Activity Report 2013

Team ALPINES

Algorithms and parallel tools for integrated numerical simulations

IN COLLABORATION WITH: Laboratoire Jacques-Louis Lions

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Team ALPINES

Keywords: Scientific Computation, Finite Elements, Linear Algebra, Parallel Algorithms, Large Scale, Parallel Solver, Domain-specific Languages

Creation of the Team: 2013 January 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.

2.2. Highlights of the Year

- Frédéric Hecht was awarded the EADS Foundation's annual prize for Information Science and its Applications, attributed by the French Academy of Science.

- Best paper finalist at IEEE/ACM Supercomputing 2013 conference, P. Jolivet, F. Hecht, F. Nataf, C. Prud'homme, *Scalable Domain Decomposition Preconditioners For Heterogeneous Elliptic Problems*.

- Best student paper finalist at IEEE/ACM Supercomputing 2013 conference, L. Qu, L. Grigori, F. Nataf, *Parallel Design and Performance of Nested Filtering Factorization Preconditioner*.

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,
- prototype 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 CO_2 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 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 the Moore's Law. Planck (http://www.rssd.esa.int/index.php?project=PLANCK) 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. Software and Platforms

5.1. Software and Platforms

5.1.1. Platforms

5.1.1.1. FreeFem++, http://www.freefem.org/ff++/

`FreeFem++` is a PDE 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. There are more than 2000 users, and on the mailing list there are 430 members. Among those, we are aware of at least 10 industrial companies, 8 french companies and 2 non-french companies. It is used for teaching at Ecole Polytechnique, Ecole Centrale, Ecole des Ponts, Ecole des Mines, University Paris 11, University Paris Dauphine, La Rochelle, Nancy, Metz, Lyon, etc. Outside France, it is used for example at universities in Japan (Tokyo, Kyoto, Hiroshima, there is a userguide FreeFem++ in japan), Spain (Sevilla, BCAM, userguide available in spanish), UK (Oxford), Slovenia, Switzerland (EPFL, ETH), China. For every new version, there are 350 regression tests, and we provide a rapid correction of reported bugs. The licence of FreeFem++ is LGPL.

5.1.1.2. Library for preconditioned iterative methods

In the project-team we develop a library that integrates the direction preserving and low rank approximation preconditioners for both approached factorizations and domain decomposition like methods. It will be available through `FreeFem++` and also as a stand alone library, and we expect to have one version of this library available in 2014.

6. New Results

6.1. Integral equations on multi-screens

We developed a new functional framework for the study of scalar wave scattering by objects, called multi-screens, that are arbitrary arrangements of thin panels of impenetrable materials. From a geometric point of view, multi-screens are a priori non-orientable non-Lipschitz surfaces. We use our new framework to study boundary integral formulations of the scattering by such objects.

6.2. Second-kind Galerkin boundary element method for scattering at composite objects

In the context of scattering of time-harmonic acoustic waves at objects composed of several homogeneous parts with different material properties, a novel second-kind boundary integral formulation for this scattering problem was proposed in [X. Claeys, A single trace integral formulation of the second kind for acoustic scattering, Report 2011-14, SAM, ETH Zürich]. We recasted it into a variational problem set in L2 and investigated its Galerkin boundary element discretization from a theoretical and algorithmic point of view. Empiric studies demonstrate the competitive accuracy and superior conditioning of the new approach compared to a widely used Galerkin boundary element approach based on a first-kind boundary integral formulation.

6.3. Instability phenomenon for a rounded corner in presence of a negative material

We studied a 2D transmission problem between a positive material and a negative material. In electromagnetics, this negative material can be a metal at optical frequencies or a negative metamaterial. We highlighted an unusual instability phenomenon in some configurations: when the interface between the two materials presents a rounded corner, it can happen that the solution depends critically on the value of the rounding parameter. To prove this result, we provided an asymptotic expansion of the solution, when it is well-defined, in the geometry with a rounded corner. Then, we demonstrated that the asymptotic expansion is not stable with respect to the rounding parameter. We also conducted obtained numerical experiments with finite element methods to validate these results.

6.4. Parallel design and performance of direction preserving preconditioners

In the context of preconditioned iterative methods, our work has focused on so called direction preserving preconditioners. In [9] we consider the parallel design and performance of nested filtering factorization (NFF), a multilevel parallel preconditioning technique for solving large sparse linear systems of equations by using iterative methods. NFF is based on a recursive decomposition that requires first to permute the input matrix, which can have an arbitrary sparsity structure, into a matrix with a nested block arrow structure. This recursive factorization is a key feature in allowing NFF to have limited memory requirements and also to be very well suited for hierarchical parallel machines. NFF is also able to preserve some directions of interest of the input matrix A. Given a set of vectors T which represent the directions to be preserved, the preconditioner M satisfies a right filtering property $MT = AT$. This is a property which has been exploited in different contexts, as multigrid methods [Brandt et al., 2011, SIAM J. Sci. Comput.], semiseparable matrices [Gu et al, 2010, SIAM J. Matrix Anal. Appl.], incomplete factorizations [Wagner, 1997, Numer. Math] , or nested factorization [Appleyard and Cheshire, 1983, SPE Symposium on Reservoir Simulation]. It is well known that for difficult problems with heterogeneities or multiscale physics, the iterative methods can converge very slowly, and this is often due to the presence of several low frequency modes. By preserving the directions corresponding to these low frequency modes in the preconditioner, their effect on the convergence is alleviated and a much faster convergence is often observed. NFF can be seen as an extension of nested factorization that can be used for matrices with arbitrary sparsity structure and for which the computation can be performed in parallel. While the algebra of NFF has been introduced previously [Grigori et al, 2010, Inria tech. report], we relate the arithmetic complexity of NFF to the depth of recursion of its decomposition, and with our data distribution and implementation, we estimate its arithmetic and communication complexity. We also discuss the convergence of NFF on a set of matrices arising from the discretization of a boundary value problem with highly heterogeneous coefficients on three-dimensional grids. Our results show that on a $400 \times 400 \times 400$ regular grid, the number of iterations with NFF increases slightly while increasing the number of subdomains up to 2048. In terms of runtime performance on Curie, a Bullx system formed by nodes of two eight-core Intel Sandy Bridge processors, NFF scales well up to 2048 cores and it is 2.6 times faster than the domain decomposition preconditioner Restricted Additive Schwarz (RAS) as implemented in PETSc http://www.mcs.anl.gov/petsc/. The choice of the filtering vectors plays an important role in direction preserving preconditioners. There are problems for which we have prior knowledge of the near kernel of the input matrix, and this is indeed the case for the problems tested in this paper. They can also be approximated by using techniques similar to the ones used in deflation, however we do not discuss further this option here.

6.5. New resuls in communication avoiding algorithms for sparse linear algebra

In the context of sparse linear algebra algorithms, our recent results focus on two operations, incomplete LU factorization preconditioners and sparse matrix-matrix multiplication.

In [12] 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 was no communication avoiding preconditioner available 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 k-way or nested dissection. We show that the reordering does not affect the convergence rate of the ILU0 preconditioned system as compared to k-way 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.

In [6] we consider a fundamental problem in combinatorial and scientific computing, the sparse matrix-matrix multiplication problem. Obtaining scalable algorithms for this operations is difficult, since this operation has a poor surface to volume ratio, that is a poor data re-use. We consider that the input matrices are random, corresponding to Erdos-Renyi random graphs. We determine new lower bounds on communication for this case, in which we assume that the algorithm is sparsity independent, where the computation is statically partitioned to processors independent of the sparsity structure of the input matrices. We show in this paper that existing algorithms for sparse matrix-matrix multiplication are sub-optimal in their communication costs, and we obtain new algorithms which are communication optimal, communicating less than the previous algorithms and matching new lower bounds.

6.6. New resuls in communication avoiding algorithms for dense linear algebra

In the context of dense linear algebra algorithms, we have focused on two operations, LU factorization and rank revealing QR factorization.

In [4] we present block LU factorization with panel rank revealing pivoting (block LU_PRRP), a decomposition algorithm based on strong rank revealing QR panel factorization. Block LU_PRRP is more stable than Gaussian elimination with partial pivoting (GEPP), with a theoretical upper bound of the growth factor of $(1 + \tau b)^{(n/b)-1}$, where b is the size of the panel used during the block factorization, τ is a parameter of the strong rank revealing QR factorization, n is the number of columns of the matrix, and for simplicity we assume that n is a multiple of b. We also assume throughout all the paper that $2 \leq b \leq n$. For example, if the size of the panel is $b = 64$, and $\tau = 2$, then $(1 + 2b)^{(n/b)-1} = (1.079)^{n-64} \ll 2^{n-1}$, where 2^{n-1} is the upper bound of the growth factor of GEPP. Our extensive numerical experiments show that the new factorization scheme is as numerically stable as GEPP in practice, but it is more resistant to pathological cases. The block LU_PRRP factorization does only $O(n^2 b)$ additional floating point operations compared to GEPP.

We also present block CALU_PRRP, a version of block LU_PRRP that minimizes communication, and is based on tournament pivoting, with the selection of the pivots at each step of the tournament being performed via strong rank revealing QR factorization. Block CALU_PRRP is more stable than CALU, the communication avoiding version of GEPP, with a theoretical upper bound of the growth factor of $(1 + \tau b)^{\frac{n}{b}(H+1)-1}$, where H is the height of the reduction tree used during tournament pivoting. The upper bound of the growth factor of CALU is $2^{n(H+1)-1}$. Block CALU_PRRP is also more stable in practice and is resistant to pathological cases on which GEPP and CALU fail.

We have also introduced CARRQR (paper submitted to SIAM Journal on Matrix Analysis and Applications), a communication avoiding rank revealing QR factorization with tournament pivoting. 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 commmunication is a major bottleneck that highly impacts the performance of an algorithm.

6.7. Scalable Schwarz domain decomposition methods

Domain decomposition methods are, alongside multigrid methods, one of the dominant paradigms in contemporary large-scale partial differential equation simulation. A lightweight implementation [8] of a theoretically and numerically scalable preconditioner was developed in the context of overlapping methods. The performance of this work is assessed by numerical simulations executed on thousands of cores, for solving various highly heterogeneous elliptic problems in both 2D and 3D with billions of degrees of freedom. Such problems arise in computational science and engineering, in solid and fluid mechanics.

For example, in 3D, the initial highly heterogeneous problem of 74 million unknowns is solved in 200 seconds on 512 threads. Using 16384 threads, the problem is now made of approximately 2.3 billions unknowns, and it is solved in 215 seconds, which yields an efficiency of $\approx 90\%$. In 2D, the initial problem of 695 million unknowns is solved in 175 seconds on 512 threads. Using 16384 threads, the problem is now made of approximately 22.3 billions unknowns, and it is solved in 187 seconds, which yields an efficiency of $\approx 96\%$.

6.8. Schur domain decomposition methods

We have introduced spectral coarse spaces for the BDD and FETI methods in [5]. These coarse spaces are specifically designed for the two-level methods to be scalable and robust with respect to the coefficients in the equation and the choice of the decomposition. We achieve this by solving generalized eigenvalue problems on the interfaces between subdomains to identify the modes which slow down convergence. Theoretical bounds for the condition numbers of the preconditioned operators which depend only on a chosen threshold and the maximal number of neighbours of a subdomain were proved. For FETI there are two versions of the two-level method: one based on the full Dirichlet preconditioner and the other on the, cheaper, lumped preconditioner. Some numerical tests confirm these results.

6.9. Non conforming domain decomposition methods

We have designed and analyzed a new non-conforming domain decomposition method, named the NICEM method, based on Schwarz-type approaches that allows for the use of Robin interface conditions on nonconforming grids. The method is proven to be well posed. The error analysis is performed in 2D and in 3D for P1 elements. Numerical results in 2D illustrate the new method. This work is in collaboration with C. Japhet and Y. Maday.

6.10. Quadratic finite elements with non-matching grids for the unilateral boundary contact

We analyze in [3] a numerical model for the Signorini unilateral contact, based on the mortar blue method, in the quadratic finite element context. The mortar frame enables one to use non-matching grids and brings facilities in the mesh generation of different components of a complex system. The convergence rates we state here are similar to those already obtained for the Signorini problem when discretized on conforming meshes. The matching for the unilateral contact driven by mortars preserves then the proper accuracy of the quadratic finite elements. This approach has already been used and proved to be reliable for the unilateral contact problems even for large deformations. We provide however some numerical examples to support the theoretical predictions with FreeFem++ (http://www.freefem.org/ff++).

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Grants with Industry

BPI France (ex OSEO) supports our work on superresolution methods in acoustics. It enabled us to establish a collaboration with Laboratoire d'Acoustique du Mans (LAUM).

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR

8.1.1.1. PETALh

ANR Cosinus project - *PETascale ALgorithms for preconditioning for scientific applications* January 2011 - September 2013 (http://petal.saclay.inria.fr/). The global cost of the project is $1,350,910$, the funding from ANR is $304,232$. The total personne.mois is 140. Collaboration with Laboratoire Lions - UPMC, IFPEN, Inria Bordeaux and CEA, UC Berkeley. This project can be seen as a continuation of ANR funded PETAL project, the goal is to design parallel algorithms for the preconditioning techniques proposed during PETAL suitable for heterogeneous architectures based on multicore processors and accelerators.

8.1.1.2. 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.

8.2. European Initiatives

8.2.1. FP7 Projects

8.2.1.1. EXA2CT

Type: COOPERATION

Instrument: Specific Targeted Research Project

Objectif: NC

Duration: September 2013 - August 2016

Coordinator: Imec, Belgium

Partner: UA Belgium, USI Switzerland, Intel France, NAG England, UVSQ France, T-Systems SfR Germany, IT4Inovations Czech Republic.

Inria contact: Luc Giraud

Abstract: The goal of this project is to develop novel algorithms and programming models to tackle what will otherwise be a series of major obstacles to using a crucial component of many scientific codes at exascale, namely solvers and their constituents. The results of this work will be combined in running programs that demonstrate the application-targeted use of these algorithms and programming models in the form of proto-applications. The application targeting will be done by an analysis of a representative selection of scientific applications using solvers and/or the constituent parts that we target. The results of the project will be disseminated to the reference application owners through a scientific and industrial board (SIB), and board-partner specific code targeting activities, to help generate momentum behind our approach in the HPC community. The proto-applications will serve as a proof-of-concept, a benchmark for doing machine/software co-design, and as a basis for constructing future exascale full applications. In addition, the use of the SIB is a means to extract the commonalities of a range of HPC problems from different scientific domains and different industrial sectors to be able to concentrate on maximising the impact of the project by improving precisely those parts that are common across different simulation needs.

Alpines role: in charge of the Task "Preconditioners" in the working group focusing on numerical algorithms.

8.3. International Initiatives

8.3.1. Inria Associate Teams

8.3.1.1. COALA Inria associated team, Alpines and UC Berkeley

COALA associated team https://who.rocq.inria.fr/Laura.Grigori/COALA2010/coala.html focuses on communication optimal algorithms for linear algebra. We have a long term collaboration with Prof. J. Demmel, which focuses currently on communication avoiding algorithms. Since 2010, this collaboration takes place in the context of COALA Inria Associated team, and every year students visit our groups in both directions.

8.3.2. Inria International Partners

8.3.2.1. Informal International Partners

A collaboration focused on the theoretical and numerical analysis for the simulation of wave scattering by means of boundary integral formulation has been in place for several years between Xavier Claeys and the group of Ralf Hiptmair from the Seminar of Applied Mathematics at ETH Zürich.

8.3.3. Inria International Labs

Joint Laboratory for Petascale Computing, JLPC Etats-Unis. We take part in this joint effort, in the numerical libraries aspects of the joint laboratory. We collaborate and interact in particular with B. Gropp, UIUC, and J. Brown and M. Knepley, Argonne.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- Euan Spence from the University of Bath visited Xavier Claeys for one week to discuss about his work on high frequency wave scatering, and to see wether this work could apply to the formulations developed by Xavier Claeys.

- Grey Ballard from U.C. Berkeley, USA, visit of 2 weeks in January 2013. In the context of COALA Inria associated team, Grey has visited us to finalize our joint work on the publication [6].

8.4.1.1. Internships

- Sebastien Cayrols, Master 2 student Paris 11 University, March - August 2013, supervisor L. Grigori. Sebastien worked on communication avoiding ILU0 preconditioner.

- Antoine Liandrat, Ecole Centrale Lyon 2nd year, June-July 2013, supervisor L. Grigori. Antoine has worked in the context of Petalh project.
- Clement Guerin, ENS Lyon, L3 student, Mai-Juin 2013, supervisor L. Grigori. Clement's objective was to understand some of the numerical problems in communication avoiding algorithms.

8.4.2. Visits to International Teams

- L. Grigori, visit to U.C. Berkeley for 1 month (August 2013) in the context of COALA Inria associated team.

9. Dissemination

9.1. Scientific Animation

Xavier Claeys reviewed articles for the following journals:

- American Mathematical Society
- Comptes Mathématiques de l'Académie des Sciences
- BIT Numerical Mathematics
- Numerical Methods for Partial Differential Equations
- Differential Equations and Applications

Laura Grigori's scientific animation activities are:

- Area Co-chair, Algorithms, IEEE/ACM SuperComputing 2013.
- Area editor for Parallel Computing Journal, Elsevier, since June 2013.
- Member of Program Committee of IEEE International Parallel and Distributed Processing Symposium, IPDPS 2013.

Frederic Hecht's scientific animation activities are:

- Organization of FreeFem++ days, December 2013, UPMC. There were around 60 participants from different countries (France, Italy, Spain, Slovenia).

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Master : Xavier Claeys, MM009: Informatique de base, 72 hrs de travaux pratiques en programmation C++, niveau M1, Université Pierre et Marie Curie, France

Master : Xavier Claeys, NM406: Résolution des EDP par la méthode des éléments finis, 18 hrs de travaux pratiques en programmation C++, niveau M2, Université Pierre et Marie Curie, France

Master : Xavier Claeys, MM031: Informatique Scientifique, 44 hrs de de cours magistral, niveau M1, Université Pierre et Marie Curie, France

Master : Laura Grigori, High performance computing, 12 hours, Master Universite Paris XI, France

Master : Laura Grigori, Course on Parallel Computing, 30 hours IFIPS, Ingenieurs 3, Polytech, Université Paris XI, France

Master : Frederic Hecht, Tutorials of practical C++ programming for the course *Informatique de Base*, 36 hours, Master 1 Mathématiques et Applications, UPMC, France

Master : Frederic Hecht, Course on Numerical methods for fluid mechanics, 30 hours, Master 2 Mechanics, UPMC, France.

Master : Frederic Hecht, From PDEs to their resolution by finite element methods, 36 hours per year, Master 2 UPMC, France.

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.

9.2.2. Supervision

PhD : Amal Khabou, Dense matrix computations : communication cost and numerical stability, University Paris-Sud 11, February 2013, advisor Laura Grigori

PhD in progress : Sebastien Cayrols, since October 2013 (funded by Maison de la simulation), adivsor L. Grigori.

PhD in progress : Pierre Jolivet, since October 2011 (funded by University of Grenoble), advisors F. Nataf, C. Prudhome and F. Hecht

PhD in progress : Sophie Moufawad, since October 2011 (funded by Inria), advisor L. Grigori

PhD in progress : Nicole Spillane, since December 2010 (funded by Michelin), co-advisor F. Nataf

PhD in progress : Ryadh Haferssas, since October 2013 (funded by Ecole Doctorale, UPMC), co-advisor F. Nataf

PhD in progress : Sylvain Auliac, since October 2009 (funded by UPMC), advisor F. Hecht

PhD in progress : Pierre-Henri Tournier, since October 2011 (funded by UPMC), advisor F. Hecht and M. Comte

9.2.3. Juries

- Laura Grigori: Phd thesis of Soleiman Youssef, UPMC, December 2013, Invited member.
- Laura Grigori: HDR habilitation of Stef Graillat, UPMC, December 2013, Examinateur.
- Laura Grigori: PhD thesis Mouraid Gouicem, defended on 14 October 2013, LIP6, Paris 6, examinatrice, president of the jury.
- Frederic Nataf : PhD thesis of Paul-Marie Berthe, defended on 18 December 2013, University Paris XIII.
- Frédéric Hecht: Phd thesis Charles Dapogny, defended on 29 december 2013, Univ Rouen, examinateur
- Frédéric Hecht: HDR BENNIS Chakib , defended on 29 november 2013, UMPC, examinateur.
- Frédéric Hecht: Phd thesis Charles Dapogny, defended on 4 december 2013, UMPC, Président.
- Frédéric Hecht: Phd thesis Nicolas Kowalski, defended on 5 december 2013, UMPC, examinateur.
- Frédéric Hecht: Phd thesis Brahim Yahioui, defended on 17 december 2013, UTT, Rapporteur.

9.3. Popularization

Xavier Claeys dedicated an afternoon to participation to the "fête de la science".

10. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

[1] X. CLAEYS, R. HIPTMAIR. *Integral Equations on Multi-Screens*, in "Integral Equations and Operator Theory", August 2013, vol. 77, nᵒ 2, pp. 167-197 [*DOI :* 10.1007/s00020-013-2085-x], http://hal.inria.fr/hal-00910327

[2] P. Have, R. Masson, F. Nataf, M. Szydlarski, H. Xiang, T. Zhao. *Algebraic Domain Decomposition Methods for Highly Heterogeneous Problems*, in "SIAM Journal on Scientific Computing", 2013, vol. 35, n⁰ 3, C284 p. , http://hal.inria.fr/hal-00611997

[3] F. Hecht, S. Auliac, F. Ben Belgacem, Z. Belhachmi. *Quadratic finite elements with non-matching grids for the unilateral boundary contact*, in "ESAIM: Mathematical Modelling and Numerical Analysis", June 2013, vol. 47, n⁰ 4, pp. 1185-1205 [*DOI :* 10.1051/M2AN/2012064], http://hal.inria.fr/hal-00933248

[4] A. Khabou, J. Demmel, L. Grigori, M. Gu. *LU Factorization with Panel Rank Revealing Pivoting and its Communication Avoiding Version*, in "SIAM Journal on Matrix Analysis and Applications", 2013, vol. 34, n⁰ 3 [*DOI :* 10.1137/120863691], http://hal.inria.fr/hal-00872145

[5] S. Nicole, D. Victorita, H. Patrice, F. Nataf, R. Daniel. *Solving generalized eigenvalue problems on the interfaces to build a robust two-level FETI method*, in "Comptes Rendus de l Académie des Sciences - Series I - Mathematics", 2013, vol. 351, n⁰ 5-6, pp. 197-201 [*DOI :* 10.1016/J.CRMA.2013.03.010], http://hal.inria.fr/hal-00912307

International Conferences with Proceedings

[6] G. Ballard, A. Buluc, J. Demmel, L. Grigori, B. Lipshitz, O. Schwartz, S. Toledo. *Communication Optimal Parallel Multiplication of Sparse Random Matrices*, in "25th ACM Symposium on Parallelism in Algorithms and Architectures", Montreal, Canada, ACM, 2013, http://hal.inria.fr/hal-00870940

[7] A.-S. Bonnet-BenDhia, L. Chesnel, P. Ciarlet, X. Claeys, S. Nazarov. *Negative materials and corners in electromagnetism*, in "Report No.3/2013 of Mathematisches Forschungsinstitut Oberwolfach "Computational Electromagnetism and Acoustics"", Oberwolfach, Germany, 2013, http://hal.inria.fr/hal-00937670

[8] F. Nataf, F. Hecht, P. Jolivet, C. Prud'Homme. *Scalable Domain Decomposition Preconditioners For Heterogeneous Elliptic Problems*, in "SC13 - International Conference for High Performance Computing, Networking, Storage and Analysis", Denver, Colorado, United States, ACM, November 2013, 11 p. [*DOI :* 10.1145/2503210.2503212], http://hal.inria.fr/hal-00912755

[9] L. Qu, L. Grigori, F. Nataf. *Parallel design and performance of nested filtering factorization preconditioner*, in "SuperComputing 2013", Denver, United States, IEEE/ACM, November 2013, Best student paper finalist, http://hal.inria.fr/hal-00870934

Scientific Books (or Scientific Book chapters)

[10] F. Nataf. *Absorbing boundary conditions and perfectly matched layers in wave propagation problems*, in "Direct and Inverse problems in Wave Propagation and Applications", de Gruyter, 2013, pp. 219-231, http://hal.inria.fr/hal-00799759

Research Reports

[11] X. Claeys, R. Hiptmair, E. Spindler. , *A Second-Kind Galerkin Boundary Element Method for Scattering at Composite Objects*, April 2013, 26 p. , http://hal.inria.fr/hal-00909835

[12] L. Grigori, S. Moufawad. , *Communication Avoiding ILU0 Preconditioner*, Inria, March 2013, n⁰ RR-8266, 21 p. , http://hal.inria.fr/hal-00803250

Other Publications

[13] L. CHESNEL, X. CLAEYS, S. NAZAROV. , *A curious instability phenomenon for a rounded corner in presence of a negative material*, November 2013, http://hal.inria.fr/hal-00909836

[14] L. GRIGORI, M. JACQUELIN, A. KHABOU. , *Multilevel communication optimal LU and QR factorizations for hierarchical platforms*, March 2013, http://hal.inria.fr/hal-00803718