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Activity Report 2018

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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1. Team, Visitors, External Collaborators

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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 data structures for vectors and sparse matrices from the mesh of the subdomain,
4. call to a linear solver,
5. analysis of the result.

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

3.3. Solvers for numerical linear algebra

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

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

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

3.4. Computational kernels for numerical linear 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

We focus on methods related to the blend of time reversal techniques and absorbing boundary conditions (ABC) used in a non standard way. Since the seminal paper by [M. Fink et al., Imaging through inhomogeneous media using time reversal mirrors. Ultrasonic Imaging, 13(2):199, 1991.], time reversal is a subject of very active research. The principle is to back-propagate signals to the sources that emitted them. The initial experiment was to refocus, very precisely, a recorded signal after passing through a barrier consisting of randomly distributed metal rods. In [de Rosny and Fink. Overcoming the 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. In [41], we improve this result from a numerical point of view by showing that it can be done numerically without knowing the source. This is done at the expense of not being able to recover the signal in the vicinity of the source. In [42], time dependent wave splitting is performed using ABC and time reversal techniques. We now work on extending these methods to non uniform media.

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

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

We are interested in the development of fast numerical methods for the simulation of electromagnetic waves in multi-scale situations where the geometry of the medium of propagation may be described through 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 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 characterizing the singular perturbation.

4.4. Data analysis in astrophysics

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

In CMB data analysis, astrophysicists produce and analyze multi-frequency 2D images of the universe when it was 5% of its current age. The new generation of the CMB experiments observes the sky with thousands of detectors over many years, producing overwhelmingly large and complex data sets, which nearly double every year therefore following Moore's Law. Planck (http://planck.esa.int/) is a keystone satellite mission which has been developed under auspices of the European Space Agency (ESA). Planck has been surveying the sky since 2010, produces terabytes of data and requires 100 Petaflops per image analysis of the universe. It is predicted that future experiments will collect half petabyte of data, and will require 100 Exaflops per analysis as early as in 2020. This shows that data analysis in this area, as many other applications, will keep pushing the limit of available supercomputing power for the years to come.

5. Highlights of the Year

5.1. Highlights of the Year

Laura Grigori was awarded with E. Cances, Y. Maday, and J.-P. Piquemal an ERC Syngergy Grant for the Extreme-scale Mathematically-based Computational Chemistry project (EMC2), 2018. A description of the project can be found here.

6. New Software and Platforms

6.1. FreeFem++

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

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

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

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

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

6.2. HPDDM

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

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

6.3. LORASC

LORASC preconditioner
KEYWORD: Preconditioner

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

6.4. Platforms

6.4.1. HTOOL

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

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

6.4.2. BemTool

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

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

6.4.3. Geneo4PETSc

KEYWORD: Domain decomposition method
FUNCTIONAL DESCRIPTION: Implementation of the GenEO preconditioner with PETSc and SLEPc.

- Partners: CNRS - UPMC - European project NLAFET
- Contact: Frédéric Nataf
- URL: https://github.com/geneo4PETSc/geneo4PETSc

6.4.4. ffddm

KEYWORD: Domain decomposition method
FUNCTIONAL DESCRIPTION: In the acronym ffddm, ff stands for FreeFem++ and ddm for domain decomposition methods. The idea behind ffddm is to simplify the use of parallel solvers in FreeFem++: distributed direct methods and domain decomposition methods.

- Partners: CNRS - UPMC
- Contact: Pierre-Henri Tournier and Frédéric Nataf
- URL: https://doc.freefem.org/documentation/ffddm/ffddm

6.4.5. preAlps

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

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

6.4.6. FreeFem++ v4

KEYWORD: New version of Freefem++, with new sparce matrix kernel, and with surface finite element.
FUNCTIONAL DESCRIPTION:

- Partners: UPMC - Inria
- Contact: Frederic Hecht
- URL: https://github.com/FreeFem/FreeFem-sources/tree/v4

7. New Results

7.1. First kind Galerkin boundary element method for the Hodge-Laplacian in three dimensions

Boundary value problems for the Euclidean Hodge-Laplacian in three dimension $-\Delta_{HL} = \mathbf{curl}\mathbf{curl} - \mathbf{grad}\mathrm{div}$ lead to variational formulations set in subspaces of $\mathbf{H}(\mathbf{curl}, \Omega) \cap \mathbf{H}(\mathrm{div}, \Omega)$, $\Omega \subset \mathbb{R}^3$ a bounded Lipschitz domain. Via a representation formula and Calderón identities we derive corresponding first-kind boundary integral equations set in trace spaces of $H^1(\Omega)$, $\mathbf{H}(\mathbf{curl}, \Omega)$, and $\mathbf{H}(\mathrm{div}, \Omega)$. They give rise to saddle-point variational formulations and feature kernels whose dimensions are linked to fundamental topological invariants of Ω.

Kernels of the same dimensions also arise for the linear systems generated by low-order conforming Galerkin boundary element (BE) discretization. On their complements, we can prove stability of the discretized problems, nevertheless. We prove that discretization does not affect the dimensions of the kernels and also illustrate this fact by numerical tests.

7.2. Boundary integral multi-trace formulations and Optimised Schwarz Methods

In the present contribution, we consider Helmholtz equation with material coefficients being constant in each subdomain of a geometric partition of the propagation medium (discarding the presence of junctions), and we are interested in the numerical solution of such a problem by means of local multi-trace boundary integral formulations (local-MTF). For a one dimensional problem and configurations with two subdomains, it has been recently established that applying a Jacobi iterative solver to local-MTF is exactly equivalent to an Optimised Schwarz Method (OSM) with a non-local impendance. In the present contribution, we show that this correspondance still holds in the case where the subdomain partition involves an arbitrary number of subdomains. From this, we deduce that the depth of the adjacency graph of the subdomain partition plays a critical role in the convergence of linear solvers applied to local-MTF: we prove it for the case of homogeneous propagation medium and show, through numerical evidences, that this conclusion still holds for heterogeneous media. Our study also shows that, considering variants of local-MTF involving a relaxation parameter, there is a fixed value of this relaxation parameter that systematically leads to optimal speed of convergence for linear solvers.

7.3. Poroelasticity

In [38], we design and study a fully coupled numerical scheme for the poroelasticity problem modelled through Biot's equations. The classical way to numerically solve this system is to use a finite element method for the mechanical equilibrium equation and a finite volume method for the fluid mass conservation equation. However, to capture specific properties of underground media such as heterogeneities, discontinuities and faults, meshing procedures commonly lead to badly shaped cells for finite element based modelling. Consequently, we investigate the use of the recent virtual element method which appears as a potential discretization method for the mechanical part and could therefore allow the use of a unique mesh for the both mechanical and fluid flow modelling. Starting from a first insight into virtual element method applied to the elastic problem in the context of geomechanical simulations, we apply in addition a finite volume method to take care of the fluid conservation equation. We focus on the first order virtual element method and the two point flux approximation for the finite volume part. A mathematical analysis of this original coupled scheme is provided, including existence and uniqueness results and a priori estimates. The method is then illustrated by some computations on two or three dimensional grids inspired by realistic application cases.

7.4. Hybrid discontinuous Galerkin discretisation and domain decomposition preconditioners for the Stokes problem

Solving the Stokes equation by an optimal domain decomposition method derived algebraically involves the use of nonstandard interface conditions whose discretisation is not trivial. For this reason the use of approximation methods such as hybrid discontinuous Galerkin appears as an appropriate strategy: on the one hand they provide the best compromise in terms of the number of degrees of freedom in between standard continuous and discontinuous Galerkin methods, and on the other hand the degrees of freedom used in the nonstandard interface conditions are naturally defined at the boundary between elements. In this paper, we introduce the coupling between a well chosen discretisation method (hybrid discontinuous Galerkin) and a novel and efficient domain decomposition method to solve the Stokes system. We present the detailed analysis of the hybrid discontinuous Galerkin method for the Stokes problem with non standard boundary conditions. This analysis is supported by numerical evidence. In addition, the advantage of the new preconditioners over more classical choices is also supported by numerical experiments. The full paper [18] is available at https://hal.archives-ouvertes.fr/hal-01967577

7.5. A class of efficient locally constructed preconditioners based on coarse spaces

In [14] we present a class of robust and fully algebraic two-level preconditioners for SPD matrices. We introduce the notion of algebraic local SPSD splitting of an SPD matrix and we give a characterization of this splitting. This splitting leads to construct algebraically and locally a class of efficient coarse spaces which bound the spectral condition number of the preconditioned matrix by a number defined a priori. We also introduce the notion of filtering subspace. This concept helps compare the dimension minimality of coarse spaces. Some PDEs-dependant preconditioners correspond to a special case. The examples of the algebraic coarse spaces in this paper are not practical due to expensive construction. We propose a heuristic approximation that is not costly. Numerical experiments illustrate the efficiency of the proposed method.

7.6. Enlarged Krylov methods for reducing communication

Krylov methods are widely used for solving large sparse linear systems of equations. On distributed architectures, their performance is limited by the communication needed at each iteration of the algorithm. In [34], we study the use of so-called enlarged Krylov subspaces for reducing the number of iterations, and therefore the overall communication, of Krylov methods. In particular, we consider a reformulation of the Conjugate Gradient method using these enlarged Krylov subspaces: the enlarged Conjugate Gradient method. We present the parallel design of two variants of the enlarged Conjugate Gradient method as well as their corresponding dynamic versions where the number of search directions is dynamically reduced during the iterations. For a linear elasticity problem with heterogeneous coefficients using a block Jacobi preconditioner, we show that this implementation scales up to 16,384 cores, and is up to 6,9 times faster than the PETSc implementation of PCG.

In [15] we propose a variant of the GMRES method for solving linear systems of equations with one or multiple right-hand sides. Our method is based on the idea of the enlarged Krylov subspace to reduce communication. It can be interpreted as a block GMRES method. Hence, we are interested in detecting inexact breakdowns. We introduce a strategy to perform the test of detection. Furthermore, we propose an eigenvalues deflation technique aiming to have two benefits. The first advantage is to avoid the plateau of convergence after the end of a cycle in the restarted version. The second is to have a very fast convergence when solving the same system with different right-hand sides, each given at a different time (useful in the context of CPR preconditioner). With the same memory cost, we obtain a saving of up to 50% in the number of iterations to reach convergence with respect to the original method.

7.7. Recycling Krylov subspaces and reducing deflation subspaces for solving a sequence of linear systems

In [32] we present deflation strategies related to recycling Krylov subspace methods for solving one or a sequence of linear systems of equations. Besides well-known strategies of deflation, Ritz and harmonic Ritz based deflation, we introduce an SVD-based deflation technique. We consider the recycling in two contexts, recycling the Krylov subspace between the cycles of restarts and recycling a deflation subspace when the matrix changes in a sequence of linear systems. Numerical experiments on real-life reservoir simulations demonstrate the impact of our proposed strategy.

7.8. Solving linear equations with messenger-field and conjugate gradient techniques: an application to CMB data analysis

In [26] we discuss linear system solvers invoking a messenger-field and compare them with (preconditioned) conjugate gradients approaches. We show that the messenger-field techniques correspond to fixed point iterations of an appropriately preconditioned initial system of linear equations. We then argue that a conjugate gradient solver applied to the same preconditioned system, or equivalently a preconditioned conjugate gradient solver using the same preconditioner and applied to the original system, will in general ensure at least a comparable and typically better performance in terms of the number of iterations to convergence and time-to-solution. We illustrate our conclusions on two common examples drawn from the Cosmic Microwave Background data analysis: Wiener filtering and map-making. In addition, and contrary to the standard lore in the CMB field, we show that the performance of the preconditioned conjugate gradient solver can depend importantly on the starting vector. This observation seems of particular importance in the cases of map-making of high signal-to-noise sky maps and therefore should be of relevance for the next generation of CMB experiments.

7.9. Low rank approximation of a sparse matrix based on LU factorization with column and row tournament pivoting

In [23] 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.

7.10. ALORA: affine low-rank approximations

In [17] we introduce the concept of affine low-rank approximation for an $m \times n$ matrix, consisting in fitting its columns into an affine subspace of dimension at most $k << \min(m, n)$. We show that the optimal affine approximation can be obtained by applying an orthogonal projection to the matrix before constructing its best approximation. Moreover, we present the algorithm ALORA that constructs an affine approximation by slightly modifying the application of any low-rank approximation method. We focus on approximations created with the classical QRCP and subspace iteration algorithms. For the former, we present a detailed analysis of the existing pivoting techniques and furthermore, we provide a bound for the error when an arbitrary pivoting technique is used. For the case of subspace iteration, we prove a result on the convergence of singular vectors, showing a bound that is in agreement with the one for convergence of singular values proved recently. Finally, we present numerical experiences using challenging matrices taken from different fields, showing good performance and validating the theoretical framework.

7.11. Linear-time CUR approximation of BEM matrices

In [33] we propose linear-time CUR approximation algorithms for admissible matrices obtained from the hierarchical form of Boundary Element matrices. We propose a new approach called geometric sampling to obtain indices of most significant rows and columns using information from the domains where the problem is posed. Our strategy is tailored to Boundary Element Methods (BEM) since it uses directly and explicitly the cluster tree containing information from the problem geometry. Our CUR algorithm has precision comparable with low-rank approximations created with the truncated QR factorization with column pivoting (QRCP) and the Adaptive Cross Approximation (ACA) with full pivoting, which are quadratic-cost methods. When compared to the well-known linear-time algorithm ACA with partial pivoting, we show that our algorithm improves, in general, the convergence error and overcomes some cases where ACA fails. We provide a general relative error bound for CUR approximations created with geometrical sampling. Finally, we evaluate the performance of our algorithms on traditional BEM problems defined over different geometries.

7.12. Fractional decomposition of matrices and parallel computing

In [40] we are interested in the design of parallel numerical schemes for linear systems. We give an effective solution to this problem in the following case: the matrix A of the linear system is the product of p nonsingular matrices A_i^m with specific shape: $A_i = I - h_i X$ for a fixed matrix X and real numbers h_i. Although having the special form, these matrices A_i arise frequently in the discretization of evolutionary Partial Differential Equations. The idea is to express A^{-1} as a linear combination of elementary matrices A_i^{-k}. Hence the solution of the linear system with matrix A is a linear combination of the solutions of linear systems with matrices A_i^k. These systems are solved simultaneously on different processors.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Contract with Total, February 2015 - August 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 - April 2019, that funds the Phd thesis of Zakariae Jorti on adaptive preconditioners using a posteriori error estimators. Supervisor L. Grigori.
- Contract with IFPen, October 2016 - October 2019, that funds the Phd thesis of Julien Coulet on the virtual element method (VEM). Supervisor F. Nataf and V. Girault.
- Contract with Total, February - September 2018, that funded an internship on Helmholtz domain decomposition solvers for multiple right hand sides. Supervisor F. Nataf.

9. Partnerships and Cooperations

9.1. Regional Initiatives

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

9.2. National Initiatives

9.2.1. ANR

9.2.1.1. B3DCMB

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

9.2.1.2. ANR Cine-Para

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

9.2.1.3. Non-local DD

ANR appel à projet générique October 2015 - September 2020

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

9.2.1.4. 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.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. NLAFET (197)

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

Programm: H2020

Duration: November 2015 - April 2019

Coordinator: UMEÅ Universitet

Partners:

- Science and Technology Facilities Council (United Kingdom)
- Computer Science Department, UmeåUniversitet (Sweden)
- Mathematics Department, The University of Manchester (United Kingdom)
- Inria, Alpines group

Inria contact: Laura Grigori

The 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.

9.4. International Initiatives

9.4.1. Inria International Partners

9.4.1.1. Informal International Partners

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

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Visit to Xavier Claeys of Jan Zapletal from IT4Innovation of University of Ostrava, Czech Republic from 4th to 30th of March 2018. The main topic of the visit was discussions around HPC implementation of multi-trace formulations in the BEM code of IT4Innovation.
- Visit to Laura Grigori of Agnieszka Miedlar, University of Kansas, from Jun 2018 until Jul 2018.
- Visit to Laura Grigori of Qiang Niu, Xi'an Jiaotong Liverpool University, from May 2018 until Jul 2018.
- Visit to Frédéric Nataf of Lawrence Mitchell from University of Durham (UK) from December 17th to 22nd. The main topic of the visit was to finalize the interface of the finite element software Firedrake to our library geneo4PETSc.
- Visit to Frédéric Hecht of T. Chacon of Differential equations and numerical analysis at University of Seville Rectorate form April 23th to May 4th.
- Visit to Frédéric Hecht of P. Degond of Department of Mathematics at Imperial College London form Juin 6th to 10th.

9.5.1.1. Internships

- Visit to Xavier Claeys of Michal Kravchenko from IT4Innovation of University of Ostrava, Czech Republic from 1st of October to 28th of December 2018. The main subject of the visit was effective implementation of multi-trace formulations in the BEM code of IT4Innovation.

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

- Visit of Xavier Claeys to Ralf Hiptmair at ETH Zuerich from the 19th of August to 25th of August 2018. The main subject of the visit was discussion on boundary integral equations adapted to low frequency electromagnetics.
- Visit of Xavier Claeys to Paul Escapil-Inchauspe at Pontificia Universidad Catholica at Santiago Chile for further collaboration around analysis of local multi-trace formulation for electromagnetics.
- Visit of Laura Grigori to the group of Professor J. Demmel, UC Berkeley, for 6 weeks in July and August 2018.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- Xavier Claeys was co-chair of the "Symposium of the International Association for Boundary Element Methods" in June 26-28 2018, an international conference that took place in Jussieu campus of Sorbonne Université and hosted 140 participants.
- Frederic Hecht organized the 10th FreeFem++ days (December 12-14, 2018, Paris), https://freefem.org/ff-days/

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

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

10.1.3. Invited Talks

- Xavier Claeys was invited speaker at the second national congress of the Société Mahématique de France (SMF) in June 2018.
- Laura Grigori was
  - Keynote speaker, International Symposium on Computational Science at Scale, September 2018, Erlangen-Nurnberg Germany.
  - Invited plenary speaker, SIAM Conference on Applied Linear Algebra, Hong Kong May 2018.
- Frédéric Nataf was invited speaker at
  - Workshop for Robert Scheichl’s farewell, Bath University, November 2018.
  - NUMACH 2018: Numerical Methods for Challenging Problems, Mulhouse (France) July 2018.
  - 10th International Workshop on Parallel Matrix Algorithms and Applications (PMAA’18) in ETH Zurich (Switzerland) June 2018.

- Frédéric Hecht was invited speaker at
  - XVIII Spanish-French school Jacques-Louis Lions about numerical simulation in physics and engineering, Las Palmas de Gran Canaria, 25-29 June 2018.

10.1.4. Leadership within the Scientific Community

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

10.1.5. 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.

10.1.6. Research Administration

- Laura Grigori is vice-president of the committee CE46 of ANR, September 2017 - July 2018.
- Frédéric Nataf is president of the committee CE40 of ANR, September 2017 - current.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master 2: Laura Grigori, Course on *High performance computing, large scale linear algebra, and numerical stability* (*Calcul haute performance, algorithmes parallèles d'algèbre linéaire à grande echelle, stabilité numérique* in french), https://who.rocq.inria.fr/Laura.Grigori/TeachingDocs/UPMC_Master2/Spr2018.html, Master 2nd year, Mathematics & Applications, UPMC, 24 hours of lectures per year.

Master 2: Laura Grigori, Winter 2018, Participation in the course on High Performance Computing given at UPMC, Computer Science, intervention for 8 hours per year.

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

Master 1: Xavier Claeys, supervision of a student project for a group of 4 students in the curriculum Polytech, 40hrs, UPMC.

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

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

Master 1: Xavier Claeys, Approximation of EDPs, 24 hrs of programming tutorials in Python, UPMC.

Master 2: Frédéric Nataf, Course on Domain Decomposition Methods, UPMC

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

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

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

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

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

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

10.2.2. Supervision

PhD: Alan Ayala, Complexity reduction methods applied to the rapid solution to multi-trace boundary integral formulations, Sorbonne Université, November 2018 (funded by NLAFET H2020 project), co-advisors Xavier Claeys and Laura Grigori.

PhD: Hussam Al Daas, Solving linear systems arising from reservoirs modelling, Sorbonne Université, December 2018, (funded by contract with Total), advisor Laura Grigori.

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

PhD in progress: Olivier Tissot, since October 2015 (funded by NLAFET H2020 project), advisor Laura Grigori.

PhD in progress: Rim El Dbaissy, since November 2015 (funded by Univ. St Joseph, Liban), advisors Tony Sayah, Frédéric Hecht.

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

PhD in progress: Zakariae Jorti, since February 2016 (funded by IFPen), advisor Laura Grigori.

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

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

10.2.3. Juries

- Xavier Claeys was examiner at the PhD defense of Wen Xu on the 17th of July 2018 at École Centrale Supélec. Title of the thesis: "Relevant numerical methods for mesoscale wave propagation in heterogeneous media".
- Laura Grigori was examiner of the Phd defense of Gilles Moreau, ENS Lyon, December 2018.
- Laura Grigori was president of the HDR habilitation defense of Pierre Fortin, Sorbonne University, July 2018.
- Laura Grigori was examiner of the Phd defense of Amanda Bienz, June 2018, University of Illinois at Urbana Champaign.
- Frédéric Nataf was examiner at the Phd defense of Louis Viot, 2018, ENS Cachan
- Frédéric Nataf was president of the PhD defense of H. Al Daas, 2018, UPMC
- Frédéric Hecht was referee of the HDR habilitation defense of S. Glockner, 2018, I2M, Bordeaux
- Frédéric Hecht was referee of the PhD defense of G. Dollé, 2018, Univ. Strasbourg
- Frédéric Hecht was examiner at the Phd defense of G. Morel, 2018, Sorbonne University

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

Laura Grigori is vice-president of the Evaluation Commission of Inria, March 2018 - current.

11. Bibliography

Major publications by the team in recent years

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[2] X. CLAEYS, R. HIPTMAIR. *Integral equations for electromagnetic scattering at multi-screens*, in "Integral Equations Operator Theory", 2016, vol. 84, n^{o} 1, pp. 33–68, https://doi-org.accesdistant.sorbonne-universite.fr/10.1007/s00020-015-2242-5

[3] X. CLAEYS, R. HIPTMAIR, E. SPINDLER. *Second kind boundary integral equation for multi-subdomain diffusion problems*, in "Adv. Comput. Math.", 2017, vol. 43, n^{o} 5, pp. 1075–1101, https://doi-org.accesdistant.sorbonne-universite.fr/10.1007/s10444-017-9517-0

[4] J. W. DEMMEL, L. GRIGORI, M. HOEMMEN, J. LANGOU. *Communication-optimal parallel and sequential QR and LU factorizations*, in "SIAM Journal on Scientific Computing", 2012, n^{o} 1, pp. 206-239, short version of technical report UCB/EECS-2008-89 from 2008

[5] V. DOLEAN, P. JOLIVET, F. NATAF. *An Introduction to Domain Decomposition Methods: algorithms, theory and parallel implementation*, SIAM, 2015

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[9] F. HECHT. *New development in FreeFem++*, in "J. Numer. Math.", 2012, vol. 20, n^{o} 3-4, pp. 251–265

[10] P. JOLIVET, F. NATAF. *HPDDM: High-Performance Unified framework for Domain Decomposition methods, MPI-C++ library*, 2014, https://github.com/hpddm/hpddm

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Publications of the year

Doctoral Dissertations and Habilitation Theses

[12] H. AL DAAS. *Solving linear systems arising from reservoirs modelling*, Inria Paris ; Sorbonne Université, UPMC University of Paris 6, Laboratoire Jacques-Louis Lions, December 2018, https://hal.inria.fr/tel-01984047

[13] A. A. OBREGÓN. *Complexity reduction methods applied to the rapid solution to multi-trace boundary integral formulations*, Sorbonne University , UPMC, November 2018, https://tel.archives-ouvertes.fr/tel-02004298

Articles in International Peer-Reviewed Journals

[14] H. AL DAAS, L. GRIGORI. *A class of efficient locally constructed preconditioners based on coarse spaces*, in "SIAM Journal on Matrix Analysis and Applications", 2018, https://hal.inria.fr/hal-01963067

[15] H. AL DAAS, L. GRIGORI, P. HÉNON, P. RICOUX. *Enlarged GMRES for solving linear systems with one or multiple right-hand sides*, in "IMA Journal of Numerical Analysis", August 2018, https://hal.inria.fr/hal-01963032

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[22] L. CHESNEL, X. CLAEYS, S. A. NAZAROV. *Oscillating behaviour of the spectrum for a plasmonic problem in a domain with a rounded corner*, in "ESAIM: Mathematical Modelling and Numerical Analysis", September 2018 [*DOI :* 10.1051/M2AN/2016080], https://hal.archives-ouvertes.fr/hal-01240977

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