



IN PARTNERSHIP WITH:
CNRS

**Université de Pau et des Pays de
l'Adour**

Activity Report 2016

Project-Team MAGIQUE-3D

Advanced 3D Numerical Modeling in Geophysics

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
**Earth, Environmental and Energy
Sciences**

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Project-Team MAGIQUE-3D

Creation of the Project-Team: 2007 July 01

Keywords:

Computer Science and Digital Science:

- 6. - Modeling, simulation and control
- 6.1. - Mathematical Modeling
- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.1.4. - Multiscale modeling
- 6.1.5. - Multiphysics modeling
- 6.2. - Scientific Computing, Numerical Analysis & Optimization
- 6.2.1. - Numerical analysis of PDE and ODE
- 6.2.7. - High performance computing

Other Research Topics and Application Domains:

- 3. - Environment and planet
- 3.3. - Geosciences
- 3.3.1. - Earth and subsoil
- 4. - Energy
- 4.1. - Fossile energy production (oil, gas)
- 5.5. - Materials

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2. Overall Objectives

2.1. General setting

MAGIQUE-3D is a joint project-team between Inria and the Department of Applied Mathematics (LMA) of the University of Pau, in partnership with CNRS. The mission of MAGIQUE-3D is to develop and validate efficient solution methodologies for solving complex three-dimensional geophysical problems, with a particular emphasis on problems arising in seismic imaging, in response to the local industrial and community needs. Indeed, as it is well known, the region of Pau has long-standing tradition in the Geosciences activities. However, in spite of the recent significant advances in algorithmic considerations as well as in computing platforms, the solution of most real-world problems in this field remains intractable. Hence, there is a scientific need of pressing importance to design new numerical methods for solving efficiently and accurately wave propagation problems defined in strongly heterogeneous domains.

MAGIQUE-3D program possesses an exceptional combination that is a prerequisite for accomplishing its mission: the investigator backgrounds, research interests, and technical skills complement to form a research team with a potential for significant impact on the computational infrastructure of geophysical sciences. The research record of MAGIQUE-3D group covers a large spectrum of accomplishments in the field of wave propagation including (a) the design, validation, and performance assessment of a class of DG-methods for solving efficiently high frequency wave problems, (b) the construction, convergence analysis, and performance assessment of various absorbing-type boundary conditions that are key ingredients for solving problems in infinite domains, and (c) the development of asymptotic models that are the primary candidate in the presence of heterogeneities that are small compared to the wave length. MAGIQUE-3D has built strong collaborations and partnerships with various institutions including (a) local industry (TOTAL), (b) national research centers (ONERA and CEA), and (c) international academic partnerships (e.g. Interdisciplinary Research Institute for the Sciences (IRIS) at California State University, Northridge, USA; University of Pays Basque at Bilbao, Spain; University of Novosibirsk, Russia).

3. Research Program

3.1. Introduction

Probing the invisible is a quest that is shared by a wide variety of scientists such as archaeologists, geologists, astrophysicists, physicists, etc... Magique-3D is involved in Geophysical imaging which aims at understanding the internal structure of the Earth from the propagation of waves. Both qualitative and quantitative information are required and two geophysical techniques can be used: **seismic reflection** and **seismic inversion**. Seismic reflection provides a qualitative description of the subsurface from reflected seismic waves by indicating the position of the reflectors while seismic inversion transforms seismic reflection data into a quantitative

description of the subsurface. Both techniques are inverse problems based upon the numerical solution of wave equations. Oil and Gas explorations have been pioneering application domains for seismic reflection and inversion and even if numerical seismic imaging is computationally intensive, oil companies promote the use of numerical simulations to provide synthetic maps of the subsurface. This is due to the tremendous progresses of scientific computing which have pushed the limits of existing numerical methods and it is now conceivable to tackle realistic 3D problems. However, mathematical wave modeling has to be well-adapted to the region of interest and the numerical schemes which are employed to solve wave equations have to be both accurate and scalable enough to take full advantage of parallel computing. Today, geophysical imaging tackles more and more realistic problems and we can contribute to this task by improving the modeling and by deriving advanced numerical methods for solving wave problems.

Magique-3D proposes to organize its research around three main axes:

1. Mathematical modeling of multi-physics involving wave equations;
2. Supercomputing for Helmholtz problems;
3. Construction of high-order hybrid schemes.

These three research fields will be developed with the main objective of solving inverse problems dedicated to geophysical imaging.

3.2. Mathematical modeling of multi-physics involving wave equations

Wave propagation modeling is of great interest for many applications like oil and gas exploration, non destructive testing, medical imaging, etc. It involves equations which can be solved in time or frequency domain and their numerical approximation is not easy to handle, in particular when dealing with real-world problems. In both cases, the propagation domain is either infinite or its dimensions are much greater than the characteristic wavelength of the phenomenon of interest. But since wave problems are hyperbolic, the physical phenomenon can be accurately described by computing solutions in a bounded domain including the sources which have generated the waves. Until now, we have mainly worked on imaging techniques based on acoustic or elastic waves and we have developed advanced finite element software packages which are used by Total for oil exploration. Nevertheless, research on modeling must go on because there are simulations which can still not be performed because their computational cost is much too high. This is particularly true for complex tectonics involving coupled wave equations. We then propose to address the issue of coupling wave equations problems by working on the mathematical construction of reduced systems. By this way, we hope to improve simulations of elasto-acoustic and electro-seismic phenomena and then, to perform numerical imaging of strongly heterogeneous media. Even in the simplest situation where the wavelengths are similar (elasto-acoustic coupling), the dimension of the discrete coupled problem is huge and it is a genuine issue in the prospect of solving 3D inverse problems.

The accurate numerical simulation of full wave problems in heterogeneous media is computationally intensive since it needs numerical schemes based on grids. The size of the cells depends on the propagation velocity of waves. When coupling wave problems, conversion phenomena may occur and waves with very different propagation velocity coexist. The size of the cells is then defined from the smallest velocity and in most of the real-world cases, the computational cost is crippling. Regarding existing computing capabilities, we propose to derive intermediate models which require less computational burden and provide accurate solutions for a wide-ranging class of problems including Elasto-acoustics and Electro-seismology.

When it comes to mathematical analysis, we have identified two tasks which could help us simulate realistic 3D multi-physics wave problems and which are in the scope of our *savoir-faire*. They are construction of approximate and multiscale models which are different tasks. The construction of approximate problems aims at deriving systems of equations which discrete formulation involves middle-sized matrices and in general, they are based on high frequency hypothesis. Multiscale models are based on a rigorous analysis involving a small parameter which does not depend on the propagation velocity necessarily.

Recently, we have conducted research on the construction of approximate models for offshore imaging. Elastic and acoustic wave equations are coupled and we investigate the idea of eliminating the computations inside water by introducing equivalent interface conditions on the sea bottom. We apply an On-Surface-Radiation-Condition (OSRC) which is obtained from the approximation of the acoustic Dirichlet-to-Neumann (DtN) operator [74], [53]. To the best of our knowledge, OSRC method has never been used for solving reduced coupling wave problems and preliminary promising results are available at [56]. We would like to investigate this technique further because we could form a battery of problems which can be solved quickly. This would provide a set of solutions which we could use as initial guess for solving inverse problems. But we are concerned with the performance of the OSRC method when wave conversions with different wavelengths occur. Anyway, the approximation of the DtN operator is not obvious when the medium is strongly heterogeneous and multiscale analysis might be more adapted. For instance, according to existing results in Acoustics and Electromagnetism for the modeling of wire antennas [65], multiscale analysis should turn out to be very efficient when the propagation medium includes well logs, fractures and faults which are very thin structures when compared to the wavelength of seismic waves. Moreover, multiscale analysis should perform well when the medium is strongly oscillating like porous media. It could thus provide an alternative to homogenization techniques which can be applied only when the medium is periodic. We thus propose to develop reduced multi-scale models by performing rigorous mathematical procedure based on regular and singular multiscale analysis. Our approach distinguishes itself from others because it focuses on the numerical representation of small structures by time-dependent problems. This could give rise to the development of new finite element methods which would combine DG approximations with XFEM (Extended Finite Element Method) which has been created for the finite element treatment of thin structures like cracks.

But Earth imaging must be more than using elasto-acoustic wave propagation. Electromagnetic waves can also be used and in collaboration with Prof. D. Pardo (Iker Basque Foundation and University of Bilbao), we conduct researches on passive imaging to probe boreholes. Passive imaging is a recent technique of imaging which uses natural electromagnetic fields as sources. These fields are generated by hydromagnetic waves propagating in the magnetosphere which transform into electromagnetic waves when they reach the ionosphere. This is a mid-frequency imaging technique which applies also to mineral and geothermal exploration, to predict seismic hazard or for groundwater monitoring. We aim at developing software package for resistivity inversion, knowing that current numerical methods are not able to manage 3D inversion. We have obtained results based on a Petrov-Galerkin approximation [50], but they are limited to 2D cases. We have thus proposed to reduce the 3D problem by using 1D semi-analytic approximation of Maxwell equations [78]. This work has just started in the framework of a PhD thesis and we hope that it will give us the possibility of imaging 3D problems.

Magique-3D would like to expand its know-how by considering electro-seismic problems which are in the scope of coupling electromagnetic waves with seismic waves. Electro-seismic waves are involved in porous media imaging which is a tricky task because it is based on the coupling of waves with very different wavelengths described by Biot equations and Maxwell equations. Biot equations govern waves in saturated porous media and they represent a complex physical phenomenon involving a slow wave which is very difficult to simulate numerically. In [72], interesting results have been obtained for the simulation of piezoelectric sensors. They are based on a quasi-static approximation of the Maxwell model coupled with Elastodynamics. Now, we are concerned with the capability of using this model for Geophysical Imaging and we believe that the derivation and/or the analysis of suitable modelings is necessary. Collaborations with Geophysicists are thus mandatory in the prospect of using both experimental and numerical approaches. We would like to collaborate with Prof. C. Bordes and Prof. D. Brito (Laboratory of Complex Fluids and their Reservoirs, CNRS and University of Pau) who have efficient experimental devices for the propagation of electromagnetic waves inside saturated porous media [55]. This collaboration should be easy to organize since Magique-3D has a long-term experience in collaborating with geophysicists. We then believe that we will not need a lot of time to get joint results since we can use our advanced software packages Hou10ni and Montjoie and our colleagues have already obtained data. Electro-seismology is a very challenging research domain for us and we would like to enforce our collaborations with IsTerre (Institute of Earth Science, University of Grenoble) and for that topic with Prof. S. Garambois who is an expert in Electro-seismology [80], [81], [69], [70]. A joint research program could gather Geophysicists from the University of Pau and from IsTerre and Magique-3D.

In particular, it would be interesting to compare simulations performed with Hou10ni, Montjoie, with the code developed by Prof. S. Garambois and to use experimental simulations for validation.

3.3. Supercomputing for Helmholtz problems

Probing invisible with harmonic equations is a need for many scientists and it is also a topic offering a wealth of interesting problems for mathematicians. It is well-known that Helmholtz equations discretization is very sensitive to the frequency scale which can be wide-ranging for some applications. For example, depth imaging is searching for deeper layers which may contain hydrocarbons and frequencies must be of a few tens of Hertz with a very low resolution. If it is to detect hidden objects, the depth of the explored region does not exceed a few tens of meters and frequencies close to the kiloHertz are used. High performing numerical methods should thus be stable for a widest as possible frequency range. In particular, these methods should minimize phenomena of numerical pollution that generate errors which increase faster with frequency than with the inverse of space discretization step. As a consequence, there is a need of mesh refinement, in particular at high frequency.

During the period 2010-2014, the team has worked extensively on high order discontinuous Galerkin (DG) methods. Like standard Finite Element Methods, they are elaborated with polynomial basis functions and they are very popular because they are defined locally for each element. It is thus easy to use basis polynomial functions with different degrees and this shows the perfect flexibility of the approximation in case of heterogeneous media including homogeneous parts. Indeed, low degree basis functions can be used in heterogeneous regions where a fine grid is necessary while high degree polynomials can be used for coarse elements covering homogeneous parts. In particular, Magique-3D has developed Hou10ni that solves harmonic wave equations with DG methods and curved elements. We found that both the effects of pollution and dispersion, which are very significant when a conventional finite element method is used, are limited [57]. However, bad conditioning is persisting and reliability of the method is not guaranteed when the coefficients vary considerably. In addition, the number of unknowns of the linear system is too big to hope to solve a realistic 3D problem. So it is important to develop approximation methods that require fewer degrees of freedom. Magique-3D wishes to invest heavily in the development of new approximation methods for harmonic wave equations. It is a difficult subject for which we want to develop different tasks, in collaboration with academic researchers with whom we are already working or have established contacts. Research directions that we would like to follow are the following.

First, we will continue our long-term collaboration with Prof. Rabia Djellouli. We want to continue to work on hybrid finite element methods that rely on basis functions composed of plane waves and polynomials. These methods have demonstrated good resistance to the phenomenon of numerical pollution [51], [52], but their capability of solving industrial problems has not been illustrated. This is certainly due to the absence of guideline for choosing the plane waves. We are thus currently working on the implementation of a methodology that makes the choice of plane waves automatic for a given simulation (fixed propagation domain, data source, etc.). This is up-front investigation and there is certainly a lot of remaining work before being applied to geophysical imaging. But it gives the team the opportunity to test new ideas while remaining in contact with potential users of the methods.

Then we want to work with Prof. A. Bendali on developing methods of local integral equations which allow calculation of numerical fluxes on the edges of elements. One could then use these fluxes in a DG method for reconstructing the solution throughout the volume of calculation. This research is motivated by recent results which illustrate the difficulties of the existing methods which are not always able to approximate the propagating modes (plane waves) and the evanescent modes (polynomials) that may coexist, especially when one considers realistic applications. Integral equations are direct tools for computing fluxes and they are known for providing very good accuracy. They thus should help to improve the quality of approximation of DG methods which are fully flux-dependent. In addition, local integral equations would limit calculations at the interfaces, which would have the effect of limiting the number of unknowns generally high, especially for DG methods. Again, it is a matter of long-term research which success requires a significant amount of mathematical analysis, and also the development of non-trivial code.

To limit the effects of pollution and dispersion is not the only challenge that the team wants to tackle. Our experience alongside Total has made us aware of the difficulties in constructing meshes that are essential to achieve our simulations. There are several teams at Inria working on mesh generation and we are in contact with them, especially with Gamma3 (Paris-Rocquencourt Research Center). These teams develop meshes increasingly sophisticated to take account of the constraints imposed by realistic industrial benchmarks. But in our opinion, issues which are caused by the construction of meshes are not the only downside. Indeed, we have in mind to solve inverse problems and in this case it is necessary to mesh the domain at each iteration of Newton-type solver. It is therefore interesting to work on methods that either do not use mesh or rely on meshes which are very easy to construct. Regarding meshless methods, we have begun a collaboration with Prof. Djellouli which allowed us to propose a new approach called Mesh-based Frontier Free Formulation (MF3). The principle of this method is the use of fundamental solutions of Helmholtz equations as basic functions. One can then reduce the volumic variational formulation to a surfacic variational formulation which is close to an integral equation, but which does not require the calculation of singularities. The results are very promising and we hope to continue our study in the context of the application to geophysical imaging. An important step to validate this method will be particularly its extension to 3D because the results we have achieved so far are for 2D problems.

Keeping in mind the idea of limiting the difficulties of mesh, we want to study the method of virtual elements. This method attracts us because it relies on meshes that can be made of arbitrarily-shaped polygon and meshes should thus be fairly straightforward. Existing works on the subject have been mainly developed by the University of Pavia, in collaboration with Los Alamos National Laboratory [54], [61], [60], [58], [62]. None of them mentions the feasibility of the method for industrial applications and to our knowledge, there are no results on the method of virtual elements applied to the wave equations. First, we aim at applying the method described in [59] to the scalar Helmholtz equation and explore opportunities to use discontinuous elements within this framework. Then hp-adaptivity could be kept, which is particularly interesting for wave propagation in heterogeneous media.

DG methods are known to require a lot of unknowns that can exceed the limits accepted by the most advanced computers. This is particularly true for harmonic wave equations that require a large number of discretization points, even in the case of a conventional finite element method. We therefore wish to pursue a research activity that we have just started in collaboration with the project-team Nachos (Sophia-Antipolis Méditerranée Research Center). In order to reduce the number of degrees of freedom, we are interested in "hybrid mixed" Discontinuous Galerkin methods that provides a two-step procedure for solving the Helmholtz equations [73], [77], [76]. First, Lagrange multipliers are introduced to represent the flux of the numerical solution through the interface (edge or face) between two elements. The Lagrange multipliers are solution to a linear system which is constructed locally element by element. The number of degrees of freedom is then strongly reduced since for a standard DG method, there is a need of considering unknowns including volumetric values inside the element. And obviously, the gain is even more important when the order of the element is high. Next, the solution is reconstructed from the values of the multipliers and the cost of this step is negligible since it only requires inverting small-sized matrices. We have obtained promising results in the framework of the PhD thesis of Marie Bonnasse-Gahot and we want to apply it to the simulation of complex phenomena such as the 3D viscoelastic wave propagation.

Obviously, the success of all these works depends on our ability to consider realistic applications such as wave propagation in the Earth. And in these cases, it is quite possible that even if we manage to develop accurate less expensive numerical methods, the solution of inverse problems will still be computationally intensive. It is thus absolutely necessary that we conduct our research by taking advantage of the latest advances in high-performance computing. We have already initiated discussions with the project team HIEPACS (Bordeaux Sud-Ouest research Center) to test the performance of the latest features of Mumps <http://mumps.enseciht.fr/>, such as Low Rank Approximation or adaptation to hybrid CPU / GPU architectures and to Intel Xeon Phi, on realistic test cases. We are also in contact with the team Algorithm at Cerfacs (Toulouse) for the development of local integral equations solvers. These collaborations are essential for us and we believe that they will be decisive for the simulation of three-dimensional elasto-dynamic problems. However, our scientific contribution will be limited in this area because we are not experts in HPC.

3.4. Hybrid time discretizations of high-order

Most of the meshes we consider are composed of cells greatly varying in size. This can be due to the physical characteristics (propagation speed, topography, ...) which may require to refine the mesh locally, very unstructured meshes can also be the result of dysfunction of the mesher. For practical reasons which are essentially guided by the aim of reducing the number of matrix inversions, explicit schemes are generally privileged. However, they work under a stability condition, the so-called Courant Friedrichs Lewy (CFL) condition which forces the time step being proportional to the size of the smallest cell. Then, it is necessary to perform a huge number of iterations in time and in most of the cases because of a very few number of small cells. This implies to apply a very small time step on grids mainly composed of coarse cells and thus, there is a risk of creating numerical dispersion that should not exist. However, this drawback can be avoided by using low degree polynomial basis in space in the small meshes and high degree polynomials in the coarse meshes. By this way, it is possible to relax the CFL condition and in the same time, the dispersion effects are limited. Unfortunately, the cell-size variations are so important that this strategy is not sufficient. One solution could be to apply implicit and unconditionally stable schemes, which would obviously free us from the CFL constraint. Unfortunately, these schemes require inverting a linear system at each iteration and thus needs huge computational burden that can be prohibitive in 3D. Moreover, numerical dispersion may be increased. Then, as second solution is the use of local time stepping strategies for matching the time step to the different sizes of the mesh. There are several attempts [66], [63], [79], [75], [68] and Magique 3D has proposed a new time stepping method which allows us to adapt both the time step and the order of time approximation to the size of the cells. Nevertheless, despite a very good performance assessment in academic configurations, we have observed to our detriment that its implementation inside industrial codes is not obvious and in practice, improvements of the computational costs are disappointing, especially in a HPC framework. Indeed, the local time stepping algorithm may strongly affect the scalability of the code. Moreover, the complexity of the algorithm is increased when dealing with lossy media [71].

Recently, Dolean *et al* [67] have considered a novel approach consisting in applying hybrid schemes combining second order implicit schemes in the thin cells and second order explicit discretization in the coarse mesh. Their numerical results indicate that this method could be a good alternative but the numerical dispersion is still present. It would then be interesting to implement this idea with high-order time schemes to reduce the numerical dispersion. The recent arrival in the team of J. Chabassier should help us to address this problem since she has the expertise in constructing high-order implicit time scheme based on energy preserving Newmark schemes [64]. We propose that our work be organized around the two following tasks. The first one is the extension of these schemes to the case of lossy media because applying existing schemes when there is attenuation is not straightforward. This is a key issue because there is artificial attenuation when absorbing boundary conditions are introduced and if not, there are cases with natural attenuation like in visco-elastic media. The second one is the coupling of high-order implicit schemes with high-order explicit schemes. These two tasks can be first completed independently, but the ultimate goal is obviously to couple the schemes for lossy media. We will consider two strategies for the coupling. The first one will be based on the method proposed by Dolean *et al*, the second one will consist in using Lagrange multiplier on the interface between the coarse and fine grids and write a novel coupling condition that ensures the high order consistency of the global scheme. Besides these theoretical aspects, we will have to implement the method in industrial codes and our discretization methodology is very suitable for parallel computing since it involves Lagrange multipliers. We propose to organize this task as follows. There is first the crucial issue of a systematic distribution of the cells in the coarse/explicit and in the fine/implicit part. Based on our experience on local time stepping, we claim that it is necessary to define a criterion which discriminates thin cells from coarse ones. Indeed, we intend to develop codes which will be used by practitioners, in particular engineers working in the production department of Total. It implies that the code will be used by people who are not necessarily experts in scientific computing. Considering real-world problems means that the mesh will most probably be composed of a more or less high number of subsets arbitrarily distributed and containing thin or coarse cells. Moreover, in the prospect of solving inverse problems, it is difficult to assess which cells are thin or not in a mesh which varies at each iteration.

Another important issue is the load balancing that we can not avoid with parallel computing. In particular, we will have to choose one of these two alternatives: dedicate one part of processors to the implicit computations and the other one to explicit calculus or distribute the resolution with both schemes on all processors. A collaboration with experts in HPC is then mandatory since we are not expert in parallel computing. We will thus continue to collaborate with the team-projects Hiepac and Runtime with whom we have a long-term experience of collaborations. The load-balancing leads then to the issue of mesh partitioning. Main mesh partitioners are very efficient for the coupling of different discretizations in space but to the best of our knowledge, the case of non-uniform time discretization has never been addressed. The study of meshes being out of the scopes of Magique-3D, we will collaborate with experts on mesh partitioning. We get already on to François Pellegrini who is the principal investigator of Scotch (<http://www.labri.fr/perso/pelegrin/scotch>) and permanent member of the team project Bacchus (Inria Bordeaux Sud Ouest Research Center).

In the future, we aim at enlarging the application range of implicit schemes. The idea will be to use the degrees of freedom offered by the implicit discretization in order to tackle specific difficulties that may appear in some systems. For instance, in systems involving several waves (as P and S waves in porous elastic media, or coupled wave problems as previously mentioned) the implicit parameter could be adapted to each wave and optimized in order to reduce the computational cost. More generally, we aim at reducing numeric bottlenecks by adapting the implicit discretization to specific cases.

4. Application Domains

4.1. Seismic Imaging

The main objective of modern seismic processing is to find the best representation of the subsurface that can fit the data recorded during the seismic acquisition survey. In this context, the seismic wave equation is the most appropriate mathematical model. Numerous research programs and related publications have been devoted to this equation. An acoustic representation is suitable if the waves propagate in a fluid. But the subsurface does not contain fluids only and the acoustic representation is not sufficient in the general case. Indeed the acoustic wave equation does not take some waves into account, for instance shear waves, turning waves or the multiples that are generated after several reflections at the interfaces between the different layers of the geological model. It is then necessary to consider a mathematical model that is more complex and resolution techniques that can model such waves. The elastic or viscoelastic wave equations are then reference models, but they are much more difficult to solve, in particular in the 3D case. Hence, we need to develop new high-performance approximation methods.

Reflection seismics is an indirect measurement technique that consists in recording echoes produced by the propagation of a seismic wave in a geological model. This wave is created artificially during seismic acquisition surveys. These echoes (i.e., reflections) are generated by the heterogeneities of the model. For instance, if the seismic wave propagates from a clay layer to sand, one will observe a sharp reflected signal in the seismic data recorded in the field. One then talks about reflection seismics if the wave is reflected at the interface between the two media, or talks about seismic refraction if the wave is transmitted along the interface. The arrival time of the echo enables one to locate the position of this transition, and the amplitude of the echo gives information on some physical parameters of the two geological media that are in contact. The first petroleum exploration surveys were performed at the beginning of the 1920's and for instance, the Orchard Salt Dome in Texas (USA) was discovered in 1924 by the seismic-reflection method.

4.2. Imaging complex media with ultrasonic waves

The acoustic behavior of heterogeneous or composite materials attracts considerable excitement. Indeed, their acoustic response may be extremely different from the single constituents responses. In particular, dispersions of resonators in a matrix are the object of large research efforts, both experimentally and theoretically. However it is still a challenge to dispose of numerical tools with sufficient abilities to deal with the simulation and imaging of such materials behavior. Indeed, not only acoustic simulations are very time-consuming, but they have to be performed on realistic enough solution domains, i.e. domains which capture well enough the structural features of the considered materials.

This collaboration with I2M, University of Bordeaux aims at addressing this type of challenges by developing numerical and experimental tools in order to understand the propagation of ultrasonic waves in complex media, image these media, and in the future, help design composite materials for industrial purposes.

4.3. Helioseismology

This collaboration with the Max Planck Institute for Solar System, Göttingen, Germany, which started in 2014, aims at designing efficient numerical methods for the wave propagation problems that arise in helioseismology in the context of inverse problems. The final goal is to retrieve information about the structure of the Sun i.e. inner properties such as density or pressure via the inversion of a wave propagation problem. Acoustic waves propagate inside the Sun which, in a first approximation and regarding the time scales of physical phenomena, can be considered as a moving fluid medium with constant velocity of motion. Some other simplifications lead to computational saving, such as supposing a radial or axisymmetric geometry of the Sun. Aeroacoustic equations must be adapted and efficiently solved in this context, this has been done in the finite elements code Montjoie 5.3. In other situations, a full 3D simulation is required and demands large computational resources. Ultimately, we aim at modeling the coupling with gravity potential and electromagnetic waves (MHD equations) in order to be able to better understand Sun spots.

5. New Software and Platforms

5.1. Elasticus

SCIENTIFIC DESCRIPTION Elasticus simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION Elasticus is a sequential library, independent of DIVA and developed in Fortran, to simulate wave propagation in geophysical environment, based on a DG method. It is meant to help PhD students and post-doctoral fellows to easily implement their algorithms in the library. Thus, readability of the code is privileged to optimization of its performances. Developed features should be easily transferred in the computing platform of Total. Contrary to DIVA which only computes approximate solutions with P1, P2 and P3 elements, Elasticus manages arbitrary orders for the spatial discretization with DG method.

- Participants: Simon Ettouati, Julien Diaz and Lionel Boillot
- Partner: TOTAL
- Contact: Julien Diaz

5.2. Hou10ni

SCIENTIFIC DESCRIPTION Hou10ni simulates acoustic and elastic wave propagation in time domain and in harmonic domain, in 2D and in 3D. It is also able to model elasto-acoustic coupling. It is based on the second order formulation of the wave equation and the space discretization is achieved using Interior Penalty Discontinuous Galerkin Method. Recently, the harmonic domain solver has been extended to handle Hybridizable Discontinuous Galerkin Methods.

FUNCTIONAL DESCRIPTION This software simulates the propagation of waves in heterogeneous 2D and 3D media in time-domain and in frequency domain. It is based on an Interior Penalty Discontinuous Galerkin Method (IPDGM) and allows for the use of meshes composed of cells of various order (p-adaptivity in space).

- Participants: Julien Diaz, Marie Bonnasse-Gahot and Lionel Boillot
- Contact: Julien Diaz

5.3. Montjoie

SCIENTIFIC DESCRIPTION

Montjoie is designed for the efficient solution of time-domain and time-harmonic linear partial differential equations using high-order finite element methods. This code is mainly written for quadrilateral/hexahedral finite elements, partial implementations of triangular/tetrahedral elements are provided. The equations solved by this code, come from the "wave propagation" problems, particularly acoustic, electromagnetic, aeroacoustic, elasto-dynamic problems.

FUNCTIONAL DESCRIPTION

Montjoie is a code that provides a C++ framework for solving partial differential equations on unstructured meshes with finite element-like methods (continuous finite element, discontinuous Galerkin formulation, edge elements and facet elements). The handling of mixed elements (tetrahedra, prisms, pyramids and hexahedra) has been implemented for these different types of finite elements methods. For time-domain simulations, a wide range of ODE (Ordinary Differential Equation) solvers have been implemented : high-order explicit or implicit time schemes. Several applications are currently available : wave equation, elastodynamics, aero-acoustics, Maxwell's equations.

- Participants: Marc Duruflé, Juliette Chabassier, Mamadou N'Diaye and Michaël Leguèbe
- Contact: Marc Duruflé
- URL: <http://montjoie.gforge.inria.fr/>

5.4. TMBM-DG

Time-Marching Based Methods-Discontinuous Galerkin

SCIENTIFIC DESCRIPTION TMBM-DG simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION TMBM-DG is the follow up to DIVA-DG that we develop in collaboration with our partner Total. Its purpose is more general than DIVA-DG and should contains various DG schemes, basis functions and time schemes. It models wave propagation in acoustic media, elastic (isotropic and TTI) media and elasto-acoustic media, in two and three dimensions.

- Participants: Julien Diaz, Lionel Boillot and Simon Ettouati
- Partner: TOTAL
- Contact: Julien Diaz

6. New Results

6.1. Seismic Imaging and Inverse Problems

6.1.1. Time-harmonic inverse problem

Participants: H el ene Barucq, Florian Faucher.

We study the seismic inverse problem for acoustic and elastic medium associated with the time-harmonic wave equation, and the underlying recovery of geophysical parameters. We employ Full Waveform Inversion (FWI) where the multi parameters reconstruction is based on iterative minimization techniques. This inverse problem shows a Lipschitz stability where the stability constant is related to the (conditional) lower bound of the Fr echet derivative, when assuming a piecewise constant representation of the parameters. We successively estimate the stability constant for different model partition in order to control the convergence of the scheme. Hence we define a multi-level (multi-scale, multi-frequency) algorithm where the natural progression of frequency is paired with the model partition. The method is implemented and numerical experiments are performed for elastic medium reconstruction, in particular for realistic geophysical situations.

6.1.2. Shape-reconstruction and parameter identification of an elastic object immersed in a fluid

Participants: Izar Azpiroz Irigorri, H el ene Barucq, Julien Diaz, Rabia Djellouli.

We investigate the inversion of a series of parameters in the context of a 2D elasto-acoustic scattering problem. The inverse problem is solved by using a Newton-like method, where the shape of the scatterer is assumed to be Lipschitz-continuous. Herein, we want to recover the shape and the material parameters in the case of isotropic and anisotropic materials. Based on the different influences of these parameters on the far field pattern, the final goal is to propose an iterative algorithm to retrieve the parameters separately, by devoting some iterations to the reconstruction of the shape and the others to the determination of the parameters. On the other hand, due to the difficulties to retrieve the material parameters, the penetrability of scatters have been studied. The conclusion has been that the recovery of material parameters can be feasible, provided that the scattered waves are not completely reflected. The results of this work have been presented to the conference Inverse Problems for PDE in Bremen, Germany [24].

6.2. Mathematical modeling of multi-physics involving wave equations

6.2.1. A study of the numerical robustness of single-layer method with Fourier basis for multiple obstacle scattering in homogeneous media

Participants: H el ene Barucq, Juliette Chabassier, Ha Pham, S ebastien Tordeux.

We investigate efficient methods to solve direct and inverse problems for the propagation of acoustic wave in strongly inhomogeneous media in low-frequency regime. We start our investigation with inhomogeneities created by compactly-supported and non-overlapping obstacles. With a large number of small obstacles, optimized softwares based on Finite Element Method (FEM) lose their robustness. As an alternative, we work with an integral equation method, which uses single-layer potentials and truncation of Fourier series to describe the scattered field. We limit our numerical experiments to disc-shaped obstacles. We first compare our method with Montjoie (a FEM-based software); secondly, we investigate the efficiency of different solver types (direct and iterative) in solving the dense linear system generated by the method. We observe that the optimal choice depends on the distance between obstacles, their size and number, and applications.

6.2.2. Derivation and validation of impedance transmission conditions for the electric potential across a highly conductive casing

Participants: H el ene Barucq, Aralar Erdozain, David Pardo, Victor P eron.

Borehole resistivity measurements are a common procedure when trying to obtain a better characterization of the Earth's subsurface. The possible risk of having borehole collapses makes the employment of a casing very suitable for this type of scenarios. Such casing protects the borehole but it also highly complicates the resistivity measurements due to the thinness of the casing and the large contrasts between the conductivities of the casing and the rock formations.

This work is motivated by realistic configurations where the resistivity of the casing is proportional to the cube of the thickness of the casing. In this framework, our aim is to derive Impedance Transmission Conditions (ITCs) for the electromagnetic field across such a casing. As a first approach we derive ITCs for the electric potential. We consider a transmission problem for the static case of the electric potential, set in an axisymmetric borehole shaped domain. This domain is composed of three different subdomains, the interior part of the borehole, the rock formations and the metallic casing.

In this framework, we address the issue of ITCs using two different approaches. The first one consists in deriving ITCs across the casing itself, whereas the second approach tackles the problem by deriving ITCs on an artificial interface located in the middle of the casing. We derive different models for the two considered approaches and we numerically assess them with a finite element method implementation. Then we perform a comparison on these models by showing the advantages and drawbacks of each model. Finally, we show an application to a borehole through-casing resistivity measurement scenario. This work delivers stability results and error estimates, leading to convergence of each approximate model. All the details regarding this work can be found in [43].and [10]. In addition it has been presented to the WONAPDE Conference [29].

6.2.3. *Semi-analytical solutions for asymptotic models for the electric potential across a highly conductive casing*

Participants: H el ene Barucq, Aralar Erdozain, Ignacio Muga, Victor P eron.

This work is performed in the framework of borehole through-casing resistivity measurements. A transmission problem for the electric potential is considered, where one part of the domain is a high-conductive casing. Numerical instabilities are created during the numerical simulations when such a casing is present in the configuration. Therefore, three different asymptotic models derived in [43] are considered, which are composed of impedance conditions specially designed to avoid the casing. These models correspond to approximations of orders one, two and four.

In this work, we employ analytical methods for the aforementioned asymptotic models, which provide a consistent solution to test and verify the numerical solutions (Finite Element Method). In addition, these methods are computationally cheaper than the purely numerical methods. The standard method we follow consists in employing cylindrical coordinates and assuming material homogeneity in the vertical and angular variables. The source term is represented as a Dirac distribution. Under these conditions, we represent the solution to our problem as an inverse Fourier integral in the vertical variable, and a Fourier series in the angular variable.

Numerical tests are carried out to compare with Finite Element solutions. Several difficulties have to be taken into account during the implementation of the semi-analytical solutions, like the treatment of the Dirac distribution and the presence of singularities when the Fourier variable tends to zero. These difficulties are also addressed in this work which is detailed in [10].

6.2.4. *Numerical investigation of instabilities of Perfectly Matched Layers coupled with DG-schemes in elastodynamic*

Participants: H el ene Barucq, Lionel Boillot, Henri Calandra, Julien Diaz, Simon Ettouati.

We observed long-term numerical instabilities when DG-schemes are coupled with PML in elastodynamic, even with isotropic media. To investigate the causes of this instabilities, we have led a series of numerical experiments with elasticus 5.1. The conclusion was that the instabilities only appear in truly elastodynamic media (i.e. when the velocities of S waves is positive) and that different factors impact the stability : the heterogeneities of the domain, the choice of the fluxes, the boundary conditions, the use of unstructured meshes... In the best scenario, using a cartesian grid with periodic boundary conditions for an homogeneous medium and centered fluxes, we did not observe instabilities. However, changing only one element of the configuration made the instabilities appear. Our conclusion is that we need a very particular flux in the PML that should be able to handle the heterogeneities of the domain and the structure of the mesh. This flux should also be adapted to discretize the boundary condition. We are now working on the design of this flux.

6.2.5. *Elasto-acoustic coupling*

Participants: H el ene Barucq, Lionel Boillot, Henri Calandra, Julien Diaz, Simon Ettouati.

Last year, we developed a Discontinuous Galerkin Method for the elastoacoustic coupling in time domain. The proposed solution methodology in general and can be applied to any kind of fluxes. The method had been implemented in Elasticus 5.1 and we have transferred it into the Total platform TMBM-DG 5.4.

In [23], we have considered elastoacoustic coupling with curved interfaces and we have proposed a solution methodology based on Finite Element techniques, which allows for a flexible coupling between the fluid and the solid domain by using non-conforming meshes and curved elements. Differently from other non-conforming approaches proposed so far, our technique is relatively simpler and requires only a geometrical adjustment at the coupling interface at a preprocessing stage, so that no extra computations are necessary during the time evolution of the simulation. This work, has been achieved in collaboration with Angel Rodriguez Rozas, former post-doc of the team.

6.2.6. *Atmospheric radiation boundary conditions for helioseismology*

Participants: H el ene Barucq, Juliette Chabassier, Marc Durufl e.

Modeling acoustic wave propagation inside a celestial body (as the Sun) prompts the question of imposing an adequate boundary condition. Classical atmosphere models suppose an exponential decay of the medium density and a constant wave celerity outside a given radius. This work proposes several radiation boundary conditions that mimic the presence of such an atmosphere and assesses their behavior numerically in radial and axisymmetric configurations.

6.2.7. Hybrid discontinuous finite element approximation for the elasto-acoustics.

Participants: H el ene Barucq, Henri Calandra, Julien Diaz, Elvira Shishenina.

Discontinuous finite element methods proved their accuracy and flexibility, but they are still criticized for the number of degrees of freedom which they use: it is much higher than the ones of the conventional methods based on continuous approximations.

Thus hybrid methods have been developed and their integration into the DIP is under way, both in the acoustic and elastic domains.

The global purpose of this work is to develop a new approach for solving wave equation in discontinuous function spaces. This will provide all propagators already developed in the CARBON platform. Possible directions in this research are for example the development of a Trefftz type approximation for elasto-acoustics, coupling with VEM, HDG.

Our current work is concentrated on using Trefftz method. The main idea of the method is that chosen basis functions of Trefftz approximation space are discrete local solutions of the initial equations to be solved.

The possible advantages of Trefftz type approximations compared to the standard ones are: 1) better orders of convergence; 2) flexibility in the choice of basis functions; 3) low dispersion; 4) incorporation of wave propagation directions in the discrete space; 5) adaptivity and local space-time mesh refinement.

The particularity of Trefftz methods is that in case of applying to time-dependent problems they require a space-time mesh.

We studied theory of application of the method to the coupled acoustic system, and implemented numerically Trefftz method to solve the first-order 1D acoustic wave propagation system. The obtained results were presented during annual workshop in Houston organized by Depth Imaging Partnership between Inria and Total.

6.3. Supercomputing for Helmholtz problems

6.3.1. Extend task-based node parallelism to cluster level: applications to geophysics

Participants: Emmanuel Agullo, Lionel Boillot, George Bosilca, Henri Calandra, Corentin Rossignon.

The context of this work is to replace static parallelism based on MPI + threads and/or CUDA by dynamic task-based parallelism on top of runtime systems. On a previous work, we demonstrated the speed-up of the new solution when applied to geophysics, at a node level. Moreover, this task paradigm proved its flexibility on several architectures such as ccNUMA big nodes or many-core Intel Xeon Phi co-processors.

We extended this principle to a set of nodes, eventually heterogeneous, in order to measure performance at a cluster level. Preliminary results on few homogeneous nodes were encouraging, ie still faster than pure MPI. Unfortunately, the geophysics algorithm being too repetitive, the load-balancing issue which can be removed within a node (i.e. between cores) comes back between nodes when they are numerous or few but heterogeneous. This is due to the work-stealing feature of the task paradigm which is by default enabled at the node level only.

To overcome this problem, we extended the work-stealing feature to cluster level. To do that we used the task identification by geometrical sub-meshes to detect candidates that can be exchanged between nodes. Then, we compared PAPI counters on these tasks to find the best choice. Finally, we use a separate task-based program to automatically do the main code task update. Preliminary results show clear improvement of load-balancing at cluster level.

This work has been presented to the conferences Rice Oil&Gas[34] and SIAM-PP (Parallel Processing) [35].

6.3.2. *Numerical libraries for hybrid meshes in a discontinuous Galerkin context*

Participants: H el ene Barucq, Lionel Boillot, Aurelien Citrain, Julien Diaz.

Elasticus team code 5.1 has been designed for triangles and tetrahedra mesh cell types. The first part of this work was dedicated to add quadrangle libraries and then to extend them to hybrid triangles-quadrangles (so in 2D). This implied to work on polynomials to form functions basis for the (discontinuous) finite element method, to finally be able to construct reference matrices (mass, stiffness, ...).

A complementary work has been done on mesh generation. The goal was to encircle an unstructured triangle mesh, obtained by third-party softwares, with a quadrangle mesh layer. At first, we built scripts to generate structured triangle meshes, quadrangle meshes and hybrid meshes (triangles surrounded by quadrangles). We are finalizing now the unstructured-goal.

The purpose is to use the h-adaptivity of discontinuous Galerkin method to easily encircle unstructured tetrahedra with hexahedra to form hybrid meshes (so in 3D). In addition, it would be interesting to couple numerical methods depending on the element types.

6.3.3. *Code transfer: TBM-DG/THBM into Total R&D environment*

Participants: Lionel Boillot, Julien Diaz.

The goal of the DIP collaboration between Total and Inria is to transfer the validated research codes. At first, DIVA-DG has been created in conjunction with Total developers team. It concerns the time modeling of wave propagation. Then, we forked it into Elasticus code to focus on mathematical research at the Inria side. Finally, once validated, we managed its transfer into the recent Total R&D environment (so instead of DIVA template, we moved to TBM template) to form the TBM-DG 5.4 code. The entire code has been transferred now, including unit tests and full documentation.

In the meantime, another code emerged within the DIP collaboration, THBM, concerning the frequency modeling of wave propagation. The development is directly done since the beginning in the Total R&D environment. An important part is already validated while research still continues.

6.3.4. *Hybridizable Discontinuous Galerkin methods for solving the elastic Helmholtz equations*

Participants: Marie Bonnasse-Gahot, Henri Calandra, Julien Diaz, St ephane Lanteri.

The advantage of performing seismic imaging in frequency domain is that it is not necessary to store the solution at each time step of the forward simulation. Unfortunately, the drawback of the Helmholtz equations, when considering 3D realistic elastic cases, lies in solving large linear systems. This represents today a challenging task even with the use of High Performance Computing (HPC). To reduce the size of the global linear system, we developed a Hybridizable Discontinuous Galerkin method (HDGm). It consists in expressing the unknowns of the initial problem in function of the trace of the numerical solution on each face of the mesh cells. In this way the size of the matrix to be inverted only depends on the number of degrees of freedom on each face and on the number of the faces of the mesh, instead of the number of degrees of freedom on each cell and on the number of the cells of the mesh as we have for the classical Discontinuous Galerkin methods (DGm). The solution to the initial problem is then recovered thanks to independent elementwise calculation. This results were presented in a submitted paper.

Moreover, as the HDG global matrix is very sparse, we focus on a suitable solver for this kind of matrix. We tested two linear solvers: a parallel sparse direct solver MUMPS (MUltifrontal Massively Parallel sparse direct Solver) and a hybrid solver MaPHyS (Massively Parallel Hybrid Solver) which combines direct and iterative methods. We compared the performances of the two solvers when solving 3D elastic waves propagation over HDGm. These comparisons were presented at the MATHIAS 2016 conference and at the DIP Workshop [36], [37]

6.3.5. A Symmetric Trefftz-DG Formulation based on a Local Boundary Element Method for the Solution of the Helmholtz Equation.

Participants: H el ene Barucq, Abderrahmane Bendali, M'Barek Fares, Vanessa Mattesi, S ebastien Tordeux.

A general symmetric Trefftz Discontinuous Galerkin method is built in [12] for solving the Helmholtz equation with piecewise constant coefficients. The construction of the corresponding local solutions to the Helmholtz equation is based on a boundary element method. A series of numerical experiments displays an excellent stability of the method relatively to the penalty parameters, and more importantly its outstanding ability to reduce the instabilities known as the ‘‘pollution effect’’ in the literature on numerical simulations of long-range wave propagation.

6.4. Hybrid time discretizations of high-order

6.4.1. High order time discretization for dissipative wave equations.

Participants: Juliette Chabassier, Julien Diaz, Anh-Tuan Ha, S ebastien Imperiale.

Magique-3D team is interested in numerical methods for wave propagation in realistic media, which are naturally dissipative in many application cases. In this internship, we wish to investigate several dissipation models, that lead to Partial Differential Equations with different structures. The simplest model is the scalar wave equation with homogeneous and constant damping $\frac{\partial^2 u}{\partial t^2} + R \frac{\partial u}{\partial t} - \Delta u = f$. In order to approach the complexity of the propagating medium and its geometry, high order finite elements in space are used. Once the spatial discretization is fixed, we get a differential equation of the kind $\frac{d^2 u_h}{dt^2} + B_h \frac{du_h}{dt} + A_h u_h = f_h$, where the mass matrix is the identity thanks to the mass lumping technique followed by a renormalization, B_h is the dissipation matrix and A_h the stiffness matrix. Classically, this equation is discretized in time with a centered and second order finite difference scheme known as the θ -scheme ($\theta > 0$)

$$\frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} + B_h \frac{u_h^{n+1} - u_h^{n-1}}{2\Delta t} + A_h (\theta u_h^{n+1} + (1 - 2\theta)u_h^n + \theta u_h^{n-1}) = f_h^n \quad (1)$$

In order to preserve the precision obtained with high order finite elements in space, we wish to design higher order time discretizations, while preserving some interesting mathematical properties as the dissipation of a discrete energy, and an efficiency close to the one observed for the second order scheme. More precisely, if $\theta = 0$ and B_h is diagonal, scheme (1) only requires the inversion of a diagonal matrix at each time step.

We want to use the technique of the modified equation, which consists in compensating the first term of the consistency error of a low order discretization, by adding a well chosen new term. If $\theta = 0$, this approach leads to the following fourth order accurate in time scheme

$$\left(I_h + \frac{\Delta t^2}{12} B_h \right) \frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} + \left[B_h + \frac{\Delta t^2}{12} (B_h A_h - A_h B_h) \right] \frac{u_h^{n+1} - u_h^{n-1}}{2\Delta t} + A_h u_h^n - \frac{\Delta t^2}{12} A_h^2 u_h^n = \tilde{f}_h^n$$

Even if B_h is diagonal, A_h and B_h do not commute in general. We propose to replace the matrix $B_h A_h - A_h B_h$, potentially hard to invert, by an approximated matrix, easy to invert, without deteriorating the consistency of the scheme.

An article is being written and will be submitted soon.

6.4.2. High order conservative explicit and implicit schemes for wave equations.

Participants: Juliette Chabassier, S ebastien Imperiale.

In 2016 we have studied the space/time convergence of a family of high order conservative explicit and implicit schemes for wave equations. An original proof of convergence has been proposed and provides an understanding of the lack of convergence of some schemes when the time step approaches its greatest admissible value for stability (CFL condition). An article has been submitted.

6.4.3. *Efficient high order implicit time schemes for Maxwell's equations.*

Participants: H el ene Barucq, Marc Durufl e, Mamadou N'Diaye.

The Pad e approximant is well known to be one of the best approximation of an exponential function which is involved in the exact solution of the linear ODE (Ordinary Differential Equations):

$$y'(t) = Ay(t) + F(t)$$

where A is a given matrix (usually coming from finite element discretization) and F is a term source. The numerical solution can be constructed by approximating the exponential function using the diagonal Pad e approximant:

$$R(z) = \frac{P_m(z)}{Q_m(z)}$$

The function $R(z)$ is a fraction involving two polynomial P_m and Q_m of same degree and approximating the exponential. The corresponding scheme is implicit and A-stable in the sense of Dahlquist. The associated stability function is the same as the stability function of the Gauss-Runge-Kutta schemes. However, Gauss-Runge-Kutta schemes can be used to handle non-linear ODEs, but they are too expensive to use in practice. The diagonal Pad e schemes presented here can be seen as a simplification of Gauss-Runge-Kutta schemes in the case of linear ODE. We have proposed an efficient way to implement the diagonal Pad e schemes with an accurate approximation of the source term to keep the correct order of accuracy.

The main drawback of Pad e schemes is that the denominator $Q_m(z)$ has distinct roots. It implies that we have to solve distinct linear systems at each time step. As a result, we have also studied the case where the denominator has an unique real root γ :

$$R(z) = \frac{N(z)}{(1 - \gamma z)^m}$$

The numerator N is then found to obtain the "best" approximation of the exponential under the constraint of the A-stability property of the underlying schemes. The obtained schemes have been called Linear Singly Diagonal Implicit Runge-Kutta schemes (Linear SDIRK) since they share the same property as SDIRK (a unique linear system to solve several times) but they can be applied only to linear ODEs. We provide a performance assessment of different implicit schemes (Pad e schemes, SDIRK and Linear SDIRK). The comparison criteria are based on the amplitude and phase errors which are reliable gauges of accuracy when approximating waves problems. The Linear SDIRK schemes and the diagonal Pad e schemes have been implemented in the code Montjoie. We have performed numerical experiments in 1-D and 2-D for Maxwell's equations to validate these schemes and compare their efficiency.

This work has been presented at the conference ICOSAHOM [28], the colloquium Inter' Actions en Math ematiques Lyon 2016 and the Mathias annual Total seminar [27].

6.4.4. *Optimized high-order explicit Runge-Kutta-Nystr om schemes.*

Participants: Marc Durufl e, Mamadou N'Diaye.

In this work we propose a high order time integration explicit scheme to solve a second order derivative non-linear ordinary differential equation (ODE)

$$y'' = f(t, y)$$

To solve this family of ODEs, explicit one-step Runge-Kutta-Nyström have been proposed by Hairer et al. The stability condition (CFL) associated with these schemes have been studied for order 3, 4 and 5 by Chawla and Sharma. In this work, we have extended the stability studies for high order. We proposed optimal coefficients for Runge-Kutta-Nyström schemes of order 6, 7, 8 and 10 which have been obtained by optimizing the CFL. With the obtained optimal CFL, these schemes are well suited for stiff problems where the stability condition is restrictive. These schemes have been implemented in the code Montjoie.

Numerical experiments have been conducted in 1-D for the non-linear Maxwell's equation and show that obtained Runge-Kutta-Nyström schemes of order 7 is quite efficient. This work has been presented at the conference ICOSAHOM [48].

7. Bilateral Contracts and Grants with Industry

7.1. Contracts with TOTAL

- Depth Imaging Partnership (DIP)
Period: 2014 May - 2019 April , Management: Inria Bordeaux Sud-Ouest, Amount: 120000 euros/year.
- Méthodes d'inversion sismique dans le domaine fréquentiel
Period: 2014 October - 2017 December , Management: Inria Bordeaux Sud-Ouest, Amount: 180000 euros.
- Portage de méthodes numériques de simulation de phénomènes complexes sur des architectures exascales
Period: 2016 January - 2017 December , Management: Inria Bordeaux Sud-Ouest, Amount: 150000 euros.
- Approximations hybrides par éléments finis discontinus pour l'élasto-acoustique
Period: 2016 November - 2018 October, Management: Inria Bordeaux Sud-Ouest, Amount: 165000 euros.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. Partnership with I2M in Bordeaux supported by Conseil Régional d'Aquitaine

title: Imaging complex materials.
Coordinator: Hélène Barucq
Other partners: I2M CNRS Université Bordeaux I

The detection, localization and monitoring of the defect evolution in composite materials, concrete and more generally heterogeneous materials is a challenging problem for Aeronautics and energy production. It is already possible to localize defects in homogeneous materials by using methods based on ultrasonic inspection and sometimes, they are usable in particular heterogeneous materials, most of the time in 2D. Classical methods rely on the correspondence between the distance and the propagation time of the wave traveling between the defect and the receivers. In complex media, such a correspondence may be lapsed, for instance when the velocity depends on the frequency (dispersion) or of the propagation direction (anisotropy). The defect signature can also be embedded in the acoustic field sent by the structure (multiple reflections). The complexity of the propagation in heterogeneous materials makes then difficult the accurate localization of the defect, in particular in 3D.

Topological imaging techniques can be applied to heterogeneous media. They can find the positions of defects from two simulations performed in a safe experimental medium. They have been developed at I2M laboratory to carry on 2D single/multi mode inspection in isotropic and anisotropic waveguides. They have also been applied to a highly reflecting medium observed with a single sensor. The objective of this work is to extend the technique to 3D problems. In particular, we are going to handle detection in composite plates and in highly heterogeneous media including a collection of small scatterers.

This project is supported by the Conseil Régional d'Aquitaine, for a duration of 2 years.

8.2. National Initiatives

8.2.1. Depth Imaging Partnership

Magique-3D maintains active collaborations with Total. In the context of Depth Imaging, Magique-3D coordinates research activities dealing with the development of high-performance numerical methods for solving wave equations in complex media. This project has involved 2 other Inria Team-Projects (Hiepac and Nachos) which have complementary skills in mathematics, computing and in geophysics. DIP is fully funded by Total by the way of an outline agreement with Inria .

In 2014, the second phase of DIP has begun. Lionel Boillot has been hired as engineer to work on the DIP platform. 4 PhD students have defended their PhD in 2015 and they have now post-doctoral researchers in Europe. DIP is currently employing 2 PhD students and one post-doctoral researcher.

8.2.2. ANR Num4Sun

The ANR has launched a specific program for supporting and promoting applications to European or more generally International projects. Magique-3D has been selected in 2016 after proposing a project to be applied as a FET project on the occasion of a call that will open in 2017 April. This project will gather researchers of the MPS (<https://www.mps.mpg.de/en>), of the BSC (<https://www.bsc.es/>), of the BCAM (<http://www.bcamath.org/en/>), of Heriot-Watt University (<https://www.hw.ac.uk/>) and Inria teams.

A kick-off meeting has been held in November in Strasbourg. The second one will be held in Paris in March 2017. The project is funded for 18 months starting from August 2016. The funding amounts 30000€.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. GEAGAM

Title: Geophysical Exploration using Advanced Galerkin Methods

Program: H2020

Duration: January 2015 - December 2017

Coordinator: Universidad Del Pais Vasco (EHU UPV)

Partners:

Bcam - Basque Center for Applied Mathematics Asociacion (Spain)

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)

Total S.A. (France)

Universidad Del Pais Vasco Ehu Upv (Spain)

Pontificia Universidad Catolica de Valparaiso (Chile)

Universidad de Chile (Chile)

Universidad Tecnica Federico Santa Maria (Chile)

University of Texas at Austin (USA)

Inria contact: Hélène BARUCQ

The main objective of this Marie Curie RISE action is to improve and exchange interdisciplinary knowledge on applied mathematics, high performance computing, and geophysics to be able to better simulate and understand the materials composing the Earth's subsurface. This is essential for a variety of applications such as CO₂ storage, hydrocarbon extraction, mining, and geothermal energy production, among others. All these problems have in common the need to obtain an accurate characterization of the Earth's subsurface, and to achieve this goal, several complementary areas will be studied, including the mathematical foundations of various high-order Galerkin multiphysics simulation methods, the efficient computer implementation of these methods in large parallel machines and GPUs, and some crucial geophysical aspects such as the design of measurement acquisition systems in different scenarios. Results will be widely disseminated through publications, workshops, post-graduate courses to train new researchers, a dedicated webpage, and visits to companies working in the area. In that way, we will perform an important role in technology transfer between the most advanced numerical methods and mathematics of the moment and the area of applied geophysics.

8.3.1.2. *HPC4E*

Title: HPC for Energy

Program: H2020

Duration: December 2015 - November 2017

Coordinator: Barcelona Supercomputing Center

Partners:

Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas-Ciemat (Spain)

Iberdrola Renovables Energia (Spain)

Repsol (Spain)

Lancaster University (United Kingdom)

Total S.A. (France)

Fundação Coordenação de Projetos, Pesquisas e Estudos Tecnológicos, (Brazil)

National Laboratory for Scientific Computation, (Brazil)

Instituto Tecnológico de Aeronáutica, (Brazil)

Petrobras, (Brazil)

Universidade Federal do Rio Grande do Sul, (Brazil)

Universidade Federal de Pernambuco, (Brazil)

Inria contact: Stéphane Lanteri

This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO₂ emissions, contribution to diversification of energy supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial applications using alternative fuels, which is required to design efficient furnaces, engines, clean

burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth's interior with unprecedented quality.

8.4. International Initiatives

8.4.1. Inria International Partners

8.4.1.1. Declared Inria International Partners

8.4.1.1.1. MAGIC2

Title: Advance Modeling in Geophysics

International Partner (Institution - Laboratory - Researcher):

California State University at Northridge (United States) - Department of Mathematics -
Djellouli Rabia

The Associated Team MAGIC was created in January 2006 and renewed in January 2009. At the end of the program in December 2011, the two partners, MAGIQUE-3D and the California State University at Northridge (CSUN) decided to continue their collaboration and obtained the "Inria International Partner" label in 2013.

See also: <https://project.inria.fr/magic/>

The ultimate objective of this research collaboration is to develop efficient solution methodologies for solving inverse problems arising in various applications such as geophysical exploration, underwater acoustics, and electromagnetics. To this end, the research program will be based upon the following three pillars that are the key ingredients for successfully solving inverse obstacle problems. 1) The design of efficient methods for solving high-frequency wave problems. 2) The sensitivity analysis of the scattered field to the shape and parameters of heterogeneities/scatterers. 3) The construction of higher-order Absorbing Boundary Conditions.

In the framework of Magic2, Rabia Djellouli (CSUN) visited Magique 3D in December 2016

8.5. International Research Visitors

8.5.1. Visits of International Scientists

- Antoine Chaigne (University of Music and Performing Arts Vienna) visited Magique 3D in November 2016.
- Rabia Djellouli (CSUN) visited Magique 3D in December 2016.

8.5.2. Visits to International Teams

8.5.2.1. Research Stays Abroad

- In the framework of the European project Geagam, Aralar Erdozain and Victor Péron visited Ignacio Muga, PUCV, Chile, in January and November 2016.
- In the framework of the European project Geagam, Florian Faucher and Ha Pham visited Henri Calandra, Total Houston, USA, in October 2016.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

- Hélène Barucq organized the Fourth Workshop of Strategic Action DIP in Houston, October 10-11, 2016, <http://dip.inria.fr/workshops/fourth-workshop-of-the-strategic-action-dip/> and JOSO 2016 (Wave days in South-West) in Pau, March 9-11 <https://team.inria.fr/magique3d/conference-and-workshops/joso-2016-wave-days-in-south-west/>

9.1.1.2. *Member of the Conference Program Committees*

Victor Péron was member of the Program Committee of the Conference JOSO 2016 (Wave days in South-West) in Pau, March 9-11 <https://team.inria.fr/magique3d/conference-and-workshops/joso-2016-wave-days-in-south-west/>

9.1.2. *Journal*

9.1.2.1. *Reviewer - Reviewing Activities*

Members of Magique 3D have been reviewers for the following journals:

- Annales de l'Institut Henri Poincaré / Analyse non linéaire
- Applied Mathematics and Computation
- ESAIM : Mathematical Modelling and Numerical Analysis
- Geophysical Journal International
- IMA Journal of Numerical Analysis
- International Journal for Numerical Methods in Engineering
- Journal of Computational Physics
- Journal of Scientific Computing
- Journal of Sound and Vibration
- Journal of the Acoustical Society of America
- Siam Journal on Scientific Computing
- Zeitschrift fuer Angewandte Mathematik und Physik

9.1.3. *Scientific Expertise*

- Julien Diaz was expert for the evaluation of Millennium Science Initiative project for the government of Chile.

9.1.4. *Research Administration*

- Hélène Barucq has been the chairwoman of the local jury of Inria competitive selection for Young Graduate Scientists (CR2) in Bordeaux. She participated to the selection committee for an Assistant Professor position at the University of Nantes and Paris 13. She was also part of the hiring committee for a Professor position at the University of Rennes 1. She is member of the local bureau of Inria Bordeaux Sud-Ouest focusing on scientific questions arising from research teams and of the Center Committee dealing with general questions related to the whole Research Center. She is the scientific head of the project DIP since its creation in 2009.
- Juliette Chabassier is member of the Workgroup for sustainable development at Inria Bordeaux Sud-Ouest.
- Julien Diaz is elected member of the Inria Technical Committee and of the Inria Administrative and Scientific Boards. He is appointed member of the CDT (Commission de Développement Technologique)
- Mamadou N'Diaye is member of the Center Committee of Inria Bordeaux Sud-Ouest.
- Victor Péron is appointed member of the CJC (Commission Jeunes Chercheurs) of Inria Bordeaux Sud-Ouest.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

- Licence : Izar Azpiroz, Fonctions et intégrales, 19.5 heures, MATH L1, UPPA, France
- Master : Julien Diaz, Transformées, 24h Eq. TD, M1, EISTIA, France
- Master : Marc Duruflé, Calcul scientifique en C++, 96h Eq. TD, M1, Bordeaux INP, France
- Licence : Marc Duruflé, Equations Différentielles, 20h Eq. TD, L3, Bordeaux INP, France
- Licence : Marc Duruflé, Calcul scientifique en Fortran 90, 20h Eq. TD, L3, Bordeaux INP, France
- Licence : Marc Duruflé, Algorithmique numérique, 30h Eq. TD, L3, Bordeaux INP, France
- Licence : Mamadou N'Diaye, Compléments d'algèbre, 19,5h Eq. TD, L1, UPPA, France
- Licence : Mamadou N'Diaye, Fonction de la variable réelle, 19,5h Eq. TD, L1, UPPA, France
- Licence : Mamadou N'Diaye, Développements limités - suites et séries, 19,5h Eq. TD, L2, UPPA, France
- Licence : Mamadou N'Diaye, Analyse 3A et Analyse 3B, 19,5h Eq. TD, L2, UPPA, France
- Master : Victor Péron, Analyse des EDP, 9 Eq. TD, M1, EISTI, France
- Master : Victor Péron, Analyse numérique fondamentale, 70 Eq. TD, M1, UPPA, France
- Master : Victor Péron, Analyse, 23 Eq. TD, M1, UPPA, France
- Master : Victor Péron et Sébastien Tordeux, Analyse Numérique 1: différences finies, 87 eq. TD, Master1, UPPA, FRANCE
- Master : Victor Péron et Sébastien Tordeux, Introduction aux phénomènes de propagation d'ondes, 38 eq. TD, Master 2, UPPA, FRANCE
- Licence : Sébastien Tordeux, Statistique descriptive, 55 eq. TD, L1, UPPA, FRANCE
- Licence : Sébastien Tordeux, Analyse complexe , 20 eq. TD, niveau (M1, M2), L3, UPPA, France

9.2.2. Supervision

- HDR : Julien Diaz, Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media, Université de Pau et des Pays de l'Adour, April 7th, 2016 [9].
- PhD : Aralar Erdozain, Fast inversion of 3D Borehole Resistivity Measurements using Model Reduction Techniques based on 1D Semi-Analytical Solutions, Université de Pau et des Pays de l'Adour, December 15th 2016, Hélène Barucq, David Pardo (BCAM) and Victor Péron. [10].
- PhD : Vincent Popie, Modélisation asymptotique de la réponse acoustique de plaques perforées dans un cadre linéaire avec étude des effets visqueux, ISAE, January 14th 2016 , Estelle Piot (ONERA) and Sébastien Tordeux. [11].
- PhD in progress : Izar Azpiroz Irigorri, Approximation des problèmes d'Helmholtz couplés sur maillages virtuels , October 2014, Hélène Barucq, Julien Diaz and Rabia Djellouli (CSUN).
- PhD in progress : Vincent Darrigrand, Etude d'erreur pour des problèmes d'Helmholtz approchés par des techniques de Petrov-Galerkin , October 2013, Hélène Barucq and David Pardo.
- PhD in progress : Aurélien Citrain, Déformation 3D de maillages en imagerie sismique, Méthodes d'inversion sismique dans le domaine fréquentiel , October 2016, Hélène Barucq and Christian Gout.
- PhD in progress : Florian Faucher, Méthodes d'inversion sismique dans le domaine fréquentiel , October 2014, Hélène Barucq.
- PhD in progress : Hamza Alaoui Hafidi, Imagerie ultrasonore tridimensionnelle dans les milieux hétérogènes complexes, October 2015, Encadrement : Marc Deschamps, Michel Castaings, Eric Ducasse, Samuel Rodriguez (I2M), Hélène Barucq, Marc Duruflé, Juliette Chabassier (Magique 3D).

PhD in progress : Justine Labat, Diffraction d'une onde par des petits obstacles dans des milieux complexes, October 2016, Victor Péron and Sébastien Tordeux.

PhD in progress : Mamadou N'Diaye, Analyse et développement de schémas temporels hybrides pour les équations hyperboliques du premier ordre, January 2015, Hélène Barucq and Marc Duruflé.

PhD in progress : Chengyi Shen, Approches expérimentale et numérique de la propagation d'ondes sismiques dans les roches carbonatées, October 2016, Julien Diaz and Daniel Brito (LFC).

PhD in progress : Elvira Shishenina, Approximations hybrides par éléments finis et éléments virtuels discontinus pour l'élasto-acoustique, October 2015, Hélène Barucq and Julien Diaz.

Master thesis : Aurélien Citrain, 2D hybrid meshes for a DG code, Insa de Rouen, Sept. 2016.

Master thesis : Alain Ha, High order time discretization for dissipative wave equations, Université de Rennes, Sept. 2016.

Master thesis : Justine Labat, Diffraction of an electromagnetic wave by small obstacles, Université de Pau et des Pays de l'Adour, Sept. 2016.

Master 1 internship : Baptiste Olivier, Modeling wave propagation in musical instruments, MatMeca, Sept. 2016.

9.2.3. *Juries*

- Hélène Barucq : Julien Diaz (Université de Pau et des Pays de l'Adour) "Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media", HDR, April 7th 2016
- Hélène Barucq : Vincent Deymier (ONERA Toulouse) "Etude d'une méthode d'éléments finis d'ordre élevé et de son hybridation avec d'autres méthodes numériques pour la simulation électromagnétique instationnaire dans un contexte industriel", PhD thesis, December 8th 2016
- Hélène Barucq : Asma Toumi (Université Paul Sabatier Toulouse III) "Méthodes numériques asynchrone pour la modélisation de phénomènes multi-échelles", PhD thesis, September 21th 2016
- Hélène Barucq : Romain Brossier (Université de Grenoble) "Contributions to developments and applications of Full Waveform Modeling and Inversion", HDR, November 18th 2016
- Julien Diaz : Azba Riaz (Université de Cergy Pontoise) "A new discontinuous Galerkin formulation for time dependent Maxwell's equations: a priori and a posteriori error estimation", PhD thesis, April 4th 2016
- Julien Diaz : Valentin Vinales (Université de Paris Saclay) "Problèmes d'interface en présence de métamatériaux : modélisation, analyse et simulations", PhD thesis, September 8th 2016
- Julien Diaz (reviewer): Asma Toumi (Université Paul Sabatier Toulouse III) "Méthodes numériques asynchrone pour la modélisation de phénomènes multi-échelles", PhD thesis, September 21th 2016

9.3. Popularization

- Juliette Chabassier took part in a round table around science professions in the high school of Valence d'Agen in March 2016.
- Juliette Chabassier shared her experience as a scientist during "Printemps de la Mixité" in May 2016.
- Juliette Chabassier participated in scientific "speed datings" during the "Filles et Maths" day in May 2016.
- Juliette Chabassier was co-responsible for a workshop around "Women in science" during Inria "Fête de la science" in October 2016.

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Major publications by the team in recent years

- [1] H. BARUCQ, A. BENDALI, M. FARES, V. MATTESI, S. TORDEUX. *A Symmetric Trefftz-DG formulation based on a local boundary element method for the solution of the Helmholtz equation*, in "Journal of Computational Physics", October 2016 [DOI : 10.1016/J.JCP.2016.09.062], <https://hal.archives-ouvertes.fr/hal-01395861>

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- [9] J. DIAZ. *Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media*, Université de Pau et des Pays de l'Adour, April 2016, Habilitation à diriger des recherches, <https://tel.archives-ouvertes.fr/tel-01304349>
- [10] A. ERDOZAIN. *Model Reduction Techniques for the Fast Inversion of Borehole Resistivity Measurements*, Université de Pau et des Pays de l'Adour, December 2016
- [11] V. POPIE. *Asymptotic modeling of the acoustic response of perforated plates in a linear case with a study of viscous effects*, Institut Supérieur de l'Aéronautique et de l'Espace (ISAE), January 2016, <https://hal.archives-ouvertes.fr/tel-01309272>

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- [12] H. BARUCQ, A. BENDALI, M. FARES, V. MATTESI, S. TORDEUX. *A Symmetric Trefftz-DG formulation based on a local boundary element method for the solution of the Helmholtz equation*, in "Journal of Computational Physics", October 2016 [DOI : 10.1016/J.JCP.2016.09.062], <https://hal.archives-ouvertes.fr/hal-01395861>
- [13] A. BENDALI, P.-H. COCQUET, S. TORDEUX. *Approximation by Multipoles of the Multiple Acoustic Scattering by Small Obstacles in Three Dimensions and Application to the Foldy Theory of Isotropic Scattering*, in

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