IN PARTNERSHIP WITH:
CNRS

Université Pierre et Marie Curie (Paris 6)

Activity Report 2016

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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Creation of the Team: 2013 January 01, updated into Project-Team: 2014 July 01

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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 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
  - 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 datat 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 aproach 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 developped: 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 difraction 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 caracteristic 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 caracteristics 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 pheneomena, 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 to handle numerically. The aim of this part of our reasearch 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 caracterizing 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. Awards

5.1.1.1. SIAM Siag on Supercomputing Best Paper Prize 2016

for the most outstanding paper published in 2012-2015 in a journal in the field of high performance computing. Co-authors are J. Demmel, L. Grigori, M. Hoemmen, and J. Langou, for the paper Communication-Optimal Parallel and Sequential QR and LU Factorizations, published in SIAM Journal on Scientific Computing 2012. Citation of the jury: *This is a cornerstone paper in Numerical Linear Algebra and Parallel Processing that lays down both theoretical and practical algorithmic frameworks for communication-avoiding algorithms. The paper provides powerful insights and renews attention on communication reduction both of which will have long-lasting and practical impact in parallel and distributed computing.*

5.1.1.2. Bull-Joseph Fourier 1st Prize 2015 (15 000 euros)

for our work *Imaging of cerebrovascular accident through High Performance Computing* by V. Dolean, F. Hecht, P. Jolivet, F. Nataf and P-H. Tournier. This was the sixth edition of this competition which corresponds to the French "Gordon Bell Prize".

6. New Software and Platforms

6.1. BFD

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, Remi Lacroix and Frédéric Nataf
- Partners: CNRS - UPMC
- Contact: Laura Grigori
- URL: https://who.rocq.inria.fr/Laura.Grigori/

6.2. CALU : communication optimal algorithms for linear algebra

KEYWORDS: Communication avoiding - Linear algebra
FUNCTIONAL DESCRIPTION

CALU solves linear systems of equations Ax=b using Communication Avoiding LU.

- Contact: Laura Grigori
- URL: https://who.rocq.inria.fr/Laura.Grigori/

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/

6.4. 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 2^d-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: Frédéric Hecht
- URL: http://www.freefem.org/ff++/

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

6.6. LORASC

LORASC preconditioner

KEYWORD: Preconditioner

- Participants: Laura Grigori and Remi Lacroix
- Contact: Laura Grigori
- URL: not available

6.7. NFF

NFF Nested Filtering Factorization

KEYWORDS: Preconditioner - Interactive method - Linear system

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

6.8. SparseToolbox

KEYWORDS: Preconditioner - Interactive method - Linear system

- Participants: Laura Grigori and Remi Lacroix
- Contact: Laura Grigori
- URL: not available

7. New Results

7.1. Communication avoiding algorithms

Our group continues to work on algorithms for dense and sparse linear algebra operations that minimize communication. During this year we focused on communication avoiding iterative methods and designing algorithms for computing rank revealing and low rank approximations of dense and sparse matrices.

In [9], we discuss sparse matrix-matrix multiplication (or SpGEMM), which is an important operation for many algorithms in scientific computing. In our previous work we have identified lower bounds on communication for this operation, which is the limiting factor of SpGEMM. Even though 3D (or 2.5D) algorithms have been proposed and theoretically analyzed in the flat MPI model on Erdos–Renyi matrices, those algorithms had not been implemented in practice and their complexities had not been analyzed for the general case. In this work, we present the first implementation of the 3D SpGEMM formulation that exploits multiple (intranode and internode) levels of parallelism, achieving significant speedups over the state-of-the-art publicly available codes at all levels of concurrencies. We extensively evaluate our implementation and identify bottlenecks that should be subject to further research.

In [10] we discuss algorithms that not only aim at minimizing communication, but they also aim at reducing the number of writes to secondary storage. Most of the prior work does not distinguish between loads and stores, i.e., between reads and writes to a particular memory unit. But in fact there are some current and emerging nonvolatile memory technologies (NVM) where writes can be much more expensive (in time and energy) than reads. NVM technologies are being considered for scientific applications on extreme scale computers and for cluster computing platforms, in addition to commodity computers.

This motivates us to first refine prior work on communication lower bounds of algorithms which did not distinguish between loads and stores to derive new lower bounds on writes to different levels of a memory hierarchy. When these new lower bounds on writes are asymptotically smaller than the previous bounds on the total number of loads and stores, we ask whether there are algorithms that attain them. We call such algorithms, that both minimize the total number of loads and stores (i.e., are CA), and also do asymptotically fewer writes than reads, *write-avoiding (WA)*. In this paper, we identify several classes of problems where either sequential or parallel WA algorithms exist, or provably cannot.

In [7] we introduce a new approach for reducing communication in Krylov subspace methods that consists of enlarging the Krylov subspace by a maximum of t vectors per iteration, based on the domain decomposition of the graph of A.We show in this paper that the enlarged Krylov projection subspace methods lead to faster convergence in terms of iterations and parallelizable algorithms with less communication, with respect to Krylov methods.

In this paper we focus on Conjugate Gradient (CG), a Krylov projection method for symmetric (Hermitian) positive definite matrices. We discuss two new versions of Conjugate Gradient. The first method, multiple search direction with orthogonalization CG (MSDO-CG), is an adapted version of MSD-CG with the A-orthonormalization of the search directions to obtain a projection method that guarentees convergence at least as fast as CG. The second projection method that we propose here, long recurrence enlarged CG (LRE-CG), is similar to GMRES in that we build an orthonormal basis for the enlarged Krylov subspace rather than finding search directions. Then, we use the whole basis to update the solution and the residual. We compare the convergence behavior of both methods using different A-orthonormalization and orthonormalization methods and then we compare the most stable versions with CG and other related methods. Both methods converge faster than CG in terms of iterations, but LRE-CG converges faster than MSDO-CG since it uses the whole basis to update the solution rather than only t search directions. And the more subdomains are introduced or the larger t is, the faster is the convergence of both methods with respect to CG in terms of iterations. For example, for $t = 64$ the MSDO-CG and LRE-CG methods converge in 75% up to 98 less iteration with respect to CG for the different test matrices.

In [12] we present an algorithm for computing a low rank approximation of a sparse matrix based on a truncated LU factorization with column and row permutations. We present various approaches for determining the column and row permutations that show a trade-off between speed versus deterministic/probabilistic accuracy. We show that if the permutations are chosen by using tournament pivoting based on QR factorization, then the obtained truncated LU factorization with column/row tournament pivoting, LU_CRTP, satisfies bounds on the singular values which have similarities with the ones obtained by a communication avoiding rank revealing QR factorization. Experiments on challenging matrices show that LU_CRTP provides a good low rank approximation of the input matrix and it is less expensive than the rank revealing QR factorization in terms of computational and memory usage costs, while also minimizing the communication cost. We also compare the computational complexity of our algorithm with randomized algorithms and show that for sparse matrices and high enough but still modest accuracies, our approach is faster.

7.2. Integral equation based domain decomposition

We kept on studying the convergence of classical domain decomposition strategies applied to multi-trace formulations (MTF). In the contribution [18], we present a gentle introduction to multi-trace formalism aimed at the domain decomposition community as well as analytical calculations in simple geometrical configuration where a full analysis of block-Jacoobi applied to MTF is possible. We only consider transmission problems in 1D with one or two interfaces. In [5], we generalize this analysis to arbitrary 2D or 3D transmission problems with arbitrary subdomain partitionning, only assuming that there is no junction point. The analysis holds mainly for completely homogeneous media with no material constrast, and in such a case we determine the spectrum of the multi-trace operator, as well as the spectrum of the Jacobi operator. We show that this spectrum only consists in a finite number of point values. In the more general case where the propagation medium is piecewise constant, this analysis still yields the location of the essential spectrum of the MTF and the Jacobi operator.

This analysis also led to an explicit expression for the inverse of the MTF operators for transmission problems in the case of perfectly homogeneous media. This was studied during the intership of Alan Ayala, and was described and tested numerically in 3D in the proceedings.

The analysis presented in [5] also shows that, in the case of purely homogeneous media, a block Jacobi strategy converges in a number of steps that exactly corresponds to the depth of the adjacency graph of the subdomain partition under consideration, which suggests a close relationship with Optimized Schwarz Methods (OSM), following the ideas of [20]. We investigated this point during the internship of Pierre Marchand, and we exhibited fully explicitely the exact relationship between block-Jacobi-MTF and OSM. Besides, we also generalized the analysis presented in [5] to the case of a competely heterogeneous problem, which involves abstract boundary integral operators that are not easily computable.

7.3. Multi-subdomain integral equations

In the context of boundary integral equations adapted to wave scattering in piecewise constant media in harmonic regime, we also made significant progress in the study of the single trace boundary integral formulation (STF) of the second kind originally introduced in [17]. This work was achieved in collaboration with Ralf Hiptmair and Elke Spindler (ETH Zürich). First of all, we proposed a version of this formulation for the solution to Maxwell's equations whereas, so far, it had been studied only in the context of scalar wave scattering (Helmholtz equation). In this direction, we conducted numerical experiments which confirmed the attractive properties of the matrices obtained when discretising such formulations (good accuracy, and good conditionning independent of discretisation parameters). For Maxwell's equations, we also established elementary theoretical results of STF 2nd kind such as Fredholmness of the corresponding integral operator.

So far, second kind STF had been stuudied for wave scatering problems where material contrasts only enter in the compact part of the partial differential operator, which is harmless regarding the Fredholmness of the corresponding boundary integral operator. Thus, in [19], we investigated the case where material contrasts come into play in the principal part of the operator, considering a pure diffusion-transmission problem. In this case, we have been able to establish well-posedness (hence Fredholmness). A rather naive approach leads to choose Sobolev spaces of fractionnal order (half-integer) as main functional setting for this formulation. We showed that this formulation can be extended so as to make sense in the space of square integrable trace functions. This is much more handy a functional setting that allows in particular discontinuous Galerkin discretisations of the corresponding boundary integral equations.

7.4. Asymptotics for a semi-linear convex problem with small inclusion

In [16], in collaboration with Lucas Chesnel (Inria Defi) and Sergei Nazarov (Saint-Petersbourg University), we recently investigated the asymptotics of the solution to a semi-linear problem in 2D with Dirichlet boundary condition. The partial differential operator under consideration was $-\Delta u + (u)^{2p+1}$ where p is a positive integer. The computational domain is assumed to contain a small Dirichlet obstacle of size $\delta > 0$. Using the method of matched asymptotic expansions, we compute an asymptotic expansion of the solution as δ tends to zero. Its relevance was justified by proving a rigorous error estimate. Then we construct an approximate model, based on an equation set in the limit domain without the small obstacle, which provides a good approximation of the far field of the solution of the original problem. The interest of this approximate model lies in the fact that it leads to a variational formulation which is very simple to discretize. We obtained numerical experiments to illustrate the analysis.

7.5. Time-dependent wave splitting and source separation

Starting from classical absorbing boundary conditions, we (M. Grote, M. Kray, F. Nataf and F. Assous) propose a method for the separation of time-dependent scattered wave fields due to multiple sources or obstacles. More precisely, we propose a method to determine the separate outgoing components of the incident and scattered wave fields for time-dependent scattering problems. In the case of two superposed wave fields, our method applies to the following three typical configurations: two distinct localized sources with unknown time history each, a single (unknown) localized source with a nearby scatterer, or two separate scatterers illuminated by a known incident wave field. In all three cases, our method permits to recover the individual outgoing components from measurements of the total scattered field at a distance. In doing so, the particular nature of the scatterer, be it an im- penetrable well-defined obstacle or a penetrable localized inhomogeneity, is immaterial; only the purely outgoing character of the individual wave fields matters. In contrast to previous work, our approach is local in space and time, deterministic, and also avoids any a priori assumptions on the frequency spectrum of the signal. Numerical simulations in FreeFem++ in two space dimensions illustrate the usefulness of wave splitting for time-dependent scattering problems. This work was presented to several international conferences and was published in J. Comput. Phys. (2016).

7.6. SORAS GenEO-2

Optimized Schwarz methods (OSM) are very popular methods which were introduced by P.L. Lions (1989) for elliptic problems and by B. Després (1990) for propagative wave phenomena. We (R. Haferssas, P. Jolivet and F. Nataf) give here a theory for Lions' algorithm that is the genuine counterpart of the theory developed over the years for the Schwarz algorithm. The first step is to introduce a new symmetric variant of the ORAS (Optimized Restricted Additive Schwarz) algorithm that is suitable for the analysis of a two-level method. Then we build a coarse space for which the convergence rate of the two-level method is guaranteed regardless of the regularity of the coefficients. We show scalability results for thousands of cores for nearly incompressible elasticity and the Stokes systems with a continuous discretization of the pressure.

7.7. Numerical modeling and high speed parallel computing: new perspectives for tomographic microwave imaging for brain stroke detection and monitoring

These works deals with microwave tomography for brain stroke imaging using state-of-the-art numerical modeling and massively parallel computing. Iterative microwave tomographic imaging requires the solution of an inverse problem based on a minimization algorithm (e.g. gradient based) with successive solutions of a direct problem such as the accurate modeling of a whole-microwave measurement system. Moreover, a sufficiently high number of unknowns is required to accurately represent the solution. As the system will be used for detecting the brain stroke (ischemic or hemorrhagic) as well as for monitoring during the treatment, running times for the reconstructions should be reasonable. The method used is based on high-order finite elements, parallel preconditioners from the Domain Decomposition method and Domain Specific Language with open source FreeFem++ solver. This work, for which we got the Joseph Fourier-Bull prize, is supported by ANR grant MEDIMAX (ANR-13-MONU-0012) and was granted access to the HPC resources of TGCC@CEA under the allocations 2016-067519 and 2016- 067730 made by GENCI.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Contract with Total, February 2015 - February 2018, that funds the PhD thesis of Hussam Al Daas on enlarged Krylov subspace methods for oil reservoir and seismic imaging applications. Supervisor L. Grigori.
- Contract with IFPen, February 2016 - February 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.
- Contract with MentorGraphics, March 2016, that funds the internship of T. Freiman on circuit simulations. Supervisor F. Nataf.

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. 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.

9.1.1.3. 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.

9.1.1.4. 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 “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. 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, UmeåUniversitet (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 Partners

9.3.1.1. Informal International Partners

- J. Demmel, UC Berkeley, USA
- R. Hipmair, ETH Zurich
- M. Grote (Université de Bâle, Suisse)
- F. Assous (Israel)

9.4. International Research Visitors

9.4.1. Visits to International Teams

9.4.1.1. Research Stays Abroad

- Laura Grigori has spent 5 months at UC Berkeley, from January 2016 to May 2016, as a visiting Professor/Researcher.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- SIAM Conference on Parallel Processing and Scientific Computing 2016 http://www.siam.org/meetings/pp16/, Paris. Co-chairs L. Grigori and R. Vuduc. The team Alpines as well as other members of Inria Paris and UPMC, were in charge of the local organization of this conference. There were a record number of 500 participants, 88 minisymposia sessions and 44 contributed talks.
- Frederic Hecht: Organizing the 8th FreeFem++ days (December 2016, Paris)

10.1.1.2. Member of the Organizing Committees

- Laura Grigori: Member of Program Committee of IEEE International Parallel and Distributed Processing Symposium, IPDPS 2016.
- Laura Grigori: Member of Program Committee of HiPC 2016, IEEE Int'l Conference on High Performance Computing.
- Laura Grigori: Member of Program Committee of IEEE Cluster 2016.
- Laura Grigori: Member of Organizing Committee of 5th SIAM Workshop on Combinatorial Scientific Computing (CSC) 2016.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

10.1.2.1.1. 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/.
- June 2013 – current. Area editor for Parallel Computing Journal, Elsevier
- January 2016 – current. Associate Editor, SIAM Journal on Scientific Computing.
- January 2016 – current. Editorial board, Numerical linear algebra with applications Journal, Wiley.

10.1.2.1.2. Frédéric Nataf

- 2014 – current. Associate Editor, Journal of Numerical Mathematics, de Gruyter.

10.1.3. Invited Talks

- Laura Grigori: Invited plenary speaker, Fifth IMA Conference on Numerical Linear Algebra and Optimization, Birmingham, (http://www.ima.org.uk/conferences/conferences_calendar/5th_ima_conference_on_numerical_linear_algebra_and_optimisation.cfm.html, September 7-9, 2016.
- Frederic Hecht: tutorial with FreeFem++, CEMRACS 2016 CIRM, Luminy, Marseille, july 18-22, 2016.
- Frederic Hecht: Graduate Course: An introduction to scientific computing using free software FreeFem++ , The Fields Institute for Research in Mathematical Sciences , Toronto, Canada , 7-17 March . 2016.
- Frederic Nataf: tutorial on Domain Decomposition Methods, CEMRACS 2016 CIRM, Luminy, Marseille, july 18-22, 2016.
- Frederic Nataf: Invited plenary speaker, Franco-Scottish Seminar 2016: Linear Algebra and Parallel Computing at the Heart of Scientific Computing. 21 September 2016.

10.1.4. Leadership within the Scientific Community

- Laura Grigori: Chair of the SIAM SIAG on Supercomputing (SIAM special interest group on supercomputing), January 2016 - December 2017. Nominated by a Committee and elected by the members of this SIAG.
- Laura Grigori: Member of the PRACE (Partnership for Advanced Computing in Europe, http://www.prace-ri.eu/) Scientific Steering Committee, September 2016 - current.
- Laura Grigori: Steering committee member, Challenge 7: Information and communication society, ANR (Comité de Pilotage , Défi 7), since November 2016.

10.1.5. 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.
- Xavier Claeys: Member of the hiring committee for the position of maître de conférence 26 MCF 4346 at Université Claude Bernard Lyon 1, Spring 2016

10.1.6. Research Administration

10.1.6.1. Xavier Claeys

- Correspondent of the Association pour les Mathématiques en Interactions avec les Entreprises et la Société (AMIES) for Laboratoire Jacques-Louis Lions

10.1.6.2. Laura Grigori

- Member of the Director Committee (Comité Directeur) of GIS Geosciences franciliennes, since November 2015.
- Member (nominated by Inria) of the Scientific Committee of the Mathematics Department of UPMC

10.1.6.3. Frédéric Hecht

- Assistant Director of Fédération de Recherche en Mathématiques de Paris Centre, Fédération de Recherche en Mathématiques de Paris Centre, Since 2010

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

10.2.1.1. Xavier Claeys

- Academic year 2015-2016, total number of course hours: 192 hrs
  - Licence 1: Calculus, 12hrs, UPMC
  - Licence 2: Orientation and Professional Insertion, 40 hrs, UPMC
  - Master 1: Basic computing, 72 hrs of practical works in C++, UPMC
  - Master 1: Scientific computing, 44 hrs of lectures, UPMC
  - Master 2: Solving PDEs by using finite element methods, 18 hrs of practical works in C++, UPMC

10.2.1.2. Laura Grigori

- Spring 2016, UC Berkeley: Co-teaching a class with J. Demmel on Communication Avoiding Algorithms https://who.rocq.inria.fr/Laura.Grigori/TeachingDocs/CS-294_Spr2016/CS-294_CA_Spr2016.html. The class is available for mathematics students as a *Hot Topics Course in Mathematics*, and for Computer Science students as a *Special Topics* class. It was mainly designed for graduate students.
- 4-hour lecture at the XVII Jacques-Louis Lions Spanish-French School on Numerical Simulation in Physics and Engineering, June 2016, Gijon, Spain.

10.2.1.3. Frédéric Hecht

- Academic year 2015-2016, total number of course hours: 192 hrs
  - Master 1: Initiation au C++, 24hrs, M1, Université Pierre-et-Marie Curie Paris 6, France
  - Master 2: Des EDP à leur résolution par la méthode des éléments finis (MEF), 24hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
  - Master 2: Numerical methods for fluid mechanics, 10hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
  - Master 2: Calcul scientifique 3 / projet industriel FreeFem++, 28hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
  - Master 2: Ingénierie 1 / Logiciel pour la simulation (FreeFem++), 21hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
  - Master 2: Ingénierie 2 / Projet collaboratif, 21hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
- CEMRACS 2016 : Calcul scientifique à haute performance, 3h course on Tutorial with FreeFem++. The slides are available on F. Hecht website, and videos can be found here https://www.youtube.com/watch?v=NQy2kZQGBbg.

10.2.1.4. Frédéric Nataf

- CEMRACS 2016 : Calcul scientifique à haute performance, 3h course on Domain decomposition methods The slides are available on F. Nataf's website, videos can be found here https://www.youtube.com/watch?time_continue=10672&v=t-rgIFcN6w4.
- Spring 2016: Course on *Domain Decomposition Methods*, Master 2nd year Mathematics & Applications, University Pierre and Marie Curie
- Winter 2016: Course on *Domain Decomposition Methods*, Master 2nd year, Mathematics & Applications, ENSTA and UVSQ

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), adivsor 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: Pierre Marchand, since October 2016 (funded by ANR NonLocalDD project), advisors Xavier Claeys et Frédéric Nataf.
- PhD in progress: Zakariae Jorti, since February 2016 (funded by IFPen), advisor Laura Grigori.
- PhD : Ryadh Haferssas, defended december 2016 (funded by Ecole Doctorale, UPMC), advisor F. Nataf
- PhD : Mireille El-HAddad, defended december 2016(t UPMC), advisors F. Hecht and T. Sayah.
- HDR: X. CLAEYS, Boundary integral equations of time harmonic wave scattering at complex structures, Accreditation to supervise research, (UPMC Paris 6), February 2016.

10.3. Popularization

- 2 Conferences on being a mathematicien: **Applied Mathematics, Research...**, in the high school Viollet le Duc - Villiers-Saint-Frédéric, France for 200 high school students in 11th and 12th grade, april 2016.
- Part of the teaching duty of Xavier Claeys (around 70 hours total) has been dedicated to "orientation and insertion professionnelle". This has consisted in familiarizing young students (2nd year bachelor) with potential curricula, professionnal activities and networks related to mathematics.

11. Bibliography

Publications of the year

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[1] X. CLAEYS. *Boundary integral equations of time harmonic wave scattering at complex structures*, Université Pierre et Marie Curie (UPMC Paris 6), February 2016, Habilitation à diriger des recherches, http://hal.upmc.fr/tel-01357729

Articles in International Peer-Reviewed Journals

[2] I. BAJC, F. HECHT, S. ŽUMER. *A mesh adaptivity scheme on the Landau–de Gennes functional minimization case in 3D, and its driving efficiency*, in "Journal of Computational Physics", September 2016, vol. 321, pp. 981–996 [*DOI :* 10.1016/J.JCP.2016.02.072], http://hal.upmc.fr/hal-01360423

[3] L. CHESNEL, X. CLAEYS. *A numerical approach for the Poisson equation in a planar domain with a small inclusion*, in "BIT Numerical Mathematics", March 2016, https://hal.inria.fr/hal-01109552

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[5] X. CLAEYS. *Essential spectrum of local multi-trace boundary integral operators*, in "IMA Journal of Applied Mathematics", May 2016, https://hal.inria.fr/hal-01251212

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[9] A. AZAD, G. BALLARD, A. BULUC, J. W. DEMMEL, L. GRIGORI, O. SCHWARTZ, S. TOLEDO. *Exploiting Multiple Levels of Parallelism in Sparse Matrix-Matrix Multiplication*, in "SIAM Journal on Matrix Analysis and Applications", November 2016, vol. 38, n^o^ 6, 27 p. , https://hal.inria.fr/hal-01426294

International Conferences with Proceedings

[10] C. ERIN, J. W. DEMMEL, L. GRIGORI, K. NICK, K. PENPORN, O. SCHWARTZ, V. HARSHA. *Write-Avoiding Algorithms*, in "Proceedings of IEEE International Parallel & Distributed Processing Symposium, IPDPS 2016", Chicago, United States, 2016, Short version of the technical report available at http://www.eecs.berkeley.edu/Pubs/TechRpts/2015/EECS-2015-163.pdf as Technical Report No. UCB/EECS-2015-163, https://hal.inria.fr/hal-01248678

[11] P. JOLIVET, P.-H. TOURNIER. *Block Iterative Methods and Recycling for Improved Scalability of Linear Solvers*, in "SC16 - International Conference for High Performance Computing, Networking, Storage and Analysis", Salt Lake City, Utah, United States, Proceedings of SC16: International Conference for High Performance Computing, Networking, Storage and Analysis, November 2016, https://hal.archives-ouvertes.fr/hal-01357998

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Other Publications

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