the scientific community
• Laura Grigori: Program Director of the SIAM SIAG on Supercomputing (SIAM special interest group on supercomputing), January 2014 - December 2015. Nominated by a Committee and elected by the members of this SIAG. One of the roles is to Co-Chair the SIAM Conference on Parallel Processing and Scientific Computing 2016.
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

- Frédéric Hecht: President of the selection committee of the opening 0254 MCF 26, Université de Technologie de Compiègne.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Master: Laura Grigori, Guest lecture in a class on Randomized Linear Algebra taught by Ravi Kanan, UC Berkeley, November 2015. The slides of the lecture on Algorithms for computing low rank approximations can be found on Laura Grigori’s webpage.

- Master: Laura Grigori, Spring 2015, UC Berkeley, Creation of a reading group and lectures on randomized linear algebra that gathers together students and experts interested in learning more and working on fast linear algebra algorithms for machine learning applications. More details are available at https://who.rocq.inria.fr/Laura.Grigori/RandNLA.html, including the videos of the lectures. The co-organizers of this reading group are Prof. J. Demmel (CS Department), Prof. M. Gu (Math Department), Prof. M. Mahoney (Statistics Department).

- Master: Laura Grigori, Spring 2015, UC Berkeley, Guest lecturer in CS267 Class of J. Demmel on Applications of Parallel Computing (lectures 13 to 16). The slides are available on L. Grigori’s website, videos can be found here https://www.youtube.com/playlist?list=PLkFD6_40KJ1yX8nEjk6oTLWohdVhjjP3X.
  - Lecture 13 on Communication Avoiding Algorithms in Linear Algebra
  - Lecture 14 on Graph partitioning
  - Lecture 15 on Sparse Direct Solvers
  - Lecture 16 on Iterative Solvers

- Master: Frederic Nataf, Course on Domain Decomposition Methods, 30 hours, Master 2, UPMC, France.

- Master: Frederic Nataf, Course on Domain Decomposition Methods, 15 hours, Master 2, ENSTA, France.


- Licence : Xavier Claeys, Calculus, 12hrs, L1, Université Pierre-et-Marie Curie Paris 6, France

- Licence : Xavier Claeys, Orientation et Insertion Professionnelle, 40hrs, L2, Université Pierre-et-Marie Curie Paris 6, France

- Master : Xavier Claeys, Informatique de base, 72hrs, M1, Université Pierre-et-Marie Curie Paris 6, France

- Master : Xavier Claeys, Informatique Scientifique, 44hrs M1, Université Pierre-et-Marie Curie Paris 6, France

- Master : Xavier Claeys, Résolution des EDP par éléments finis, 18hrs M2, Université Pierre-et-Marie Curie Paris 6, France

- Master : Frédéric Hecht, Informatique de base, 24hrs, M1, Université Pierre-et-Marie Curie Paris 6, France
10.2.2. Supervision

- PhD in progress: Alan Ayala, since October 2015 (funded by NLAFET H2020 project), co-advisors Xavier Claeys and Laura Grigori.
- PhD in progress: Sebastien Cayrols, since October 2013 (funded by Maison de la simulation), advisor Laura Grigori.
- PhD in progress: Hussam Al Daas, since February 2015 (funded by contract with Total), advisor Laura Grigori.
- PhD in progress: Olivier Tissot, since October 2015 (funded by NLAFET H2020 project), advisor Laura Grigori.
- PhD in progress: RyadH Haferssas, since October 2013 (funded by Ecole Doctorale, UPMC), advisor F. Nataf
- PhD in progress: Mireille El-HAddad, since March 2014 (Cotuelle l’Université Saint-Joseph de Beyrouth, Liban et UPMC), advisors F. Hecht and T. Sayah.
- PhD in progress: Gillaume Verger El-HAddad, since Sept. 2013 (funded by ANR Becasim, Université de Rouen), advisors F. Hecht and I. Danaila.

10.2.3. Juries

- Frédéric Hecht: HDR of Laurence Moreau, Rapporteur, UTT, Troyes, June 2015
- Frédéric Hecht: PhD thesis of Arnaud BERTRAND, Rapporteur, Université de Strasbourg, November 2015
- Frédéric Hecht: PhD thesis of Moussa Diédhiou, Examineur, Université de la Rochelle, December 2015

11. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

Articles in International Peer-Reviewed Journals


Invited Conferences


Other Publications

[8] L. CHESNEL, X. CLAEYS. *A numerical approach for the Poisson equation in a planar domain with a small inclusion*, January 2016, working paper or preprint, https://hal.inria.fr/hal-01251220


[10] X. CLAEYS. *Essential spectrum of local multi-trace boundary integral operators*, August 2015, working paper or preprint, https://hal.inria.fr/hal-01251212


