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Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media.

Julien Diaz

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Habilitation à Diriger des Recherches

UPPA - Université de Pau et des Pays de l'Adour

Spécialité Mathématiques Appliquées

Julien DIAZ

Chargé de Recherche, Équipe Projet Commune Magique 3D

Inria Bordeaux Sud-Ouest
et

Laboratoire de Mathématiques et de leurs Applications UMR CNRS 5142

**Modélisation et simulation Avancée de phénomènes de propagation d'ondes
dans des milieux GéophysIQUES 3D.**

soutenue le 7 avril 2016 devant le Jury composé de

Rémi Abgrall	Rapporteur
Abderrahmane Bendali	Examineur
Hélène Barucq	Examinatrice
Henri Calandra	Examineur
Patrick Joly	Examineur
Peter Monk	Rapporteur
Jeroen Tromp	Rapporteur

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Première partie

Partie Administrative

Curriculum Vitae

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Né le 5 novembre 1978
Nationalité française
Pacsé

Postes

- 2006- : Chargé de Recherche, Magique 3D, Inria Bordeaux Sud Ouest
- 2006-2007 : Post-Doctorat à l'Université de Bâle (Suisse), sous la direction de Marcus Grote
- 2005-2006 : Post-Doctorat au département SINETICS d'EDF R&D de Clamart
Sujet : Étude des phénomènes de bruit de structure,

Études

- 2001-2005 : Doctorat en Mathématiques Appliquées de l'Université Paris VI.
Effectué au projet POems de l'Inria Rocquencourt sous la direction de Patrick Joly
Sujet : Approches analytiques et numériques de problèmes de transmission en propagation d'ondes en régime transitoire. Application au couplage fluide-structure et aux méthodes de couches parfaitement adaptées.
Mention : Très honorable.
- 2001-2002 : Licence d'économétrie, Université Paris I
- 1998-2001 : Ingénieur diplômé de l'École Centrale Nantes.
 - 2000-2001 : Option Mathématiques Appliquées à l'École Centrale Paris.
 - 1998-2000 : Tronc commun à l'École Centrale Nantes
- 2000-2001 : DEA Mathématiques pour la Modélisation et la Simulation appliquées à la physique, Université de Versailles.

Curriculum Vitae

Activité dans l'Équipe Magique 3D

J'ai intégré l'équipe Magique 3D à mon arrivée à l'Inria le 1er février 2007 et j'en suis depuis le responsable permanent. Je présente dans cette section mon implication dans l'encadrement de doctorants, le transfert, le montage et le suivi de projets, l'organisation de manifestations scientifiques et les activités de vulgarisation de l'équipe.

Encadrement et coencadrement d'étudiants

Dès mon recrutement, je me suis impliqué dans l'encadrement d'étudiants au niveau master et thèse. Je ne détaille ici que la liste des thèses dont j'ai assuré le coencadrement, le plus souvent avec des chercheurs seniors. J'ai également encadré une dizaine d'étudiants en Master et je renvoie aux rapports d'activité de l'équipe disponibles à <https://team.inria.fr/magique3d/research/> pour plus de détails.

- Encadrement de la thèse de Caroline Baldassari, en codirection à 50% avec Hélène Barucq. *Modélisation et simulation numérique pour la migration terrestre par équation d'ondes*. Soutenue le 17 décembre 2009
Caroline est actuellement ingénieur de recherche en CDI chez SGI
- Encadrement de la thèse de Véronique Duprat, en codirection à 50% avec Hélène Barucq. *Conditions aux limites absorbantes enrichies pour l'équation des ondes acoustiques et l'équation d'Helmholtz*. Soutenue 6 décembre 2011.
Véronique est actuellement ingénieur de recherche en CDI dans la cellule de recherche Opéra commune à l'UPPA et à Total
- Encadrement de la thèse de Cyril Agut, en codirection à 80% avec Hélène Barucq. *Schémas numériques d'ordre élevé en espace et en temps pour l'équation des ondes*. Soutenue le 13 décembre 2011.
Cyril est actuellement ingénieur de recherche en CDI chez Total
- Encadrement de la thèse de Florent Ventimiglia, en codirection à 50% avec Hélène Barucq. *Schémas d'ordre élevé et pas de temps local pour les ondes élastiques en milieux hétérogènes*. Soutenue le 5 juin 2014.
- Encadrement de la thèse de Lionel Boillot, en codirection à 50% avec Hélène Barucq. *Contributions à la modélisation mathématique et à l'algorithmique parallèle pour l'optimisation d'un propagateur d'ondes élastiques en milieu anisotrope*. Soutenue le 12 décembre 2014.
Lionel est actuellement ingénieur expert en CDD dans le projet Inria Total DIP.
- Encadrement de la thèse de Jérôme Luquel, en codirection à 50% avec Hélène Barucq. *Imagerie de milieux complexes par Équations d'ondes élastiques*. Soutenue le 16 avril 2015.

Jérôme est actuellement professeur certifié à Niort

- Encadrement de la thèse de Marie Bonnasse Gahot, en codirection à 80% avec Stéphane Lanteri. *Méthodes de Galerkin Discontinues d'ordre élevé pour l'élastodynamique en domaine harmonique*. Soutenance le 15 décembre 2015.

Après sa soutenance, Marie sera ingénieur expert en CDD dans le projet Inria Total DIP, dans le cadre du projet européen HPC4E (HPC for Energy).

Je coencadre actuellement les thèses d'Izar Azpiroz (soutenance prévue fin 2017) et d'Elvira Shishenina (soutenance prévue fin 2018).

Développement Logiciel

J'ai participé au développement de plusieurs logiciels de l'équipe. Je décris ici brièvement leurs fonctionnalités et mon degré de participation et je donnerai plus de détails dans la partie scientifique. Tous les codes ci-dessous sont écrits en Fortran 90.

- **Hou10ni**. Ce code calcule la solution de problèmes de propagation d'ondes acoustiques et élastiques en milieux hétérogènes, en domaines temporel et harmonique (Helmholtz), en dimension deux et trois. Il permet également la modélisation du couplage élasto-acoustique. Le code se base sur la méthode de Galerkin Discontinue avec Pénalité Intérieure pour la discrétisation en espace, avec des éléments d'ordre arbitrairement élevé et la p -adaptabilité. Dans la version 2D, les éléments du maillage peuvent être courbes pour mieux approcher les interfaces. Il a été parallélisé sous MPI et OpenMP. Je suis le principal développeur de ce code. Il a été utilisé et étendu par plusieurs étudiants de l'équipe. Il a servi aux comparaisons de performance entre la méthode de Galerkin Discontinue avec Pénalité Intérieure (IPDG) et la méthode d'éléments finis spectraux qui ont effectuées par Caroline Baldassari [A7]. Cyril Agut l'a utilisé pour analyser l'influence du paramètre de pénalisation sur les performances de la méthode IPDG [A4], puis pour développer des schémas d'ordre élevé en temps [A8]. Véronique Duprat a développé et testé des Conditions aux Limites Absorbantes sur des frontières arbitraires [A9, A5] La version élasto-acoustique 2D a été mise en œuvre par Élodie Éstécahandy [17] dans le cadre de sa thèse et a été utilisée dans un solveur de type Problème Inverse pour la reconstruction d'obstacles [77]. Plus récemment, Conrad Hillairet a mis en œuvre le couplage élasto-acoustique en dimension trois dans le cadre de son stage élève ingénieur de l'Insa de Rouen.

Le code a été validé en temporel à l'aide du logiciel Gar6more (voir ci-dessous). En harmonique, Hou10ni génère ses propres solutions analytiques, qui peuvent être des ondes planes ou des solutions de problèmes de diffraction par un cercle. Dans ce dernier cas, les solutions analytiques sont calculées par développement en séries de Bessel.

La version 2D a fait l'objet d'un dépôt APP.

- **DIVA/TMBM**. La plateforme DIVA, récemment renommée TMBM (Time Marching Based Methods) est la plateforme de simulation de propagation d'ondes en temporel développée par Total. Elle est optimisée pour le HPC, principalement en utilisant MPI. Je n'interviens pas directement dans le développement de cette plateforme, mais je supervise avec Hélène Barucq l'intégration des travaux des étudiants de l'équipe. Plusieurs étudiants ont contribué au développement : Caroline Baldassari, Florent Ventimiglia, Lionel Boillot et Jérôme Luquel.
- **Elasticus**. Ce logiciel est développé principalement par Simon Ettouati et Lionel

Boillot, sous ma direction. Il a pour but de faciliter l'intégration des travaux des doctorants dans la plateforme THBM. L'idée étant d'avoir un code moins optimisé, mais plus lisible, de manière à pouvoir tester rapidement les nouvelles fonctionnalités.

- **THBM.** Cette plateforme, appelée Time Harmonic Based Methods est l'équivalent de TMBM pour l'harmonique. Son développement est plus récent que THBM, et je supervise principalement l'intégration des travaux de thèse de Marie Bonnasse Gahot sur des méthodes de Galerkin Discontinues Hybrides.
- **Gar6more.** Ce code calcule la solution analytique de problèmes de propagation d'ondes dans des milieux 2D et 3D homogènes ou bicouches, à l'aide de la méthode de Cagniard de Hoop. Dans le cas homogène, le milieu peut-être acoustique, élastique ou poroélastique, infini ou semi-infini avec une condition de surface libre ou de bord fixe. Dans le cas bicouche, les couplages suivants ont été considérés (la source est dans le premier milieu) : acoustique/acoustique ; acoustique/élastique ; acoustique/poroélastique ; élastique/acoustique ; élastique/élastique ; poroélastique/poroélastique.

Le code est opensource et téléchargeable :

<http://web.univ-pau.fr/~jdiaz1/gar62DCecill.html>

pour la version 2D et

<http://web.univ-pau.fr/~jdiaz1/gar63DCecill.html>

pour la version 3D. Les utilisateurs visés sont des chercheurs ayant besoin de solutions de référence pour valider et/ou tester les performances de leurs codes de simulation de propagation d'ondes. Dans cette optique, Gar6more a déjà été utilisé par J. Tromp et C. Morency (Princeton) [124] et par R. Sidler, K. Holliger (Université de Lausanne) et J. Carcione (OGS Trieste) [144, 145] pour valider leurs codes de propagation d'ondes poroélastiques. Je suis également en contact avec Stefan Wenk, de l'Université de Munich, pour la validation de son code de couplage élasto-acoustique. Gar6more est régulièrement utilisé pour valider les développements de l'équipe dans le domaine temporel.

Je suis le principal développeur de ce code et j'en assure la maintenance.

Aujourd'hui, je dispose de toute l'expérience nécessaire pour faire évoluer les codes de l'équipe, en vue du passage à l'exascale. À ce titre, j'ai une très forte activité d'encadrement au niveau des stagiaires accueillis par l'équipe chaque année (en moyenne deux par an), des doctorants, mais aussi des post-doctorants.

Transfert

Ma contribution aux activités de transfert de l'équipe Magique3D a été principalement réalisée dans le cadre de l'action Stratégique DIP (Depth Imaging Partnership <https://dip.inria.fr>). DIP est un partenariat entre l'Inria et Total qui a pour but de regrouper les compétences de différentes équipes Inria pour mener des actions de recherche en lien avec l'imagerie sismique. Magique 3D joue un rôle prépondérant dans DIP puisque sa chef d'équipe Hélène Barucq est à l'origine de sa création et en est la responsable scientifique. Je participe à DIP de deux façons, par l'encadrement de thèses (Caroline Baldassari, Florent Ventimiglia, Lionel Boillot, Jérôme Luquel, Marie Bonnasse et Elvira Shishenina) et par le développement logiciel (voir ci-dessus). En particulier, je supervise les développements réalisés dans les plateformes de Total et à ce titre, j'effectue des séjours fréquents à Houston où sont maintenues ces plateformes.

Montage et suivi de projets

J'ai participé au montage (rédaction des projets scientifiques et du budget) et au suivi (rédaction des rapports à mi-parcours et des rapports finals) des projets suivants

- Projet "Akellarre", du fonds commun de coopération Aquitaine/Euskadi. Montant : 14 000 euros, de février 2011 à février 2013. Coordonné par H. Barucq. En collaboration avec le BCAM.
- ANR "AHPI", de juillet 2007 à juillet 2010. Coordonné par L. Baratchart (Inria Sophia). En collaboration avec l'Université Bordeaux 1 et l'Université d'Orléans
- Projet Européen FP7 "HPCGA", International Research Staff Exchange Scheme (IRSES). De janvier 2012 à Décembre 2014. Coordonné par J.F Méhaut (Université Joseph Fourier, Grenoble). En collaboration avec le BCAM, le BRGM, ISTERre, UFRGS (Federal University of Rio Grande do Sul), Institute of Informatics, Brésil ; UNAM (National Autonomous University of Mexico) , Institute of Geophysics, Mexique.
- Projet Inria-CNPq "HOSCAR", de janvier 2012 à décembre 2015. Coordonné par Stéphane Lanteri (Inria Sophia). En collaboration avec LNCC (Laboratorio Nacional de Computação Científica), COPPE/UFRJ (Alberto Luiz Coimbra Institute for Graduate Studies and Research in Engineering, Universidade Federal do Rio de Janeiro), INF/UFRGS (Instituto de Informatica, Universidade Federal do Rio Grande do Sul) ; LIA/UFC (Laboratorios de Pesquisa em Ciancia da Computação Departamento de Computação, Universidade Federal do Ceara), Brésil.
- Projet Européen FP7, "GEAGAM", International Research Staff Exchange Scheme (IRSES). De janvier 2015 à Décembre 2017. Coordonné par David Pardo (BCAM). En collaboration avec le BCAM, l'Université du Pays Basque (UPV/EHU), Barcelona Supercomputing Center (BSC), TOTAL, Politecnica Universidad Catalica de Valparaiso (PUCV), Universidad de Chile (UCHILE), Universidad Tecnica Federico Santa Maria (USM), University of Texas at Austin (UT).
- Projet européen "HPC4E", de décembre 2015 à novembre 2017. Coordonné par Stéphane Lanteri, en collaboration avec LNCC (Laboratorio Nacional de Computação Científica), COPPE/UFRJ (Alberto Luiz Coimbra Institute for Graduate Studies and Research in Engineering, Universidade Federal do Rio de Janeiro), INF/UFRGS (Instituto de Informatica, Universidade Federal do Rio Grande do Sul) ; LIA/UFC (Laboratorios de Pesquisa em Ciancia da Computação Departamento de Computação, Universidade Federal do Ceara), Brésil.
- Projet FEDER Poctefa, soumis en novembre 2015. Coordonné par Josep de la Puente (Barcelone Supercomputing Center). En collaboration avec le BSC, le BCAM et le CERFACS.

Organisation de Conférences et Workshops

- Membre du comité d'organisation de la conférence Waves 2009 à Pau au Palais Beaumont

<http://waves-2009.bordeaux.inria.fr/>.

Cette conférence a rassemblé 250 chercheurs d'une trentaine de pays différents.

- Membre du comité d'organisation de la Journée Ondes et Problèmes Inverses en Géophysique, organisée dans le cadre de l'année mondiale "Maths et Terre".

<http://www.ensta-paristech.fr/~chaillat/MPT2013.html>.

- Membre du comité d'organisation du premier workshop franco-russe sur la géophysique mathématique, la modélisation mathématique des milieux continus et les problèmes inverses

<http://uppa-inria.univ-pau.fr/m3d/ConfFR/>.

Diffusion Scientifique

- Exposé à la fête de la science (20 octobre 2010)
- Réalisation d'un film de vulgarisation, Sonder l'invisible : du séisme au modèle :

<http://www.universcience.tv/>

[video-sonder-l-invisible-du-seisme-au-modele--5539.html](http://www.universcience.tv/video-sonder-l-invisible-du-seisme-au-modele--5539.html) (2010).

Ce film a été traduit en anglais (Probing the invisible, from the earthquake to the model). Il a été présenté lors de la journée Mathematics for Planet Earth à l'Unesco, le 5 mars 2013

<http://mpe2013.org/fr/mpe-day-at-unesco/>.

Il fait également partie de l'exposition virtuelle Mathematics of Planet Earth

<http://imaginary.org/fr/node/134>

- Rédaction d'un article dans Interstices

https://interstices.info/jcms/i_58073/sonder-linvisible-du-seisme-au-modele

(2010).

- Exposé à la "Journées jeunes chercheurs en mathématiques du lycée de Navarre / UPPA"

<http://univ-pau.fr/live/newsletter/newsletter-n46/journeesmaths?isPdf=1>
(2013).

- Réalisation d'une Étude de Documents, "Prospection pétrolière : le sous-sol révélé", pour le magazine TDC (Textes et Documents pour la classe), à destination des enseignants du secondaire :

<http://www.cndp.fr/tdc/tous-les-numeros/les-mathematiques-de-la-terre.html>

(2013).

- Intervention dans une école primaire d'Arthez de Béarn.

Participation à des tâches administratives et à des activités d'enseignement

Tâches administratives

- Membre élu de la commission d'évaluation de l'Inria(2007-2014). J'ai effectué deux mandats d'élu à la CE. Cette commission a en charge tous les aspects liés à la fonction de chercheur : recrutements, détachements/délégation, éméritats, promotions, évaluations des équipes, réflexions sur la recherche chez Inria. J'ai notamment été :
 - Membre du Groupe de Travail "Évaluation des logiciels"
 - Coordinateur du Groupe de Travail "Transfert"
 - Membre du Groupe de Travail "SELECT" (logiciel pour la gestion des recrutements Inria)
- Membre élu suppléant du Conseil d'Administration de l'Inria (2014-2018)
- Membre élu suppléant du Conseil Scientifique de l'Inria (2014-2018)
- Membre élu titulaire du Comité Technique de l'Inria (2014-2018)
- Membre élu du comité d'experts du LMA (2008-2011)
- Membre élu de l'AGOS (Association pour la Gestion des Oeuvres sociales (2011-2013)
- Jurys de Concours
 - Inria Saclay, CR1 et CR2 (2009)
 - Inria Grenoble, CR1 et CR2 (2010)
 - Inria Sophia, CR2 (2013)
 - Inria Saclay, CR2 (2013)
 - Inria Lille, CR2 (2014)
 - Inria Bordeaux, CR2 (2014)
 - Inria CR1 (2014)
 - Admission CR2 Inria (2013)
 - Mcf Toulouse (2009, 2010, 2012, 2013 et 2014)
 - Mcf Pau (2010)
- Membre élu du CLSCHT de l'Inria Bordeaux (2013-2014)

Activités d'enseignement

- Université de Pau et des Pays de l'Adour
J'ai assuré le cours de M2 MMS, *Propagation d'Ondes et Imagerie*, en collaboration

Tâches administratives

avec Hélène Barucq puis Sébastien Tordeux durant les années 2007/2008, 2009/2010, 2010/2011, 2011/2012, 2012/2013 et 2014/2015 (environ 25h équivalent TD).

- ESTIA (École d'ingénieurs, Bidart)
TD du module "Transformées" en deuxième année d'école (équivalent à un Master 1) en 2009/2010, 2012/2013, 2013/2014, 2014/2015 et 2015/2016 (environ 30h équivalent TD chaque année).
- EISTI (École d'ingénieurs, Pau)
Cours et TD du module "Résolution de systèmes linéaires" en 2009/2010 (environ 30h équivalent TD).

Participation à des jurys de thèse

- Essayed Sayari (Université de Cergy-Pontoise) "Étude numérique de quelques équations aux dérivées partielles par la méthode discontinue de Galerkin", 28 juin 2010.
- Ronan Madec (Université de Pau) "Méthode des éléments spectraux pour la propagation d'ondes sismiques en milieu géologique fluide-solide avec pas de temps locaux et couches absorbantes parfaitement adaptées C-PML", 10 décembre 2010.
- Jean-Baptiste Laurent (Université de Toulouse) "Raffinements locaux auto-adaptatifs dans une méthode Galerkin discontinu pour la résolution des équations de Maxwell", 10 juillet 2013.
- Axel Modave (Université de Liège, Belgique) "Absorbing Layers for Wave-Like Time-Dependent Problems - Design, Discretization and Optimization", 7 octobre 2013.
- Ludovic Moya (Université de Nice), "Discontinuous Galerkin time domain method for electromagnetic wave propagation in biological tissues", 16 décembre 2013.
- Vanessa Mattesi (Université de Pau et des Pays de l'Adour), "Propagation des ondes dans un domaine comportant des petites hétérogénéités : modélisation asymptotique et calcul numérique", 11 décembre 2014.

Publications

Articles dans des revues internationales avec comité de lecture

- [A1] J. Diaz and M. J. Grote. Multi-level explicit local time-stepping methods for second-order wave equations. *Computer Methods in Applied Mechanics and Engineering*, 291, pp. 240–265, Juil. 2015.
- [A2] J. Diaz, K. Schmidt, and C. Heier. Non-conforming Galerkin finite element method for symmetric local absorbing boundary conditions. *Computers and Mathematics with Applications*, page 22, 2015. to appear.
- [A3] M. Amara, S. Chaudhry, J. Diaz, R. Djellouli, and S. Fiedler. A local wave tracking strategy for efficiently solving mid-and high-frequency Helmholtz problems. *Computer Methods in Applied Mechanics and Engineering*, 276, pp. 473–508, 2014.
- [A4] C. Agut and J. Diaz. Stability analysis of the Interior Penalty Discontinuous Galerkin method for the wave equation. *ESAIM : Mathematical Modelling and Numerical Analysis*, 47(3), pp. 903–932, 2013.
- [A5] H. Barucq, J. Diaz, and V. Duprat. Long-Time Stability Analysis of Acoustic Absorbing Boundary Conditions for Regular-Shaped Surfaces. *Mathematical Models and Methods in Applied Sciences*, 23(11), pp. 2129–2154, 2013.
- [A6] H. Barucq, T. Chaumont Frelet, J. Diaz, and V. Péron. Upscaling for the Laplace problem using a discontinuous Galerkin method. *Journal of Computational and Applied Mathematics*, Nov. 2012.
- [A7] C. Baldassari, H. Barucq, H. Calandra, B. Denel, and J. Diaz. Performance Analysis of a High-Order Discontinuous Galerkin Method. Application to the Reverse Time Migration. *Communications in Computational Physics*, 11(2), pp. 660–673, Jan. 2012.
- [A8] C. Agut, J. Diaz, and A. Ezziani. High-Order Schemes Combining the Modified Equation Approach and Discontinuous Galerkin Approximations for the Wave Equation. *Communications in Computational Physics*, 11(2), pp. 691–708, Fev. 2012.
- [A9] H. Barucq, J. Diaz, and V. Duprat. Micro-differential boundary conditions modelling the absorption of acoustic waves by 2D arbitrarily-shaped convex surfaces. *Communications in Computational Physics*, 11(2), pp. 674–690, 2012.
- [A10] C. Baldassari, H. Barucq, H. Calandra, and J. Diaz. Numerical performances of a hybrid local-time stepping strategy applied to the reverse time migration. *Geophysical Prospecting*, 59(5), pp. 907–919, Sept. 2011.
- [A11] H. Barucq, J. Diaz, and M. Tlemcani. New absorbing layers conditions for short water waves. *Journal of Computational Physics*, 229, pp. 58–72, 2010.

Publications

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Publications

Deuxième partie

Partie Scientifique

Introduction

Most of my research activities in the Inria team Magique-3D are linked to 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 my goal is to contribute to this task by improving the modeling and by deriving advanced numerical methods for solving wave problems.

A The Reverse Time Migration

In order to give an overview of my research activities, I will first describe briefly the principle of Seismic Reflection Imaging. I refer the reader to the SEG short course of Biondo Biondi for more details on this technique [33]. Seismic Reflection Imaging is a process that consists in three steps. The first step is called the “acquisition”. It is the acquisition of series of recordings obtained during a seismic acquisition campaign, where elastic waves are generated by the successive explosions of N_s sources, $(s_i(\mathbf{x}, t))_{i=1..N_s}$, placed all over the region to be explored. Then the variations of a given quantity u are registered at N_r receivers $(r_j)_{j=1..N_r}$. This quantity can be scalar (the vertical component of the displacement or of the velocity, the pressure, ...), or vectorial (the displacement or the velocity fields). In the following, we denote by $u_{ij}(\mathbf{x}, t)$ the recordings obtained at receiver r_{ji} after the explosion of source s_i . Once these recordings are obtained, the next step is called “velocity estimation” and consists in defining an approximate model of the subsurface. This step is usually performed using tomography by Velocity Analysis [70, 34, 149, 31, 32] or by Migration Velocity Analysis [79, 166, 148, 49, 137, 37]. This can be done for an acoustic or elastodynamic model. In the case of an acoustic model, only the velocities of the P-waves (the compressional waves) will be reconstructed. In

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the case of an elastic model, it is necessary to construct also an initial model for S waves (the shear waves), and possibly a model for the Thomsen parameters if one wishes to consider imaging of anisotropic media. I will give more details on the different kind of waves and on the anisotropy in the last part of this section and I refer to [163, 165] for discussions on the issues related to seismic imaging of anisotropic media.

The velocity model will be used as an initial model for the last step, which is called “migration”. This step can be performed by different methods. Kirchhoff migration [35, 48] has been very popular during the past decades, because it is based on an approximation of the wave equation, which reduces strongly the computational costs. However, in order to improve the accuracy of the images, geophysicists are now interested in the Reverse Wave Equation (RTM), which is based on the full wave equation [19, 172].

The algorithm of RTM reads as

1. For each source (i.e. for i from 1 to N_s) :
 - (a) Forward step : Propagate a numerical wave generated by the source s_i in the initial model, and register a quantity v_i^f at each point of the mesh and at each time step of the simulation. We denote by $v_i^f(x, y, z, t)$ the value of this quantity at (x, y, z) and at t . The exponent f is the abbreviation of 'forward'. Note that the registered quantity v_i^f is not necessarily the quantity that has been registered during the acquisition campaign. It is for instance possible to register the vertical component of the displacement at the receivers during the acquisition campaign and the complete velocity field during the forward step.
 - (b) Backward step : Backpropagate a numerical wave generated by all the receivers $(r_{ij})_{j=1..N_r}$ in the initial model. To do so, we use the following as a source :

$$s_i^*(x, t) = \sum_{j=1..N_r} u_{ij}(\mathbf{x}, T - t),$$

where T is the final time of the experiment. We register then a quantity v_i^b at each point of the mesh and at each time of the simulation. This quantity should be the same that the one registered during the forward step. We denote by $v_i^b(x, y, z, t)$ the value of this quantity at point (x, y, z) and at time t . The exponent b is the abbreviation of 'backward'.

- (c) Imaging Condition : At each point (x, y, z) , compute the imaging condition $I_i(x, y, z)$. In [48], Claerbout proposed the condition

$$I_i(x, y, z) = \int_0^T v_i^f(x, y, z, t) v_i^b(x, y, z, t) dt \quad (\text{A.1})$$

2. The total imaging condition is then obtained by summing up the conditions obtained for each source :

$$I(x, y, z) = \sum_{i=1}^{N_s} I_i(x, y, z) \quad (\text{A.2})$$

The above algorithm, which is specific to time-domain problems, can be adapted to frequency domain. One has then to preprocess the registered signals at the receivers by a Fourier transform in time. We suppose here that, for each $i \in \{1..N_s\}$ and each $j \in \{1..N_r\}$, the discrete

Fourier transform of u_{ij} has been computed at N_ω frequencies $(\omega_k)_{k=1..N_\omega}$. We denote by $\hat{u}_{ij}(\mathbf{x}, \omega_k)$ the value of \hat{u}_{ij} at point \mathbf{x} and at frequency ω_k .

The algorithm of RTM in frequency domain reads then as :

1. For each frequency (i.e. for i from 1 to N_ω) :
 - (a) For each source (i.e. for i from 1 to N_s) :
 - i. Forward step : Propagate a numerical wave generated by the source $\hat{s}_i(\omega_k)$ in the initial model, and register a quantity $\hat{v}_{i,k}^f$ at each point of the mesh. We denote by $v_{i,k}^f(x, y, z)$ the value of this quantity at point (x, y, z) .
 - ii. Backward step : Backpropagate a numerical wave generated by all the receivers $(\hat{r}_{ijk})_{j=1..N_r}$ in the initial model. To do so, we use the following as a source

$$\hat{s}_i^*(x, \omega_k) = \sum_{j=1..N_r} \bar{\hat{u}}_{ijk}(\mathbf{x}).$$

The complex conjugation is the “*harmonic*” equivalent of the reverse time operator $t \mapsto T - t$.

We register then a quantity $\hat{v}_{i,k}^b$ at each point of the mesh. We denote by $\hat{v}_{i,k}^b(x, y, z)$ the value of this quantity at point (x, y, z) .

- iii. Imaging Condition : At each point (x, y, z) , compute the imaging condition $I_{ik}(x, y, z)$. For instance, the condition proposed by Claerbout becomes

$$I_{ik}(x, y, z) = \hat{v}_{i,k}^f(x, y, z) \hat{v}_{i,k}^b(x, y, z) \tag{A.3}$$

- (b) The imaging condition for a given frequency is then computed by summing up the conditions obtained for each source :

$$I_k(x, y, z) = \sum_{i=1}^{N_s} I_{ik}(x, y, z) \tag{A.4}$$

- (c) The full imaging condition is computed by summing up the conditions obtained for each frequency :

$$I(x, y, z) = \sum_{i=1}^{N_s} \alpha_k I_k(x, y, z) \tag{A.5}$$

where the coefficients α_k are weights associated to each frequency. Usually, we set $\alpha_k = 1$.

Note that the computation of the imaging condition is much simpler in frequency domain than in time domain. Indeed, the solution for a given frequency ω_k can be computed independently of the solutions for the other frequencies, while the computation of a time-domain solution at time t depends on the solution at all the previous time steps. Since the computational domains are huge, the computation of time-domain imaging conditions requires the implementation of sophisticated algorithms in order to limit as much as possible the storage and computational costs. Moreover, for a given frequency, the solution of a Helmholtz problem for each source can be obtained by solving a multi-right hand side linear system where each right hand side corresponds to one source. Hence, if one considers a direct solver, it is sufficient to perform

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one single factorization to model both forward and backward propagation for all the sources. Last, the frequency domain is much more convenient to deal with dissipative media where the attenuation depends on the frequency, since time-domain modeling would require the introduction of convolution product to handle this kind of dissipation.

Unfortunately, when considering 3D industrial problems, the size of the computational domains is so huge that the factorization of the global matrix is still out of reach, even with the help of the most advanced supercomputing facilities. That is why harmonic RTM has been until now mostly used for small computational domains or in two dimensions, while time-domain RTM is preferred for larger problems.

A.1 The wave equations

In the algorithms presented above, I did not detail the equations modeling the wave propagation. The simplest model is the acoustic wave equation, which models only the propagation of P-waves compressional waves (P-waves). Acoustic media are characterized by two parameters, the density ρ and the wave speed V_P . A more accurate model is given by the isotropic elastodynamic wave equation that also takes into account the propagation of shear waves (S-waves). In isotropic media the velocity of waves does not depend on the direction of propagation, and geophysics media are generally anisotropic. To handle the anisotropy, it is necessary to introduce additional parameters known as Thomsen parameters [162]. Of course, the more accurate the model is, the higher the computational costs are. There exist more accurate models, taking into account attenuation or the porosity of the media, but the computational costs are still too high to be implemented in a Reverse Time Migration. Therefore, I will only focus in the following on acoustic and elastodynamic wave equations, which were my main interests during the past years. These equations can be written either as a first order formulation, involving only first-order space and time derivatives, or as a second order formulation, involving second order space and time derivatives.

The first order formulation of the acoustic wave equation reads as

$$\left\{ \begin{array}{ll} \frac{1}{\mu(\mathbf{x})} \frac{\partial p}{\partial t}(t, \mathbf{x}) - \operatorname{div} \mathbf{u}(t, \mathbf{x}) = f(t, \mathbf{x}), & (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \rho(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}) - \nabla p(t, \mathbf{x}) = 0, & (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \mathcal{B}_1(p(t, \mathbf{x}), \mathbf{u}(t, \mathbf{x})) = 0, & (t, \mathbf{x}) \in]0, T[\times \partial\Omega, \\ p(0, \mathbf{x}) = p_0(\mathbf{x}), & \mathbf{x} \in \Omega, \\ \mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}), & \mathbf{x} \in \Omega, \end{array} \right. \quad (\text{A.6})$$

where

- Ω is a bounded open domain of \mathbb{R}^d , with $d = 1, 2$ or 3 ;
- $p : [0, T] \times \Omega \rightarrow \mathbb{R}$ is the pressure in Ω , in Pa;
- $\mathbf{u} : [0, T] \times \Omega \rightarrow \mathbb{R}^d$ is the velocity of the particles in Ω , in $\text{m}\cdot\text{s}^{-1}$;
- $\mu : \Omega \rightarrow \mathbb{R}^+$ is the bulk modulus, in Pa.
It is such that $0 < \mu(\mathbf{x}) < \mu_\infty$, with $\mu_\infty \in \mathbb{R}^+$;
- $\rho : \Omega \rightarrow \mathbb{R}^+$ is the mass density, in $\text{kg}\cdot\text{m}^{-3}$.
It is such that $0 < \rho(\mathbf{x}) < \rho_\infty$, with $\rho_\infty \in \mathbb{R}^+$;

- $f : [0, T] \times \Omega \longrightarrow \mathbb{R}$ is the source term, in s^{-2} ;
- \mathcal{B}_1 is a differential operator representing the boundary conditions. For a free surface condition, we have $\mathcal{B}_1(p, \mathbf{u}) = p$; for a wall condition, we have $\mathcal{B}_1(p, \mathbf{u}) = \mathbf{u} \cdot \mathbf{n}$, where \mathbf{n} denotes the unit normal vector outward to $\partial\Omega$. The expression of \mathcal{B}_1 is more complicated in the case of an absorbing boundary condition, and we will give more details in Chapter 1.
- p_0 and \mathbf{u}_0 are the initial conditions. If their support is not in Ω , they have to satisfy a compatibility condition such that $\mathcal{B}_1(p(t, \mathbf{x}), \mathbf{u}_0) = 0$ for any $\mathbf{x} \in \partial\Omega$.

The first order formulation of the elastodynamic wave equation reads as

$$\left\{ \begin{array}{l} \frac{\partial \underline{\underline{\sigma}}}{\partial t}(t, \mathbf{x}) - \underline{\underline{C}} \underline{\underline{\varepsilon}} \mathbf{u}(t, \mathbf{x}) = \underline{\underline{f}}(t, \mathbf{x}), \quad (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \rho(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}) - \nabla \underline{\underline{\sigma}}(t, \mathbf{x}) = 0, \quad (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \mathcal{B}_2(\underline{\underline{\sigma}}(t, \mathbf{x}), \mathbf{u}(t, \mathbf{x})) = 0, \quad (t, \mathbf{x}) \in]0, T[\times \partial\Omega, \\ \underline{\underline{\sigma}}(0, \mathbf{x}) = \underline{\underline{\sigma}}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{array} \right. \quad (\text{A.7})$$

where

- Ω is a bounded open domain of \mathbb{R}^d , with $d = 1, 2$ or 3 ;
- $\underline{\underline{\sigma}} : [0, T] \times \Omega \longrightarrow \mathbb{R}^{d^2}$ is the stress tensor in Ω , in Pa. It is a second order symmetric tensor, i.e. $\sigma_{ij} = \sigma_{ji}$;
- $\mathbf{u} : [0, T] \times \Omega \longrightarrow \mathbb{R}^d$ is the velocity of the particles in Ω , in $\text{m} \cdot \text{s}^{-1}$;
- $\underline{\underline{\varepsilon}}$ is the infinitesimal strain tensor. It is an operator defined as $\underline{\underline{\varepsilon}}(\mathbf{u}) = \frac{1}{2} (\underline{\underline{\nabla}} \mathbf{u} + \underline{\underline{\nabla}}^T \mathbf{u})$, i.e. $\varepsilon_{ij}(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$;
- $\underline{\underline{C}} : \Omega \longrightarrow \mathbb{R}^{d^4}$ is the stiffness tensor, in Pa. It is a fourth-order tensor that possesses the following symmetry properties : $C_{ijkl} = C_{jikl} = C_{ijlk}$ and $C_{ijkl} = C_{klij}$ for $(i, j, k, l) \in \{1..d\}$. Moreover, it satisfies $\underline{\underline{C}} \underline{\underline{\xi}} : \underline{\underline{\xi}} > 0$ for all symmetric second order tensor $\underline{\underline{\xi}}$.
- $\rho : \Omega \longrightarrow \mathbb{R}^+$ is the mass density, in $\text{kg} \cdot \text{m}^{-3}$. It is such that $0 < \rho(\mathbf{x}) < \rho_\infty$, with $\rho_\infty \in \mathbb{R}^+$;
- $\underline{\underline{f}} : [0, T] \times \Omega \longrightarrow \mathbb{R}$ is the source term, in $\text{Pa} \cdot \text{s}^{-2}$;
- \mathcal{B}_2 is a differential operator representing the boundary conditions. For a free surface condition, we have $\mathcal{B}_2(\underline{\underline{\sigma}}, u) = \underline{\underline{\sigma}} \mathbf{n}$, where \mathbf{n} denotes the unit normal vector outward to $\partial\Omega$; for a wall condition, we have $\mathcal{B}_2(\underline{\underline{\sigma}}, u) = u$. The expression of \mathcal{B}_2 is more complicated in the case of an absorbing boundary condition, and we will give more details in Chapter 1.
- $\underline{\underline{\sigma}}_0$ and \mathbf{u}_0 are the initial conditions. If their support is not in Ω , they have to satisfy a compatibility condition such that $\mathcal{B}_2(\underline{\underline{\sigma}}_0(t, \mathbf{x}), \mathbf{u}_0) = 0$ for any $\mathbf{x} \in \partial\Omega$.

Using the first symmetry property of the tensor $\underline{\underline{C}}$, we associate it to a $d \times d$ matrix \mathcal{C} , using the Voigt notation. This notation links each pair $\{i, j\}$ to a unique index I as indicated in Tabs. 1

Introduction

and 2, respectively in two and in three dimensions. For instance, in 3D, $C_{34} = C_{3323} = C_{3332}$. Moreover, \mathcal{C} is symmetric, because of the second symmetry property of $\underline{\underline{C}}$. The tensor $\underline{\underline{C}}$

$\{i, j\}$	$\{1, 1\}$	$\{2, 2\}$	$\{1, 2\}$	$\{i, j\}$	$\{1, 1\}$	$\{2, 2\}$	$\{3, 3\}$	$\{2, 3\}$	$\{1, 3\}$	$\{1, 2\}$
I	1	2	3	I	1	2	3	4	5	6

TABLE 1 – Voigt notation in 2D

TABLE 2 – Voigt notation in 3D

defines a general elastodynamic medium. For modeling seismic wave propagation, we are particularly interested in two kinds of media, the isotropic media and the transverse isotropic media. Isotropic media are such that the wave speed is independent of the direction of the wave propagation. In such a case, the stiffness tensor can be expressed with the help of only two parameters, λ and μ , that are called the Lamé parameters. We have (in 3D)

$$C_{11}^{iso} = C_{22}^{iso} = C_{33}^{iso} = \lambda + 2\mu, \quad C_{44}^{iso} = C_{55}^{iso} = C_{66}^{iso} = \mu, \quad \text{and} \quad C_{12}^{iso} = C_{13}^{iso} = C_{23}^{iso} = \lambda,$$

and the remaining parameters vanish.

In isotropic media, the volumic waves are of two kinds :

- the P-waves, also defined as pressure waves, or primary waves, or compressional waves, or longitudinal waves. They are such that the velocity \mathbf{u} is parallel to the direction of propagation of the waves and they satisfy $\text{curl} \mathbf{u} = 0$. Their wave speed is $V_p = \sqrt{\lambda + 2\mu\rho}$;
- the S-waves, also defined as shear waves, or secondary waves, or transverse waves. They are such that the velocity \mathbf{u} is orthogonal to the direction of propagation of the waves and they satisfy $\nabla \cdot \mathbf{u} = 0$. Their wave speed is $V_s = \sqrt{\mu\rho}$;

In order to model accurately the seismic wave propagation, it may be necessary to take the anisotropy into account. Most of geophysical media are transversely isotropic media, which means that they are isotropic in one plane orthogonal to an axis called anisotropy axis. If this axis is the vertical axis (the z axis), then the medium is Vertically Transverse Isotropic (VTI) and the stiffness tensor can be expressed thanks to six parameters : ρ , V_p , V_s and three additional parameters ϵ , δ , and μ introduced by Thomsen in[162]. We then have

$$C_{11}^{VTI} = C_{22}^{VTI} = \rho V_p^2 (1 + 2\epsilon), \quad C_{33}^{VTI} = \rho V_p^2, \quad C_{44}^{VTI} = C_{55}^{VTI} = \rho V_s^2, \quad C_{66}^{VTI} = \rho V_s^2 (1 + 2\gamma),$$

$$C_{12}^{VTI} = C_{11}^{VTI} - 2C_{66}^{VTI}, \quad \text{and} \quad C_{13}^{VTI} = C_{23}^{VTI} = \rho \sqrt{(V_p^2 - V_s^2)^2 + 2V_p^2 \delta (V_p^2 - V_s^2)} - \rho V_s^2.$$

and the remaining parameters vanish.

Note that the number of non zero elements is the same for VTI and for isotropic media. However, we will see in the next sections that because VTI media require more parameters, the computational costs of numerical simulations in VTI media are often higher than the costs of numerical simulations in isotropic media.

If the axis of anisotropy is not aligned with the vertical axis, then the media is called Tilted Transverse Isotropic. Besides the six previous parameters, it is then necessary to add two angles, θ and ϕ which are respectively the polar and azimuth angle of the axis of anisotropy. The TTI stiffness is then computed from the VTI stiffness tensor by using the relation

$$C_{ijkl}^{TTI} = \sum_{p=1}^d \sum_{q=1}^d \sum_{r=1}^d \sum_{s=1}^d R_{pi} R_{qj} R_{rk} R_{sl} C_{ijkl}^{VTI},$$

where, if $d = 3$,

$$R = \begin{bmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \theta & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{bmatrix}.$$

Except for particular values of θ and ϕ , the TTI stiffness tensor is full, which induces a big increase of the computational costs.

In three dimensions, the solution to the first order acoustic system requires to compute and to store one pressure and the three components of the velocity, while the solution of the first order elastodynamic system requires to compute and to store the six components of the stress (thanks to the symmetry of $\underline{\underline{\sigma}}$, we do not have to compute the nine components) and the three components of the velocity. It is possible to reduce these costs by considering only one of the two unknowns, thanks to the second order formulation of these systems. Of course, we will focus on the formulation that involves the “smallest” unknown : the pressure in Acoustics and the velocity in Elastodynamics.

The acoustic second order formulation is obtained by derivating the first and the third equation of (A.6) with respect to time and by using the equation in order to replace $\frac{\partial u}{\partial t}$

$$\left\{ \begin{array}{l} \frac{1}{\mu(\mathbf{x})} \frac{\partial^2 p}{\partial t^2}(t, \mathbf{x}) - \operatorname{div} \left(\frac{1}{\rho(\mathbf{x})} \nabla p(t, \mathbf{x}) \right) = \frac{\partial f}{\partial t}(t, \mathbf{x}), \quad (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \mathcal{B}_1 \left(\frac{\partial p}{\partial t}(t, \mathbf{x}), \nabla p(t, \mathbf{x}) \right) = 0, \quad (t, \mathbf{x}) \in]0, T[\times \partial\Omega, \\ p(0, \mathbf{x}) = p_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \frac{\partial p}{\partial t}(0, \mathbf{x}) = \operatorname{div} \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{array} \right. \quad (\text{A.8})$$

Similarly, the second order formulation of the elastodynamic wave equation reads as

$$\left\{ \begin{array}{l} \rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(t, \mathbf{x}) - \nabla \underline{\underline{C}} \underline{\underline{\varepsilon}} \mathbf{u}(t, \mathbf{x}) = \nabla \underline{\underline{f}}(t, \mathbf{x}), \quad (t, \mathbf{x}) \in]0, T[\times \Omega, \\ \mathcal{B}_2(\nabla \underline{\underline{\sigma}}(t, \mathbf{x}), \frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x})) = 0, \quad (t, \mathbf{x}) \in]0, T[\times \partial\Omega, \\ \mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \frac{\partial \mathbf{u}}{\partial t}(0, \mathbf{x}) = \nabla \underline{\underline{\sigma}}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{array} \right. \quad (\text{A.9})$$

Since these formulation are second-order in time, their solution requires to store at each time step the unknown and the first order time derivative of the unknown. If we have N degrees of freedom, we then have to store $2N$ values for Acoustics and $6N$ value for 3D Elastodynamics. For the first-order formulation, we only have to store the values of the unknowns. There are N values for the pressure and $3N$ values for the velocity in 3D Acoustics and $3N$ values for the velocity and $6N$ values for the stress in Elastodynamics. Hence, using the second order formulation allows for dividing the computational costs by two in Acoustics and by 1.5 in Elastodynamics. However, the first order formulation has several advantages. First, as we will see later, the imaging condition presented above can be improved by taking into account the divergence and the curl of the velocity in order to separate P waves from S waves. This can

be easily computed by the first order formulation, since we compute the space derivatives of the velocity to obtain the stress. With the second order formulation, it is necessary to postprocess the solution at each time step. Second, Absorbing Boundary Conditions and Perfectly Matched Layers are easier to implement in the first order formulation. Third, the extension to viscoelastic media is more natural with the first order formulation. Last, when one considers Discontinuous Galerkin Methods, the second order formulation requires the computation of the trace of the space derivatives of the solution on each face of the mesh, while the first order formulation only requires the trace of the solution.

This is probably because of all these advantages, that the first order formulation is the most popular for geophysical applications in time domain. In harmonic domain, since the bottleneck is here the solution of the linear system, it is more efficient to compute the solution to the second order formulation and to postprocess it to obtain its space derivatives.

B Improving the efficiency of RTM

The algorithm of RTM described in the previous section requires a huge computational burden, and the design of new advanced numerical methods is mandatory to improve the efficiency of the method and to tackle 3D realistic geophysical media. Here, “improving the efficiency of the method” means to increase its accuracy and/or reducing its computational costs. To do so, various research topics can be considered :

- **Design of efficient Artificial Boundary Conditions.** Geophysical media are so large compared to the wavelengths that they can be considered as infinite. However, since computers are not able to handle the concept of infinity, it is necessary to reduce the computational domain to a box. The boundaries of these boxes should be as transparent as possible, in order to minimize spurious reflections. I describe in Chapter 1 my contributions to the design of Absorbing Boundary Conditions and of Perfectly Matched Layers.
- **Design of numerical schemes in space.** I am particularly interested in the design of efficient schemes for time-domain and time-harmonic equations. The ultimate goal is to implement these schemes in order to solve realistic direct and inverse problems in a High Performance Computing framework. For that purpose, I adopted the following guidelines : the schemes are rigorously analyzed and validated by performing convergence analysis and the associated computational burdens are also estimated, including computational time, memory consumption, communications and load balancing. I have distributed my efforts in two directions : 1) the development of mature solution methodologies that can be almost immediately implemented in industrial codes and 2) the design and the analysis of prototype methods which require much more developments before being applied to industrial problems. I explain in Chapter 2 why I have chosen to consider a particular class of Finite element methods, the Discontinuous Galerkin method, and I detail my contributions to this topic.
- **Mesh Generation.** Finite Element Methods are based on meshes whose design is a crucial issue for the efficiency of the simulation. Indeed, only one very small cell inside a mesh of very large cells will strongly deteriorate the CFL condition of explicit time schemes or the condition number of the linear system in harmonic domain. Low quality cells, such as very elongated cells, will also increase the computational time while hampering the accuracy of the solution.

Mesh generation is outside of my research field. However, thanks to the strategic action DIP I am in close touch with Inria teams which are experts of this topic, and I have started to collaborate with researchers from Inria team Gamma3 on the design of efficient meshes for realistic geological simulations.

- **Time Discretization.** The design of higher order time schemes has been one of my main interests during the past ten years. I have mainly focused on two directions : 1) The development of local time stepping methods, which allow for using locally very small time steps where the cells of the mesh are very fine and large time steps where the cells are coarse; 2) The development of new global high-order time schemes, by considering an alternative approach to the ADER [108, 73]. Instead of using auxiliary variables, I have proposed to directly discretize the high-order space operators that appear after the Taylor expansion in time of the wave equation. This discretization is easily achieved thanks to DG methods.

I detail my contributions on these topics in Chapter 3.

- **Design of Efficient Linear Solvers.** The main bottleneck of numerical simulations for seismic waves propagation in harmonic domain is the solution of a huge linear system. Until now, we have chosen to consider direct solvers, mostly because we have to solve a linear system with a huge number of right hand sides and also because of the large condition number of the system. However, the amount of memory required by direct solvers for realistic simulations is still out of the reach of the most powerful supercomputer. It is then necessary to consider alternative strategies and I am now collaborating with the Inria team Hiepac (Luc Giraud, Emmanuel Agullo and Stojce Nakov) in order to implement hybrid solvers in the software of Magique 3D. Hybrid solvers combine Direct and Iterative solvers by mimicking Domain Decomposition strategies.
- **Improvement of Imaging Condition.** The Imaging Condition I have described above is the simplest one, and it does not take wave conversions into account. Since P-wave and S-wave interact with each other, it might be relevant to use an imaging condition including these interactions. In [134], it has been observed that with the vectorial version of Claerbout condition the images are polluted by interferences between the various modes. Following the publication of this paper, many works proposed to isolate P-waves from S-waves. In [78, 175], it has been proposed to distinguish the two kinds of waves at the acquisition step, by approximating the propagation trajectory. In [150], the authors proposed to record the whole elastic fields and then to apply a decomposition in P- and S-waves. In [44, 45] the separation is performed P et S just before the computation of the imaging condition. It is obviously possible to construct a RTM image by combining different imaging conditions. In the framework of the Ph.D. thesis of Jérôme Luquel [120], various conditions have been tested and it has been observed that though the conditions based on P- and S- waves improve the classical Claerbout conditions, they are not good enough to provide an accurate image of the subsurface.

In the eighties, Lailly [115] and Tarantola [154] showed that Claerbout Imaging principle could be rewritten as a local optimization problem in which the cost function is defined as the difference between observed data (obtained during the acquisition campaign) and computed data (obtained during the simulation). This theory was extended later to elastic waves by Tarantola in [155, 156] and it has been implemented by Gauthier in [85] using finite differences. Tarantola's works have been followed by

numerous authors, for instance [20, 138, 46, 133, 142, 116]. During the past decade, Jeroen Tromp and his collaborators have considered the imaging of the Earth by using a Spectral Finite Element method [119, 123, 164] and by considering sensitivity kernels. These works raised the possibility to apply the sensitivity kernels to RTM and the objective of Jérôme was to exploit this link by using Discontinuous Finite Element, which enables easily to compute the derivatives of the waves fields. The results he obtained showed that the sensitivity kernels improve the final images on simple 2D test cases. It now remains to extend these results to more realistic 3D geophysical domains

- **Computation of the Imaging condition.** If the choice of the imaging condition clearly impacts on the accuracy of the RTM, the design of the algorithm is crucial to reduce the computational costs. To emphasize this point, let us suppose that the computational grid contains N grid points and that the time interval has been divided in M time steps. We only consider here the case of one source, since each source can be modeled independently of the others.

The most simple algorithm for computing the Imaging condition consists in **(a)** computing and storing the whole forward field at each time step and at each point ; **(b)** computing and storing the whole backward field at each time step and at each point ; and **(c)** computing the imaging condition.

Steps **(a)** and **(b)** would require to store $2N \times M$ values, which is intractable since N can reach 10 000 000 and M can be 10 000.

A second possibility could be **(a)** compute and store the whole backward field at each time step and at each point ; **(b)** compute the whole forward field and the imaging condition on the fly.

This algorithm would require to store $N \times M$ values, which is still too heavy for practical applications.

An alternative consists in **(a)** computing the whole backward field at each point and **(b)** at each time step of the simulation, computing the corresponding value of the forward field and computing the imaging condition.

This approach only requires to store the field at one time step, but it is necessary to recompute the forward field from the beginning. Hence, it requires to compute $N(N+1)/2$ iterations of the forward field, which is not possible for realistic configurations.

Hence it is necessary to find a trade-off between the two previous approaches, which has been proposed by Symes [151], using an algorithm developed by Griewank [88].

It reads as : **(a)** compute the forward field and store it at M_c given time steps called “*checkpoints*” ; **(b)** compute the whole backward field ; and **(c)** at each time step of the simulation, compute the corresponding value of the forward field from the closest checkpoint and compute the imaging condition on the fly.

This algorithm requires to store only M_c time steps where M_c is usually much smaller than M , while the amount of computation depends on the position of the checkpoint. To optimize the computational time, we place them following the method proposed by Griewank [88].

Another technique [76, 50, 173], relies on the following remark. If we know the value of the forward field at the final time step M and its value on the boundaries at each time step, then we are able to reconstruct the forward field from M to 1 and the algorithm reads as : **(a)** compute the forward field, store its values on the boundaries of the domain at each time step and store its values at each point of the grid at the final time step M ; **(b)** compute the whole backward field and the whole forward field from M

to 1 and compute the imaging condition on the fly.

If N_b denotes the number of grid points on the boundaries, this algorithm reduces the storage cost to $N + M \times N_b$ and the computations to $3M$ iterations. This method has two drawbacks that have convinced us to focus on the Griewank algorithm. First of all, even if N_b is much smaller than N , it is not marginal in 3D problems. Second, this method is very sensitive to the quality of the absorbing boundary conditions imposed on the boundary and it is often necessary to store the value of the forward field not only on the boundary, but also on a ring surrounding the computational domain [50], which strongly increases the storage costs.

- **High Performance Computing.** All the methods and algorithms that are developed for geophysical applications have to be compatible with High Performance Computing. For instance, one motivation of favoring Discontinuous Galerkin Methods was the fact that all the computations at one time step can be performed locally, element by element, which reduces the communications when compared with finite element methods. As for the solution of linear system or the mesh generation, I am far from being an expert in that field and I do not pretend to propose new techniques. However, I try to keep up to date with the advances in the domain, and I collaborate with specialists of Computer Science in order to improve the performance of the software I developed. For instance, the Ph.D. thesis of Lionel Boillot [36] that I co-advised with H el ene Barucq, gave us the opportunity to collaborate with George Bosilca (University of Tennessee) and Emmanuel Agullo (Hiepacs), on the implementation of task programming strategies in the software DIVA of Total.

I have implemented most of the numerical methods I developed in numerical codes that I describe in Chapter 5. In order to benchmark and to validate these codes, I considered the computation of analytical solution using the Cagniard-de Hoop method, and I calculated these solutions for poroelastic media. I detail my contribution in Chapter 4.

Chapter 1

Design of Artificial Boundary Conditions

Most of the problems I am interested in are set in infinite domains or in domains so large with respect to the wavelengths that they can be considered infinite. Since a computer can not achieve calculations on an infinite set of points, it is mandatory to limit the computation to a domain containing the sources, the receivers and the obstacles. A first obvious solution is to choose the computational domain large enough so that the waves do not have time to hit the boundary and to come back to the receivers. Unfortunately, since the computational costs grow with L^d where d is the dimension of the problem and L the characteristic length of the problem, this solution is intractable.

Note that these problems are very close to the problems of oceanographic experiments in tank tests. The tank is necessarily finite and the reflections of the waves at its boundary interfere with the experiment. Two solutions can be envisaged to limit these reflections and they are very similar to the ones that we use in numerical simulations.

1. **To surround the basin by a damping material in order to absorb the waves.**
There are no physical materials allowing for a perfect absorption, but for numerical simulations we can fortunately design non physical materials with such properties. These materials are known as Perfectly Matched Layers (PML) proposed in 1994 by Bérenger [26, 27]. These layers became rapidly very popular because they are relatively easy to implement and they absorb the waves very efficiently : the amplitude of waves decreases exponentially as a function of the distance to the layer. However, they induce a high computational burden, they deteriorate the scalability of parallel codes and they may be unstable, in particular when coupled with TTI media or in aeroacoustics.
2. **To vibrate the boundaries as the waves arrive in order to absorb them.**
The mathematical equivalent of this technique is the Absorbing Boundary Condition technique, which consists in imposing on the exterior boundary a boundary condition representing an infinite domain. However, the transparent boundary condition, which generate no reflections, is non-local and requires to store the whole history of the solution on the boundary. In order to reduce the computational costs, we prefer to use approximate boundary conditions, that are local and less computationally expensive but produce spurious reflections. The most accurate conditions, known as “*higher-order boundary conditions*” involve high-order operators in space and in time, which reduce significantly the amplitude of the reflections, but increase the computational

costs and the difficulty of implementation.

There exist other kinds of technique that do not have any physical equivalent, such as the integral equation technique. As for the transparent boundary condition, this technique allows for an exact modeling of infinite media, but the computational are a very high price to pay in an industrial context. Another technique is the technique of infinite elements, which consists in using finite elements whose size tends to infinity, but this technique is difficult to implement.

1.1 Absorbing Boundary Conditions for Transverse Tilted Isotropic Media

One of the main drawbacks of Perfectly Matched Layers is their instability when applied to Anisotropic Media [102, 21]. These instabilities can be removed for some particular media, in which only one kind of waves can propagate [1, 103, 101, A17]. In elastodynamic media, such as TTI media, where two kinds of waves, the P-waves and the S-waves, propagate, the regular technique does not apply and its extension is still an open question. Indeed, removing the instabilities of the P-waves induces more instabilities on the S-waves and vice-versa. This is why, in collaboration with Lionel Boillot, H el ene Barucq and Henri Calandra, we have proposed a low order absorbing boundary condition for elliptic media, preserving the system stability. The construction is based on comparing and then connecting the slowness curves for isotropic and elliptic TTI waves.

In [B1], we have described how to construct this ABC in two dimensions. This paper is given page 6 of the Appendix and can be downloaded at

<https://hal.inria.fr/hal-01085442/>?

When applied in a TTI medium, this new ABC performs well with the same level of accuracy than the standard isotropic ABC set in an isotropic medium. The condition demonstrates also a good robustness when applied for large times of simulation. The extension to three-dimensional TTI elastodynamic media will be presented in a paper to be submitted soon.

1.2 Absorbing Boundary Condition for curved boundary

PMLs are probably one of the most popular methods because they are easier to implement than high-order ABCs and they provide exact modeling of infinite domains before discretization. However, the simplicity of implementation is proved for flat boundaries only and there are applications for which using piecewise linear boundaries is not optimal. In case of arbitrarily-shaped boundaries, the difficulty of implementing ABCs and PMLs is similar which implies that both approaches stand up. Nevertheless, both conditions do not demonstrate the same properties of stability. It is even surprising that PMLs are difficult to connect to energy estimates which can generally be established with ABCs. This is why, in collaboration with H el ene Barucq, we have defined a research program which aims at constructing high-order ABCs for curved boundaries and stable ABCs for media in which PMLs are known to be unstable. Our works are characterized by arbitrarily-shaped boundaries and by stability. Regarding high-order ABCs, there are results obtained by Hagstrom, Warburton, Givoli et al who proposed a new solution methodology to facilitate the implementation of high-order ABC

1.3 Perfectly Matched Layers for Aeroacoustic media

for plane boundary [15, 97, 96]. Regarding ABCs set where PMLs are unstable, we have considered anisotropic media. To the best of our knowledge, the ABCs that we have constructed are new. Our works distinguish themselves from others because we apply micro-local analysis techniques for the construction of ABCs. Here again, our mathematical background allows us to apply tools of fundamental analysis. The pseudo-differential calculus provides us a smart way to compute out-going waves in contact with curved boundaries. In [A9], which is given page 17 of the Appendix and available online at

<https://hal.inria.fr/hal-00649837>,

we have constructed a new family of absorbing boundary conditions from the micro-local factorization of the acoustic wave equation, following M.E. Taylor theory. By this way, we can generate an infinite number of boundary conditions which can not be obtained via the Nirenberg's factorization method. The conditions can be applied on arbitrarily-shaped surfaces and involve second-order derivatives. In order to easily include the boundary conditions inside a variational formulation, we then proposed in [A5], which is given page 34 of the Appendix and available online at

<https://hal.inria.fr/hal-00759451>

a reduced formulation of the wave equation using an auxiliary unknown which is defined on the regular surface only. The corresponding boundary value problem remains well-posed in suitable Hilbert spaces and we gave a demonstration in a framework that is suitable to applications. We then studied the long-time behavior of the wave field and we showed that it tends to 0 as time tends to infinity. This provided a weak stability result that we improved by performing a quantitative study of the energy. We have then shown that the energy is exponentially decaying if the obstacle is star-shaped and the external boundary is convex.

1.3 Perfectly Matched Layers for Aeroacoustic media

In collaboration with H el ene Barucq and Mounir Tlemcani (University of Oran, Algeria), we have proposed in [A11], which is given page 60 of the Appendix and available online at

<https://hal.inria.fr/inria-00418317>,

a new Perfectly Matched Layer for Shallow Water equations, based on a transformation proposed by Hu [103]. This layer required the computation of an auxiliary variable in the whole computational domain. We are now considering a new strategy, which only requires the computation of the auxiliary variable inside the layer. Moreover, the new methodology seems to be well-adapted to the non-linear shallow water equations. A publication is now being prepared.

Chapter 2

Analysis of Spatial Discretization Schemes

There exists a large variety of numerical methods to discretize the wave equation in space. Finite Difference Methods are very popular in the geophysical community and have been widely used during the past four decades, mainly for two reasons. First, they are relatively easy to implement in a numerical code ; second, when applied to transient wave equation they lead to diagonal mass matrices, which means that the solution at each time step does not require the solution of a (huge) linear system. I refer to the seminal works of Madariaga [121] and Virieux [171] for details on the design of Finite Difference Schemes in a geophysical context and to [87] for an example of application to 3D realistic domain. However, the main drawback of Finite Difference Methods is that they are based on regular cartesian grids, which severely complicates to modeling of rough topography or strong heterogeneities (see [127, 135]).

Based on unstructured meshes, FEM have the required flexibility to reproduce correctly the topography of the environment and the geometry of the various interfaces of the subsurface. FEM approximations are not only very accurate but they are also able to easily combine different orders of approximations. This important feature allows for reducing the computational cost while maintaining the level of accuracy. However, FEM methods are rarely used for time domain geophysical problems because they often deliver an implicit representation of the solution. In harmonic domain, they suffers from pollution effect [12, 13, 86]. I also refer to [100] for a review of finite element methods for harmonic acoustics.

To overcome the difficulty in time domain, mass condensation procedures were suggested [47, 104]. These techniques have however the effect of blocking the order of approximation. On the other hand, the spectral element methods (SEM) are based on the Gauss Lobatto quadrature formula, which allows for the diagonalization of the mass matrix without affecting the order of convergence. SEM was thus successfully applied to the wave equation [139, 53, 54] and more specifically for problems arising in Geophysics [110, 113, 112, 64]. We also refer to the paper of de Basabe and Sen [64] which is a very interesting state of the art for finite element techniques applied to the propagation of seismic waves. SEM methods are often applied on meshes with quadrilateral or hexahedral elements. Such meshes are often hard to generate, particularly when the topography and/or interfaces are complex. Note that SEM methods have been applied to meshes with triangular elements [160, 52, 136, 141]. Nevertheless, their implementation with high-order finite element remains difficult, and to the best of my knowledge, the transition to 3D is still an open problem. This is a major drawback for SEM since

most mesh generators have been developed for tetrahedral elements. Last, this technique does not solve the problem of pollution effect in harmonic domain, which explains why SEM are mostly used for time-domain problems.

In the two last decades, a new class of methods, called Discontinuous Galerkin Methods (DGM) emerged. DGM methods employ discontinuous functions, and therefore combine much more easily different levels of approximation on a single mesh. Furthermore, DGM can be applied to both hexahedral and tetrahedral elements. The approximate solution is expressed in a quasi-explicit way because the mass matrix is block diagonal even when its entries are evaluated analytically. DGM are also naturally adapted to parallel computing since all volume integrals are computed locally and the communications between the cells are ensured by integrals over the faces of the elements. In [9], the authors provide a detailed review of the various Discontinuous Galerkin approximations of the Laplacian operator. They show that the so-called Interior Penalty Discontinuous Galerkin Method (IPDGM), also known as Symmetric Interior Penalty (SIP) [10, 18], is one of the most suitable since it is stable and adjoint consistent, which guarantees the optimal order of convergence of the scheme. This explains why this method has been successfully used to solve Helmholtz equation [3, 4] and the wave equation [3, 91, 93, 92, 94].

DGM methods are also widely used for solving the first order wave equation. In [68], Delcourt, Fezoui and Glinsky have proposed a DGM with centered fluxes for Elastodynamics. This formulation is based on the one proposed in [132, 82]. It has been applied to model seismic waves propagation in [80, 152]. Another very popular approach in seismology, the ADER method, is based on upwind fluxes [108, 73, 73, 74].

2.1 Performance analysis and optimization of Discontinuous Galerkin methods.

In [A7], which is given page 82 of the Appendix and available online at

<https://hal.archives-ouvertes.fr/hal-00643334>,

we have shown, in collaboration with Caroline Baldassari, H el ene Barucq, Henri Calandra and Bertrand Denel, that the Interior Penalty Discontinuous Galerkin Method (IPDGM) is well-suited for RTM in heterogeneous media in spite the widespread belief that DGM methods are not competitive. This work can be compared to [A12], which contains, as far as I know, the only other comparisons between DGM and SEM in a geophysical context. The authors concluded that SEM is more efficient than DGM. This observation is however valid only for regular quadrilaterals covering homogeneous media. We have shown here that, using triangular-shaped elements, IPDGM exhibits the same level of performance as SEM, for both homogeneous and heterogeneous media. We have concluded that IPDGM is more versatile since it accommodates unstructured meshes with arbitrarily-shaped elements. Last, we have applied IPDGM to RTM to highlight its potential efficiency. Numerical experiments are performed in the case where the velocity varies strongly. The results reported in the paper have shown that we can recover all the interfaces of the considered subsurface. This work has been done in the framework of the PhD thesis of Caroline Baldassari [16].

One of the main drawbacks of IPDGM is its dependence on a penalty parameter which could have a negative impact on the CFL condition of explicit time schemes. Except for

2.2 Operator Based Upscaling for Discontinuous Galerkin Methods.

regular quadrilateral or cubic meshes, the optimal value of this parameter was not known explicitly. Moreover, there was no explicit expression of the CFL condition as a function of the penalization parameter, even for regular meshes. We have obtained an analytical expression of the optimal penalization parameter for regular triangular meshes. This expression is a function of both the radius of the inscribed circle and of the angle values of the triangle. This study was one of the topics of the PhD thesis of Cyril Agut [2]. We have also obtained an analytical expression of the CFL as a function of the penalization parameter for quadrilateral and cubic meshes, which is published in [A4]. This paper is given page 96 of the appendix and available online at

<https://hal.inria.fr/hal-00759457>.

We have considered numerical schemes for the discretization of the first order formulation of the wave equation, which seems to be more appropriate than the second order formulation to obtain realistic seismic images of elastic media. For the space discretization, we implemented the DG formulation with centered fluxes proposed in [68]. However, we observed that seismic images were often polluted by spurious waves. Thanks to a dispersion analysis, we showed that the DG-centered Flux formulation admits spurious modes for particular frequencies, and that these modes could be suppressed by adding a non-dissipative penalization term similar to the one proposed in [3]. This penalization term has enabled us to remove the spurious waves from the seismic images and to improve the order of convergence of the schemes. These results are part of Florent Ventimiglia PhD thesis [169].

2.2 Operator Based Upscaling for Discontinuous Galerkin Methods.

Realistic numerical simulations of seismic wave propagation are difficult to handle because they must be performed in strongly heterogeneous media. The heterogeneities are currently very small when compared to the characteristic dimensions of the propagation medium and to get accurate numerical solutions, engineers are then forced to use meshes that match the finest scale of the media. But meshing the whole domain with a fine grid leads to huge linear systems and the computational cost of the numerical method is then too high to consider 3D realistic simulations. Since it is hp-adaptive, DG method is however a good candidate to approximate Helmholtz problems with discontinuous coefficients but it still generates high computational costs. It was thus relevant to find a way of reducing the computational burden. Since we wanted to avoid homogenization techniques, we have been attracted by the operator-based upscaling method which has been developed first for elliptic flow problems [8] and then extended to hyperbolic problems [114, 167, 168]. We have then addressed the question of knowing if it could be interesting to apply operator-based upscaling with DG elements. In [A6], in collaboration with H el ene Barucq, Th eophile Chaumont Frelet and Victor P eron, we have presented a preliminary attempt of using operator-based upscaling with a DG method. We have considered the Laplace problem and we have compared the performance of our numerical scheme with the Lagrange finite elements. By performing the numerical analysis of the problem, we have shown that there is an interest in combining DG method with upscaling. This paper is given page 127 of the Appendix and available online at

<https://hal.inria.fr/hal-00757098>.

2.3 Efficient solution methodologies for high-frequency Helmholtz problems.

In collaboration with Mohamed Amara and Rabia Djellouli (CSUN) we proposed two new solution methodologies for solving high-frequency Helmholtz problems. The first one is a procedure for selecting basis function orientation in order to improve the efficiency of discretization methods based on local plane-wave approximations. The numerical results obtained for the case of a two-dimensional rigid scattering problem indicate that the proposed approach reduce the size of the resulting system by up to two orders of magnitude, depending on the frequency range, with respect to the size of the standard Least Square Method system. These results have been presented in [A3], which is given page 139 of the Appendix and available online at

<https://hal.inria.fr/hal-01010465>.

The second proposed solution method employs a boundary-type formulation without however involving Green functions and/or incurring singular integrals. In addition, this approach does not necessitate the use of a mesh. For these reasons, the method is named Mesh Free Frontier-based Formulation (MF3). Furthermore, the sought-after field is locally approximated using a set of basis functions that consist of Bessel-kind functions computed at a prescribed finite set of points. The preliminary numerical results obtained in the case of 2D-Helmholtz problems in the high-frequency regime illustrate the computational efficiency of MF3 (the method delivers results with high accuracy level, about 10^{-8} on the L^2 relative error, while requiring the solution of small linear systems). In addition, these results tend to suggest that MF3 is pollution free. These results have been presented at [C8]. A paper is in preparation.

Chapter 3

Design of Higher-Order Time Schemes

The main advantage of discontinuous approximations is their capability of allowing for space hp-adaptivity. They contribute thus to reduce the computational costs by computing the numerical solution on grids composed of fitted cells. However, local-time stepping schemes should also be considered to fully exploit the flexibility of discontinuous elements to reduce the computational burden. Indeed, a mesh that is composed of a collection of fine and coarse cells defines implicitly a local Courant-Friedrichs-Levy (CFL) condition and suggests thus to employ the corresponding local time step. Using the global time step that would be determined from the smallest cell obviously involves too many computations and thus limits the interest of using discontinuous elements. Moreover, it is well-known that a too small time step can create spurious dispersion effects. A local time stepping scheme can thus improve both the accuracy of the solution and the computational performances of the numerical code.

Locally implicit methods build on the long tradition of hybrid implicit-explicit (IMEX) algorithms for operator splitting in computational fluid dynamics (see [128, 11] and the references therein). Here, a linear system needs to be solved inside the refined region at every time-step, which becomes not only increasingly expensive with decreasing mesh size, but also increasingly ill-conditioned as the grid-induced stiffness increases [107]. Moreover, even when each individual method has order two, the implicit-explicit component splitting can reduce by one the overall space-time convergence rate of the resulting scheme [71, 69]. Recently, Descombes, Lanteri and Moya[69] remedied that unexpected loss in accuracy and hence recovered second-order convergence, by using the LF/CN-IMEX approach of Verwer [170] instead, yet at the price of a significantly larger albeit sparse linear system.

In contrast, locally explicit time-stepping methods remain fully explicit by taking smaller time-steps in the “fine” region, that is precisely where the smaller elements are located. In the mid-to late 80s, Berger and Oliger [30] and Berger and Colella [28] proposed a space-time adaptive mesh refinement (AMR) strategy for nonlinear hyperbolic conservation laws. Based on a hierarchy of rectangular finite-difference grids, it was later extended to hyperbolic equations not necessarily in conservation form by using wave propagation algorithms [29]. Higher accuracy was achieved more recently by combining the AMR approach with weighted essentially non-oscillatory (WENO) reconstruction techniques [14, 75].

In [83], Flaherty *et al.* proposed probably the first local time-stepping (LTS) strategy for a DG-FEM, where each element selects its time-step according to the local CFL stability

condition. By using the Cauchy-Kovalevskaya procedure within each element, arbitrary high-order (ADER) DG schemes achieve high-order accuracy both in space and time [118] and also permit each element to use its optimal time-step determined by the local stability condition. They were also successfully applied to electromagnetic [159] and elastic wave propagation [74]. In the absence of forcing and dissipation, the classical wave equation conserves the total energy. When a symmetric spatial FD or FE discretization is combined with a centered time-marching scheme, such as the standard leap-frog (LF) (also known as Newmark or Störmer-Verlet) method, the resulting fully discrete formulation will also conserve (a discrete version of) the energy. Highly efficient in practice, centered time discretizations also display remarkably high accuracy over long times and remain even nowadays probably the most popular methods for the time integration of wave equations. In particular, in [22, 55, 56, 105], the authors proposed energy conserving local-time stepping methods. Their approach, which is based on the introduction of a Lagrange multiplier, conserves a discrete energy. However, it requires the solution of a linear system on the interface between the coarse and the fine meshes. By combining a symplectic integrator with a DG discretization of Maxwell's equations, [131] proposed an explicit local time-stepping scheme, which also conserves a discrete energy. All of these methods are second-order accurate in time and the extension to higher order schemes is not obvious. Alternatively, domain decomposition methods permit the use of different numerical methods or time steps in separate subdomains [84, 99].

3.1 Higher order local time stepping for the wave equation

In [A15], given page 204 of the Appendix and available online at

<https://hal.inria.fr/inria-00409233>,

I have proposed, in collaboration with Marcus Grote, a local time-stepping method for second-order wave equations of arbitrarily high order of accuracy. The method is fully explicit and requires no additional storage. With a symmetric finite element discretization in space and a (block-)diagonal mass matrix, the resulting fully discrete scheme is not only explicit and, thus, inherently parallel but also conserves (a discrete version of) the energy. We have also shown via numerical experiments how a small overlap between the fine and the coarse regions achieves an optimal CFL condition.

In [A10], given page 235 of the Appendix and available online at

<https://hal.archives-ouvertes.fr/hal-00627603>,

I have proposed, in collaboration with Caroline Baldassari, H el ene Barucq and Henri Cailandra, an hp-version of the method, where not only the time-step but also the order of approximation is adapted within different regions of the mesh. This method has been later applied to a realistic geological model [122].

Finally, in [A1], given page 248 of the appendix and available online at

<https://hal.inria.fr/hal-01184090>,

I have proposed with Marcus Grote a Multi-Level Local Time-Stepping (MLTS) method. When a region of local refinement contains itself sub-regions of further refinement, those

3.2 Local time stepping for fluid structure coupling

“very fine” elements yet again will dictate the time-step, albeit local, to the entire “fine” region. Then, it becomes more efficient to let the time-marching strategy mimic the multilevel hierarchy of the mesh organized into tiers of “coarse”, “fine”, “very fine”, etc. elements by introducing a corresponding hierarchy into the time-stepping method. Hence, the resulting MLTS method will advance in time by using within each tier of equally sized elements the corresponding optimal time-step. In this paper, we present a numerical experiment where the small time step is up to 150 times smaller than the coarse time step.

It is worth noting that the methods I have proposed can also be applied to finite difference methods, to the spectral element method or to any other discontinuous Galerkin formulation. It is a major difference as compared to the ADER method.

3.2 Local time stepping for fluid structure coupling

A key issue in the numerical modeling of fluid-solid models in the time domain is that it is often desirable to resort to time substepping because the stability condition in the solid part of the medium can be more stringent than in the fluid. This comes from the combination of two reasons :

- in many cases of practical interest, for instance in the oil industry, the value of the shear wave velocity at the ocean bottom on the solid side is similar to the value of the pressure wave velocity on the fluid side (in the ocean) and thus a spatially conforming mesh is needed to keep a similar mesh resolution,
- but the maximum pressure wave speed, which governs the stability condition of explicit time schemes, is often much higher in the solid than in the fluid, which is often water ; the ratio can typically be between 2 and 5.

Therefore, being able to use a significantly larger time step on the fluid side is useful in order to save computational time. Several schemes or approximations are available in the literature to do that, for instance [41] and references therein, or [147] in the context of finite difference-finite element coupling. At an interface across which the time step changes, energy conservation should be ensured along the interface, otherwise instabilities and/or inaccuracies can arise. But this is often not done in the available literature and approximate techniques that do not enforce the conservation of energy are used instead. For instance Tessmer [161] does not explicitly enforce energy conservation and observes that small spurious reflected and refracted waves arise in his snapshots of wave propagation. In the case of fluid-solid coupling, one should therefore enforce the conservation of energy along the fluid-solid interface in the time-marching algorithm in order to ensure the accuracy and the stability of the time scheme. Some classical time integration schemes ensure the conservation of energy inside a given domain, see e.g. [146, 158, 51, 106, 55, 56, 98, 126, 42]. But when coupling two different domains in a non conforming way (in time or in space) one must in addition enforce the conservation of total energy along the interface explicitly.

In [A16], given page 274 of the Appendix and available online at

<https://hal.inria.fr/inria-00436429>,

I have introduced in collaboration with Ronan Madec and Dimitri Komatitsch, such an energy-conserving local time stepping method, which is both accurate and numerically stable. To implement it we need to solve a linear system along the fluid-solid interface. We validated it based on numerical experiments performed using a spectral-element method and checked

that energy conservation along the fluid-solid interface is ensured from a numerical point of view.

3.3 Explicit high-order time schemes.

In conjunction with my works on DG method, I have developed new explicit high order time schemes, in order to make the best use of the high order space discretization, by considering an alternative approach to the ADER schemes. Instead of using auxiliary variables, I have proposed, in collaboration with Cyril Agut, to directly discretize the high-order space operators that appear after the Taylor expansion in time of the wave equation. This discretization is easily achieved thanks to DG methods. We have applied this method to the second order wave equation in [A8], which is given page 301 of the Appendix and available online at

<https://hal.inria.fr/hal-00646421>.

The numerical results showed that this technique induced less computational burden than the modified equation scheme or the ADER scheme. These results are part of the PhD thesis of Cyril Agut [2]. Then, in collaboration with H el ene Barucq, Henri Calandra and Florent Ventimiglia, we have extended this strategy to the first order formulation of the wave equation, which is the formulation used in the DIVA platform of TOTAL. In [B2], given at page 319 of the Appendix and available online at

<https://hal.inria.fr/hal-01111071>,

we have adapted the DG formulation with centered fluxes proposed in [68] to higher order operators. Numerical results showed once again that this method requires less computational costs and less storage than the High-Order ADER Scheme. These results are part of Florent Ventimiglia PhD thesis [169].

Chapter 4

Computation of Analytical Solution

Even if the geophysical problems I am considering are too complicated to be solved analytically, the computation of analytical solutions for wave propagation problems is of high importance for the validation of the numerical computational codes. It also provides a better understanding of the reflection/transmission properties of the media. Cagniard-de Hoop method [40, 66] is a useful tool to obtain such solutions and permits to compute each type of waves (P wave, S wave, head wave...) independently. Although it was originally dedicated to the solution of elastodynamic wave propagation, it can be applied to any transient wave propagation problem in stratified media.

I started to develop a software based on the Cagniard-de Hoop method during a visit of Cristina Morency in the team Magique 3D. In collaboration with Jeroen Tromp, they were implementing a code for poroelastic wave propagation and wished to validate in the case of bilayered poroelastic media and in the case of poroelastic/acoustic coupling. Together with Abdelaaziz Ezziani, we developed a first version in 2D and then in 3D, and we parallelized it with the help of Nicolas Le Goff who was engineer in the team. The results produced by the code have been used by Morency and Tromp to benchmark their software [124].

The computation of the analytical solution in 2D is detailed in [A13], given at page 328 of the Appendix and available online at

<https://hal.inria.fr/inria-00404224>,

while the 3D results are given in [A14], given at page 352 of the Appendix and available online at

<https://hal.inria.fr/inria-00404228>.

Later, I extended the code to Elastodynamics, and to Acoustics, which give rise to Gar6more2D and Gar6more3D that I describe with more details in the next chapter. It has been used by R. Sidler, K. Holliger (University of Lausanne) and J. Carcione (OGS Trieste) [144, 145] to validate their codes of poroelastic wave propagation. We have also been contacted by Stefan Wenk, from the University of Munich, in order to validate his elasto-acoustic code. Gar6more is routinely used in the team in order to validate our numerical codes.

I now intend to develop an equivalent of Gar6more in harmonic domain.

Chapter 5

Software

In this Chapter, I detail the software packages I contributed to develop. Two of them (TMBM and Elasticus) are specifically devoted to transient problems, one (THBM) is specifically devoted to harmonic problems, one (Hou10ni) is adapted both to transient and harmonic problems and one (Gar6more) is designed to compute analytical solutions.

5.1 Hou10ni

This software, written in FORTRAN 90, simulates wave propagation in 2D and 3D heterogeneous media in time domain and in frequency domain. It is based on the Interior Penalty Discontinuous Galerkin Method (IPDGM). It is able to deal with both acoustic and elastodynamic media, but also to model elastoacoustic problems. In 2D, the surfaces between the different media can be approximated by curved elements. Elements up to P^{15} order are available for curved elements while there is no limitation (except the one related to machine precision) of order when dealing with non-curved elements. It has been parallelized using hybrid MPI/OpenMP parallelism. This code has been also implemented in an inversion solver which determines the shape of an elastic obstacle from the knowledge of its scattered field.

The 2D Frequency Domain version has been registered in 2013 at APP (Agency for the Protection of Programs). I do not plan to distribute it widely, but I wish to use it to build collaboration with research teams in geophysics. I have recently started discussions with IsTerre in Grenoble on that topic.

I am the main developer of Hou10ni, which has been used and extended by various students of the team. It has been used for the performance comparisons between IPDGM and SEM by Caroline Baldassari [A7]. Cyril Agut analyzed the impact of the penalization parameter on the performances of IPDGM [A4], and then developed high order time schemes [A8]. Véronique Duprat developed and tested Absorbing Boundary Conditions on arbitrarily-shaped boundary [A9, A5].

The 2D elasto-acoustic version has been implemented by Élodie Éstécahandy [17] and employed in an inverse problem solver for shape reconstruction of obstacles [77]. More recently, Conrad Hillairet implemented the 3D elasto-acoustic coupling in the framework of his Master Internship.

The code has been validated in time-domain thanks to the software Gar6more (see below). In harmonic domain, Hou10ni generates its own analytical solutions which can be plane waves or solution of problems of diffraction by a circle. In this latter configuration, the analytical

solutions are computed using Bessel series.

5.2 DIVA/TMBM

The platform DIVA, now renamed as TMBM (Time Marching Based Methods) is a seismic imaging software in time-domain developed by Total. It is a research platform available for Inria team projects and Magique-3D contributes mainly to the implementation of Discontinuous Galerkin Methods. The first version of this software relied on Finite Differences for solving the direct problems and we have implemented a new version based on a Discontinuous Galerkin Method. The DGM version, based on the DG centered fluxes formulation [68] can solve acoustic, isotropic elastic, and TTI elastic wave propagation problems in 2D or in 3D. Several PhD and post-doc students and one engineer of Magique 3D are involved in the development of TMBM. We validated the code with analytic solutions provided by Gar6more. The code is optimized in a High Performance Computing framework, principally by using MPI. I do not program directly into the platform, but I supervise with H el ene Barucq the integration of the student works. Many students contributed to the development of the platform : Caroline Baldassari, Florent Ventimiglia, Lionel Boillot et J er ome Luquel.

5.3 Elasticus

This software is mainly developed by Simon Ettouati and Lionel Boillot under my supervision. It aims at facilitating the integration of the student works into THBM. The objective is to develop a code less optimized than THBM, but more readable, in order to test more rapidly each of the new features we propose.

5.4 THBM

This platform, called Time Harmonic Based Methods is the equivalent of TMBM in harmonic domains. Its development is more recent than TMBM and I principally supervise the integration of the works of Marie Bonnasse Gahot on Hybrid Discontinuous Galerkin Methods.

5.5 Gar6more

This software package compute the analytical solution of problems of waves propagation in two layered 2D or 3D media, based on the Cagniard-de Hoop method. In the homogeneous case, the medium can be acoustic, elastic or poroelastic ; infinite or semi-infinite with a free boundary or a wall boundary condition at its end. In the bilayered case, the following coupling are implemented (the source is assumed to be in the first medium) :

- acoustic/acoustic ;
- acoustic/elastic ;
- elastic/acoustic ;
- acoustic/poroelastic ;
- poroelastic/poroelastic,

The code is freely distributed under a CECILL license and can be downloaded online :

<http://web.univ-pau.fr/~jdiaz1/gar62DCecill.html>

for the 2D version and

<http://web.univ-pau.fr/~jdiaz1/gar63DCecill.html>

for the 3D version.

The targeted users are researchers who need reference solutions in order to validate and/or benchmark numerical codes simulating wave propagation.

Gar6more has been already used by J. Tromp and C. Morency (Princeton) [124] and by R. Sidler, K. Holliger (University of Lausanne) and J. Carcione (OGS Trieste) [144, 145] to validate their codes of poroelastic wave propagation. I have also been contacted by Stefan Wenk, from the University of Munich, in order to validate his elastoacoustic code. Gar6more is routinely used in the team in order to validate our numerical codes. As far as I know, the main competitor of this code is EX2DELDEL (available on <http://www.spice-rtn.org>), but this code only deals with 2D acoustic or elastic media. Gar6more seem to be the only one able to deal with bilayered poroelastic media and to handle three dimensional cases.

Chapter 6

Perspectives

To conclude this dissertation, I present the research directions I want to pursue during the next four years. In particular, I wish to consider innovative solution methodologies for solving Helmholtz equations; to couple regular grids with irregular grids; to go deeper in the performance analysis of Discontinuous Galerkin methods for geophysical simulations; and to consider hybrid time discretizations by coupling implicit and explicit schemes.

6.1 Advanced numerical techniques for solving the Helmholtz equations

In the framework of DIP, I am more and more involved in the solution of Helmholtz equation. In particular, I co-advised with Stéphane Lanteri (Inria team project Nachos) the Ph.D. thesis of Marie Bonnasse-Gahot, who derived a new class of Discontinuous Galerkin Method, the Hybridizable Discontinuous Galerkin method, for the harmonic elastic wave equation. This technique provides a two-step procedure for solving the Helmholtz equations [109, 117, 125]. 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 solutions 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 that 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. The results that Marie obtained emphasized the efficiency of the technique and we want to apply it now to the simulation of complex phenomena such as the 3D viscoelastic wave propagation.

I also want to pursue my collaboration with Rabia Djellouli, both on the selection of the basis functions for local plane-wave approximations and on the Mesh Free Frontier-based Formulation. 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 both methods will be particularly the extension to 3D because the results we have achieved so far are for 2D problems. This is up-front investigation and there is a lot of remaining work before being applied to geophysical imaging. It will give me the opportunity of testing new ideas while remaining in contact with potential users of the methods.

Keeping in mind the idea of limiting the difficulties of mesh, we want to study the method of

virtual elements. This method attracts me 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 [24, 39, 61, 60, 38, 25]. None of them mentions the feasibility of the method for industrial applications and to my knowledge, there are no results on the method of virtual elements applied to the elastodynamic wave equations. First, I aim at applying the method described in [130] to the elastodynamic Helmholtz equation and to 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.

6.2 Coupling regular and irregular grids

The geophysical subsurface is so heterogeneous that we cannot envisage to create a mesh following all the interfaces, especially if we want to update the mesh at each iteration of an inverse problem. Therefore, it might be more efficient to use an unstructured mesh to model only the topography, that we know prior to the experiment, and to use a structured cartesian mesh for the bottom of the subsurface. We did a first attempt in [B4] by coupling a finite difference scheme (for the bottom) to a Discontinuous Galerkin scheme (for the top). The major limitation of the method was the fact that we had to use P^0 in order to ensure the coupling between the two meshes. This reduces drastically the accuracy of the computation. I now wish to use Discontinuous Galerkin Method both for the structured and the unstructured grids. By doing so, the transmission condition between the two grids will be taken into account naturally, and we will keep the possibility to use hp -adaptivity on the regular grid, and possibly to consider physical velocities that varies inside the mesh. Finally, we will take advantages of the structural grids by using all the algorithms that have been implemented to optimize Finite Differences.

This topic could bring benefit both to solutions of time-domain and of harmonic-domain problems.

6.3 Performance analysis of discontinuous Galerkin methods for geophysical simulations

There exists a large variety of Discontinuous Galerkin Methods, the main differences being the type of numerical fluxes that are used at the interface between two cells. There also exists a large variety of time schemes to discretize transient problems. It is therefore necessary to compare the different methods in a geophysical context. For instance, the ability to accurately handle point source is of high importance in seismic imaging, and this point is rarely discuss in mathematical papers, the authors focusing mainly on the generation of very regular solutions. I already performed comparisons between IPDGM and SEM in [A10] and comparisons between IPDGM, and DG with centered fluxes in the framework of the Ph.D. thesis of Florent Ventimiglia [169]. I now intend to compare DG with centered fluxes with DG with upwind fluxes and to compare the efficiency of various time schemes (mainly Leap-Frog and Runge-Kutta formulation).

6.4 Higher-order hybrid time discretizations

Despite a very good performance assessment in academic configurations, I have observed to my detriment that the implementation of local-time stepping algorithm 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 [90].

Recently, Dolean *et al* [71] 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 first task should be 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 viscoelastic media. The second task would be 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. Two strategies could be considered for the coupling. The first one is based on the method proposed by Dolean *et al*, the second one consists 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, I will have to implement the method in industrial codes and the discretization methodology should be very suitable for parallel computing since it involves Lagrange multipliers. I 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 my experience on local time stepping, I claim that it is necessary to define a criterion which discriminates thin cells from coarse ones. Indeed, I 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 I am not expert in parallel computing.

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