



IN PARTNERSHIP WITH:
CNRS

**Université Pierre et Marie Curie
(Paris 6)**

Activity Report 2017

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**

Table of contents

1. Personnel	1
2. Overall Objectives	2
3. Research Program	2
3.1. Overview	2
3.2. Domain specific language - parallel FreeFem++	2
3.3. Solvers for numerical linear algebra	3
3.4. Computational kernels for numerical linear algebra	3
4. Application Domains	4
4.1. Compositional multiphase Darcy flow in heterogeneous porous media	4
4.2. Inverse problems	4
4.3. Numerical methods for wave propagation in multi-scale media	4
4.4. Data analysis in astrophysics	5
5. Highlights of the Year	5
6. New Software and Platforms	5
6.1. FreeFem++	5
6.2. HPDDM	6
6.3. LORASC	6
6.4. Platforms	6
6.4.1. HTOOL	6
6.4.2. BemTool	6
7. New Results	7
7.1. Communication avoiding algorithms for preconditioned iterative methods	7
7.2. Communication avoiding algorithms for low rank matrix approximation	7
7.3. Domain decomposition preconditioning for high frequency wave propagation problems	8
7.4. First kind boundary integral formulation for the Hodge-Helmholtz equation	8
7.5. Integral equation based optimized Schwarz method for electromagnetics	8
7.6. Quasi-local Multi-Trace formulations for electromagnetics	9
7.7. Domain decomposition preconditioning with approximate coarse solve	9
8. Bilateral Contracts and Grants with Industry	9
9. Partnerships and Cooperations	10
9.1. National Initiatives	10
9.1.1.1. B3DCMB	10
9.1.1.2. Medimax	10
9.1.1.3. ANR Cine-Para	10
9.1.1.4. Non-local DD	10
9.1.1.5. Soil μ -3D	10
9.2. European Initiatives	11
9.2.1.1. NLAFET	11
9.2.1.2. EXA2CT	12
9.3. International Initiatives	12
9.4. International Research Visitors	13
9.4.1. Visits of International Scientists	13
9.4.2. Visits to International Teams	13
10. Dissemination	13
10.1. Promoting Scientific Activities	13
10.1.1. Scientific Events Organisation	13
10.1.2. Journal	13
10.1.2.1.1. Laura Grigori	13
10.1.2.1.2. Frédéric Nataf	13

10.1.3. Invited Talks	13
10.1.4. Leadership within the Scientific Community	14
10.1.5. Scientific Expertise	14
10.1.6. Research Administration	14
10.2. Teaching - Supervision - Juries	14
10.2.1. Teaching	14
10.2.1.1. Xavier Claeys	14
10.2.1.2. Laura Grigori	14
10.2.1.3. Frédéric Hecht	14
10.2.1.4. Frédéric Nataf	15
10.2.2. Supervision	15
10.2.3. Juries	15
11. Bibliography	15

Project-Team ALPINES

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

Other Research Topics and Application Domains:

- B3.3.1. - Earth and subsoil
- B9.4.2. - Mathematics
- B9.4.3. - Physics

1. Personnel

Research Scientists

Laura Grigori [Team leader, Inria, Senior Researcher, HDR]
Frédéric Nataf [CNRS, Senior Researcher]

Faculty Members

Xavier Claeys [Univ Pierre et Marie Curie, Associate Professor]
Frédéric Hecht [Univ Pierre et Marie Curie, Professor]

Post-Doctoral Fellows

Jan Papez [Inria, from Mar 2017]
Amin Rafiei [Ambassade de France, from Nov 2017]

PhD Students

Hussam Al Daas [Inria]
Alan Ayala Obregon [Inria]
Sebastien Cayrols [Inria]
Igor Chollet [Univ Pierre et Marie Curie, from Oct 2017]
Zakariae Jorti [IFPEN]
Pierre Marchand [Inria]
Van Thanh Nguyen [Inria, from Nov 2017]
Olivier Tissot [Inria]

Technical staff

Simplice Donfack [Inria]
Franck Houssen [Inria, from Apr 2017]
Ange Toulougoussou [Inria, until Feb 2017]
Pierre-Henri Tournier [CNRS]

Interns

Igor Chollet [Inria, from Mar 2017 until Jul 2017]
Alaeddine Jlaiel [Inria, from May 2017 until Aug 2017]
Hao Song [Inria, from Mar 2017]
David Wobrock [Inria, from Sep 2017]

Administrative Assistant

Laurence Bourcier [Inria]

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

3.4. Computational kernels for numerical linear algebra

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

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

4. Application Domains

4.1. Compositional multiphase Darcy flow in heterogeneous porous media

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

4.2. Inverse problems

The research of F. Nataf on inverse problems is rather new since this activity was started from scratch in 2007. Since then, several papers were published in international journals and conference proceedings. All our numerical simulations were performed in FreeFem++.

We focus on methods related to time reversal techniques. Since the seminal paper by [M. Fink et al., Imaging through inhomogeneous media using time reversal mirrors. *Ultrasonic Imaging*, 13(2):199, 1991.], time reversal is a subject of very active research. The main idea is to take advantage of the reversibility of wave propagation phenomena such as it occurs in acoustics, elasticity or electromagnetism in a non-dissipative unknown medium to back-propagate signals to the sources that emitted them. Number of industrial applications have already been developed: touchscreen, medical imaging, non-destructive testing and underwater communications. The principle is to back-propagate signals to the sources that emitted them. The initial experiment was to refocus, very precisely, a recorded signal after passing through a barrier consisting of randomly distributed metal rods. In [de Rosny and Fink. Overcoming the diffraction limit in wave physics using a time-reversal mirror and a novel acoustic sink. *Phys. Rev. Lett.*, 89 (12), 2002], the source that created the signal is time reversed in order to have a perfect time reversal experiment. Since then, numerous applications of this physical principle have been designed, see [Fink, Renversement du temps, ondes et innovation. Ed. Fayard, 2009] or for numerical experiments [Larmat et al., Time-reversal imaging of seismic sources and application to the great sumatra earthquake. *Geophys. Res. Lett.*, 33, 2006] and references therein.

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

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

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

4.4. Data analysis in astrophysics

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

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

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards and Recognitions

5.1.1.1. Laura Grigori elected Member of the SIAM Council

January 2018 - December 2020.

6. New Software and Platforms

6.1. FreeFem++

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

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

7. New Results

7.1. Communication avoiding algorithms for preconditioned iterative methods

Our group continues to work on algorithms for dense and sparse linear algebra operations that minimize communication, introduced in [1], [4]. An overview of communication avoiding algorithms for dense linear algebra operations is presented in [18]. During this year we focused on communication avoiding iterative methods and designing algorithms for computing rank revealing and low rank approximations of dense and sparse matrices.

Iterative methods are widely used in industrial applications, and in the context of communication avoiding algorithms, our research is related to increasing the scalability of Krylov subspace iterative methods. Indeed the dot products related to the orthogonalization of the Krylov subspace and performed at each iteration of the Krylov method require collective communication among all processors. This collective communication does not scale to very large number of processors, and thus is a main bottleneck in the scalability of Krylov subspace methods. Our research focuses on enlarged Krylov subspace methods, a new approach that we have introduced in the recent years [5] that consists of enlarging the Krylov subspace by a maximum of t vectors per iteration, based on a domain decomposition of the graph of the input matrix. The solution of the linear system is searched in the enlarged subspace, which is a superset of the classic subspace. The enlarged Krylov projection subspace methods lead to faster convergence in terms of iterations and parallelizable algorithms with less communication, with respect to Krylov methods.

In [20] we propose an algebraic method in order to reduce dynamically the number of search directions during block Conjugate Gradient iterations. Indeed, by monitoring the rank of the optimal step α_k it is possible to detect inexact breakdowns and remove the corresponding search directions. We also propose an algebraic criterion that ensures in theory the equivalence between our method with dynamic reduction of the search directions and the classical block Conjugate Gradient. Numerical experiments show that the method is both stable, the number of iterations with or without reduction is of the same order, and effective, the search space is significantly reduced. We use this approach in the context of enlarged Krylov subspace methods which reduce communication when implemented on large scale machines. The reduction of the number of search directions further reduces the computation cost and the memory usage of those methods.

In [19] 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.

7.2. Communication avoiding algorithms for low rank matrix approximation

Our work focuses on computing the low rank approximation of a sparse or dense matrix, while also minimizing communication, [3].

In [21] we introduce an URV Factorization with Random Orthogonal System Mixing. The unpivoted and pivoted Householder QR factorizations are ubiquitous in numerical linear algebra. A difficulty with pivoted Householder QR is the communication bottleneck introduced by pivoting. In this paper we propose using random orthogonal systems to quickly mix together the columns of a matrix before computing an unpivoted QR factorization. This method computes a URV factorization which forgoes expensive pivoted QR steps in exchange for mixing in advance, followed by a cheaper, unpivoted QR factorization. The mixing step typically reduces the variability of the column norms, and in certain experiments allows us to compute

an accurate factorization where a plain, unpivoted QR performs poorly. We experiment with linear least-squares, rank-revealing factorizations, and the QLP approximation, and conclude that our randomized URV factorization behaves comparably to a similar randomized rank-revealing URV factorization, but at a fraction of the computational cost. Our experiments provide evidence that our proposed factorization might be rank-revealing with high probability.

7.3. Domain decomposition preconditioning for high frequency wave propagation problems

This work studies preconditioning the Helmholtz and Maxwell equations, where the preconditioner is constructed using two-level overlapping Additive Schwarz Domain Decomposition. The coarse space is based on the discretisation of the PDE on a coarse mesh. The PDE is discretised using finite-element methods of fixed, arbitrary order. The theoretical part of this work is the Maxwell analogue of a previous work for Helmholtz equation, and shows that for Maxwell problems with absorption, if the absorption is large enough and if the subdomain and coarse mesh diameters are chosen appropriately, then classical two-level overlapping Additive Schwarz Domain Decomposition preconditioning performs optimally – in the sense that GMRES converges in a wavenumber-independent number of iterations. An important feature of the theory is that it allows the coarse space to be built from low-order elements even if the PDE is discretised using high-order elements. This theory is presented in [24] and is illustrated by numerical experiments, which also (i) explore replacing the PEC boundary conditions on the subdomains by impedance boundary conditions, and (ii) show that the preconditioner for the problem with absorption is also an effective preconditioner for the problem with no absorption. The numerical results include two substantial examples arising from applications; the first (a problem arising in medical imaging from the Medimax ANR project) shows the robustness of the preconditioner against heterogeneity, and the second (scattering by a COBRA cavity) shows good scalability of the preconditioner with up to 3000 processors. The parallel implementation was done using FreeFem++ and HPDDM. We performed additional numerical studies of this two-level Domain Decomposition preconditioner for the Maxwell equations in [23], and for the Helmholtz equation (in 2D and 3D) in [25], where we also compare it to another two-level Domain Decomposition preconditioner where the coarse space is built by solving local eigenproblems on the interface between subdomains involving the Dirichlet-to-Neumann (DtN) operator.

7.4. First kind boundary integral formulation for the Hodge-Helmholtz equation

We adapt the variational approach to the analysis of first-kind boundary integral equations associated with strongly elliptic partial differential operators from [M. COSTABEL, *Boundary integral operators on Lipschitz domains: Elementary results*, SIAM J. Math. Anal., 19 (1988), pp. 613–626.] to the (scaled) Hodge-Helmholtz equation $\operatorname{curl} \operatorname{curl} \mathbf{u} - \eta \nabla \operatorname{div} \mathbf{u} - \kappa^2 \mathbf{u} = 0$, $\eta > 0$, $\operatorname{Im} \kappa^2 \geq 0$, on Lipschitz domains in 3D Euclidean space, supplemented with natural complementary boundary conditions, which, however, fail to bring about strong ellipticity.

Nevertheless, a boundary integral representation formula can be found, from which we can derive boundary integral operators. They induce bounded and coercive sesqui-linear forms in the natural energy trace spaces for the Hodge-Helmholtz equation. We can establish precise conditions on η, κ that guarantee unique solvability of the two first-kind boundary integral equations associated with the natural boundary value problems for the Hodge-Helmholtz equations. Particular attention needs to be given to the case $\kappa = 0$.

7.5. Integral equation based optimized Schwarz method for electromagnetics

The optimized Schwarz method (OSM) is recognised as one of the most efficient domain decomposition strategies without overlap for the solution to wave propagation problems in harmonic regime. For the Helmholtz equation, this approach originated from the seminal work of Després, and led to the development of an abundant literature offering more elaborated but more efficient transmission conditions. Most contributions focus on transmission conditions based on local operators.

In recent years, F. Collino, P. Joly and M. Lecouvez introduced non-local transmission conditions that can drastically improve the convergence rate of OSM. The performance of this strategy seems to remain robust at high frequency. Such an approach was proposed only for the Helmholtz equation, and has still not been adapted to electromagnetics.

In this work we investigated such an approach for Maxwell's equations in a simple spherical geometry that allows explicit calculus by means of separation of variables. The transmission condition that we propose involves a non-local operator that is a dissipative counterpart of the so-called Electric Field integral operator (EFIE) which is a classical object in electromagnetic potential theory. We show that the iterative solver associated to our strategy converges at an exponential rate.

7.6. Quasi-local Multi-Trace formulations for electromagnetics

Multi-trace formulations (MTF) are a general methodology to derive first kind boundary integral formulations for harmonic wave scattering problems posed in multi-domain geometrical configurations. There exists both a local and a global variant of MTF that only differ through the way transmission conditions are imposed across interfaces. Global MTF is easier to analyse but, from a computational viewpoint, local MTF appears more appealing because it looks computationally cheaper.

As regards local MTF, a decent stability theory has been developed for acoustic scalar wave propagation, but no such result as Garding inequality or uniform discrete inf-sup condition has been established so far for local MTF in the case of electromagnetics. Whether or not local MTF is stable for electromagnetics is actually an open question presently.

In this work, we have adopted a slightly modified version of local MTF where transmission conditions are imposed by means of an operator that is non-local, but with a kernel whose support can be as small as desired. This so-called quasi-local MTF approach has previously been developed for acoustics and we adapted it to the case of electromagnetics. We could in particular prove a Garding inequality for quasi-local MTF applied to electromagnetics, and thus obtain uniform discrete inf-sup condition.

7.7. Domain decomposition preconditioning with approximate coarse solve

Convergence of domain decomposition methods relies heavily on the efficiency of the coarse space used in the second level. The GenEO coarse space has been shown to lead to a fully robust two-level Schwarz preconditioner which scales well over multiple cores [9], [2] as has been proved rigorously in [9]. The robustness is due to its good approximation properties for problems with highly heterogeneous material parameters. It is available in the finite element packages FreeFem++ [7], Feel++ [31] and recently in Dune [30] and is implemented as a standalone library in HPDDM [8]. But the coarse component of the preconditioner can ultimately become a bottleneck if the number of subdomains is very large and exact solves are used. It is therefore interesting to consider the effect of approximate coarse solves. In [28], robustness of GenEO methods is analyzed with respect to approximate coarse solves. Interestingly, the GenEO-2 method introduced in [6] has to be modified in order to be able to prove its robustness in this context.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Contract with Total, February 2015 - February 2018, that funds the PhD thesis of Hussam Al Daas on enlarged Krylov subspace methods for oil reservoir and seismic imaging applications. Supervisor L. Grigori.
- Contract with IFPEN, February 2016 - February 2019, that funds the PhD thesis of Zakariae Jorti on adaptive preconditioners using a posteriori error estimators. Supervisor L. Grigori.
- Contract with IFPEN, October 2016 - October 2019, that funds the PhD thesis of Julien Coulet on the virtual element method (VEM). Supervisor F. Nataf and V. Girault.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

9.1.1.1. 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.

9.1.1.2. 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.

9.1.1.3. ANR Cine-Para

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

9.1.1.4. Non-local DD

ANR appel à projet générique October 2015 - September 2020

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

9.1.1.5. Soil μ -3D

ANR appel à projet générique October 2015 - September 2020

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

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

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

9.2. European Initiatives

9.2.1. FP7 & H2020 Projects

9.2.1.1. NLAFET

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

Programm: H2020

Duration: November 2015 - November 2018

Coordinator: UMEÅUniversitet

Partners:

Science and Technology Facilities Council (United Kingdom)

Computer Science Department, UmeåUniversitet (Sweden)

Mathematics Department, The University of Manchester (United Kingdom)

Infria contact: Laura Grigori

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

9.2.1.2. EXA2CT

Title: EXascale Algorithms and Advanced Computational Techniques

Programm: FP7

Duration: September 2013 - August 2016

Coordinator: IMEC

Partners:

Fraunhofer-Gesellschaft Zur Foerderung Der Angewandten Forschung E.V (Germany)

Interuniversitair Micro-Electronica Centrum Vzw (Belgium)

Intel Corporations (France)

Numerical Algorithms Group Ltd (United Kingdom)

T-Systems Solutions for Research (Germany)

Universiteit Antwerpen (Belgium)

Universita della Svizzera italiana (Switzerland)

Université de Versailles Saint-Quentin-En-Yvelines. (France)

Vysoka Skola Banska - Technicka Univerzita Ostrava (Czech Republic)

Inria contact: Luc Giraud

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

9.3. International Initiatives

9.3.1. Inria International Partners

9.3.1.1. Informal International Partners

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

9.4. International Research Visitors

9.4.1. Visits of International Scientists

- Ralf Hiptmair (ETH Zürich) came to visit Xavier Claeys for a sabbatical semester, from January to June 2017.
- Mahadevan Ganesh (Colorado School of Mines) came to visit Xavier Claeys from the 4th of July 2017 to 18th of July 2017.
- Carlos Jerez-Hanckes (Pontificia Universidad Catholica, Santiago, Chile) came to visit Xavier Claeys from the 3rd of December to the 16th of December 2017.

9.4.2. Visits to International Teams

9.4.2.1. Research Stays Abroad

- Laura Grigori has spent 3 weeks at UC Berkeley, from July 21, 2016 to August 13, 2016.
- Xavier Claeys visited Catalin Turc (New Jersey Institute of Technology) from the 5th of November to the 14th of November 2017.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- Frederic Hecht: Organized the 9th FreeFem++ days (December 2017, Paris)
- Xavier Claeys was main organiser (together with S. Fliss, B. Delourme and J. Diaz) of the 3 days colloquium "Waves Diffracted by Patrick Joly", in honour of P. Joly's 60th birthday, that took place in Saclay and Gif-sur-Yvette.
- Xavier Claeys and Frédéric Nataf were the main organisers (together with V. Dolean) of a workshop on "Numerical methods for wave propagation and applications" held in Jussieu campus of UPMC on 31st of August and 1st of September.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

10.1.2.1.1. Laura Grigori

- March 2014 – current. Member of the editorial board for the SIAM book series Software, Environments and Tools. See <http://bookstore.siam.org/software-environments-and-tools/>.
- June 2013 – current. Area editor for Parallel Computing Journal, Elsevier
- January 2016 – current. Associate Editor, SIAM Journal on Scientific Computing.
- January 2017 – current. Associate Editor, SIAM Journal on Matrix Analysis and Applications.
- January 2016 – current. Editorial board, Numerical linear algebra with applications Journal, Wiley.

10.1.2.1.2. Frédéric Nataf

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

10.1.3. Invited Talks

- Laura Grigori: Keynote speaker, 46th International Conference on Parallel Processing (ICPP-2017), <http://www.icpp-conf.org/2017/index.php>, Bristol, UK, August 14-17, 2017.

- Laura Grigori: Keynote speaker, Power-Aware Computing Workshop - PACO2017, <https://www2.mpi-magdeburg.mpg.de/mpcsc/events/paco2017/index.php>, July 2017, Germany.
- Laura Grigori: Plenary talk, Householder Symposium XX on Numerical linear algebra, <http://www.math.vt.edu/HHXX/>, June 2017, Virginia Tech.
- Laura Grigori: Invited plenary speaker, International Conference on Domain Decomposition Methods DD XXIV, <http://www.ddm.org/dd24/invited.html>, February 2017, Longyearbyen, Norway.

10.1.4. Leadership within the Scientific Community

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

10.1.5. Scientific Expertise

- Laura Grigori: November 2015 - current, expert to the Scientific Commission of IFPEN (French Petroleum Institute). Evaluation of research programs, PhD theses, work representing a total of 5 days per year.
- Xavier Claeys was member of a hiring committee for a position of maître de conférence in section CNU 60/61 for the Institut de Recherche de Coordination Acoustique et Musicale (IRCAM) and Université Pierre-et-Marie Curie Paris 6, in Spring 2017.

10.1.6. Research Administration

- Laura Grigori: Member of the Director Committee (Comité Directeur) of GIS Geosciences franciliennes, since November 2015.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

10.2.1.1. Xavier Claeys

- Academic year 2017-2018, total number of course hours: 192 hrs
 - Master 1: supervision of a student project for a group of 4 students in the curriculum Polytech, 80hrs, UPMC.
 - Master 1: Initiation to C++, 36 hrs of programming tutorials in C++, UPMC.
 - Master 1: Computational Linear Algebra, 32 hrs of lectures, UPMC.
 - Master 1: Practical programming of the finite element method, 12 hrs of lectures, UPMC.
 - Master 1: Approximation of EDPs, 24 hrs of programming tutorials in Python, UPMC.

10.2.1.2. Laura Grigori

- Spring 2017, Course on *High performance computing, large scale linear algebra, and numerical stability* (*Calcul haute performance, algorithmes parallèles d'algèbre linéaire à grande échelle, stabilité numérique* in french), https://who.rocq.inria.fr/Laura.Grigori/TeachingDocs/UPMC_Master2/Spr2017.html, Master 2nd year, Mathematics & Applications, University Pierre and Marie Curie, 20 hours per year.
- Winter 2017, Participation in the course on High Performance Computing given at University Pierre and Marie Curie, Master 2nd year, Computer Science, intervention for 8 hours per year.

10.2.1.3. Frédéric Hecht

- Academic year 2016-2017, total number of course hours: 192 hrs
 - Master 1: Initiation au C++, 24hrs, M1, Université Pierre-et-Marie Curie Paris 6, France
 - Master 2: Des EDP à leur résolution par la méthode des éléments finis (MEF), 24hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
 - Master 2: Numerical methods for fluid mechanics, 10hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
 - Master 2: Calcul scientifique 3 / projet industriel FreeFem++, 28hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
 - Master 2: Ingénierie 1 / Logiciel pour la simulation (FreeFem++), 21hrs, M2, Université Pierre-et-Marie Curie Paris 6, France
 - Master 2: Ingénierie 2 / Projet collaboratif, 21hrs, M2, Université Pierre-et-Marie Curie Paris 6, France

10.2.1.4. Frédéric Nataf

- Spring 2017: Course on *Domain Decomposition Methods*, Master 2nd year Mathematics & Applications, University Pierre and Marie Curie
- Winter 2017: Course on *Domain Decomposition Methods*, Master 2nd year, Mathematics & Applications, ENSTA and UVSQ

10.2.2. Supervision

- PhD in progress: Alan Ayala, since October 2015 (funded by NLAFFET H2020 project), co-advisors Xavier Claeys and Laura Grigori.
- PhD in progress : Sebastien Cayrols, since October 2013 (funded by Maison de la simulation), advisor Laura Grigori.
- PhD in progress: Hussam Al Daas, since February 2015 (funded by contract with Total), advisor Laura Grigori.
- PhD in progress: Olivier Tissot, since October 2015 (funded by NLAFFET 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 et 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

- Frédéric Hecht, President of the Jury for the PhD thesis of Alexandre LIMAR, Applied Mathematics, UTT, October 2017.
- Laura Grigori, President of the Jury for the PhD thesis of Chaoyu Quan, Applied Mathematics, UPMC, November 2017.
- Frédéric Hecht, President of the Jury for the PhD thesis of Roberto Molina, Applied Mathematics, UPMC, December 2017.

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Major publications by the team in recent years

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- [4] L. GRIGORI, J. DEMMEL, H. XIANG. *CALU: a communication optimal LU factorization algorithm*, in "SIAM Journal on Matrix Analysis and Applications", 2011, vol. 32, pp. 1317-1350
- [5] L. GRIGORI, S. MOUFAWAD, F. NATAF. *Enlarged Krylov Subspace Conjugate Gradient methods for Reducing Communication*, in "SIAM Journal on Matrix Analysis and Applications", 2016, vol. 37, n^o 2, pp. 744-773
- [6] R. HAFERSSAS, P. JOLIVET, F. NATAF. *An Additive Schwarz Method Type Theory for Lions's Algorithm and a Symmetrized Optimized Restricted Additive Schwarz Method*, in "SIAM J. Sci. Comput.", 2017, vol. 39, n^o 4, pp. A1345–A1365, <http://dx.doi.org/10.1137/16M1060066>
- [7] F. HECHT. *New development in FreeFem++*, in "J. Numer. Math.", 2012, vol. 20, n^o 3-4, pp. 251–265
- [8] P. JOLIVET, F. NATAF. *HPDDM: High-Performance Unified framework for Domain Decomposition methods, MPI-C++ library*, 2014, <https://github.com/hpddm/hpddm>
- [9] N. SPILLANE, V. DOLEAN, P. HAURET, F. NATAF, C. PECHSTEIN, R. SCHEICHL. *Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps*, in "Numer. Math.", 2014, vol. 126, n^o 4, pp. 741–770, <http://dx.doi.org/10.1007/s00211-013-0576-y>

Publications of the year

Articles in International Peer-Reviewed Journals

- [10] M. BONAZZOLI, V. DOLEAN, F. RAPETTI, P.-H. TOURNIER. *Parallel preconditioners for high order discretizations arising from full system modeling for brain microwave imaging*, in "International Journal of Numerical Modelling: Electronic Networks, Devices and Fields", 2017 [DOI : 10.1002/JNM.2229], <https://hal.archives-ouvertes.fr/hal-01328197>
- [11] L. A. CHESNEL, X. CLAEYS, S. A. NAZAROV. *Small obstacle asymptotics for a 2D semi-linear convex problem*, in "Applicable Analysis", February 2017, 20 p. [DOI : 10.1080/00036811.2017.1295449], <https://hal.archives-ouvertes.fr/hal-01427617>
- [12] X. CLAEYS, R. HIPTMAIR, E. SPINDLER. *Second-kind boundary integral equations for electromagnetic scattering at composite objects*, in "Computers & Mathematics with Applications", December 2017, vol. 74, n^o 11, pp. 2650 - 2670 [DOI : 10.1016/j.camwa.2017.08.014], <https://hal.inria.fr/hal-01671147>
- [13] X. E. CLAEYS, R. E. HIPTMAIR, E. E. SPINDLER. *Second Kind Boundary Integral Equation for Multi-Subdomain Diffusion Problems*, in "Advances in Computational Mathematics", October 2017, vol. 43, n^o 5, 26 p. , <https://hal.archives-ouvertes.fr/hal-01427625>

- [14] M. J. GROTE, M. KRAY, F. NATAF, F. ASSOUS. *Time-dependent wave splitting and source separation*, in "Journal of Computational Physics", 2017, vol. 330, pp. 981–996, <https://hal.archives-ouvertes.fr/hal-01216117>
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- [18] L. GRIGORI. *Introduction to Communication Avoiding Algorithms for Direct Methods of Factorization in Linear Algebra*, in "SEMA SIMAI Springer Series", M. MATEOS, P. ALONSO (editors), Computational Mathematics, Numerical Analysis and Applications, Springer, 2017, vol. 13, pp. 153-185 [DOI : 10.1007/978-3-319-49631-3_4], <https://hal.inria.fr/hal-01669315>

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- [19] H. AL DAAS, L. GRIGORI, P. HÉNON, P. RICOUX. *Enlarged GMRES for reducing communication*, Inria Paris, March 2017, n^o RR-9049, <https://hal.inria.fr/hal-01497943>
- [20] L. GRIGORI, O. TISSOT. *Reducing the communication and computational costs of Enlarged Krylov subspaces Conjugate Gradient*, Inria Paris, February 2017, n^o RR-9023, <https://hal.inria.fr/hal-01451199>

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- [21] S. BECKER, J. FOLBERTH, L. GRIGORI. *URV Factorization with Random Orthogonal System Mixing*, 2017, working paper or preprint, <https://hal.inria.fr/hal-01669915>
- [22] I. BEN GHARBIA, M. BONAZZOLI, X. CLAEYS, P. MARCHAND, P.-H. TOURNIER. *Fast solution of boundary integral equations for elasticity around a crack network: a comparative study*, November 2017, working paper or preprint, <https://hal.inria.fr/hal-01644518>
- [23] M. BONAZZOLI, V. DOLEAN, I. G. GRAHAM, E. A. SPENCE, P.-H. TOURNIER. *A two-level domain-decomposition preconditioner for the time-harmonic Maxwell's equations*, November 2017, working paper or preprint, <https://hal.archives-ouvertes.fr/hal-01525438>
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