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2023

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Exploration of the Solid Earth across Short and Long Spatial and Temporal Scales.

by

Sevan Adourian

A dissertation submitted in partial satisfaction of the

requirements for the degree of

Doctor of Philosophy

in

Earth and Planetary Science

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Barbara Romanowicz, Chair

Professor Michael Manga

Professor Per-Olof Persson

Summer 2023

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Abstract

Exploration of the Solid Earth across Short and Long Spatial and Temporal Scales.

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Sevan Adourian

Doctor of Philosophy in Earth and Planetary Science

University of California, Berkeley

Professor Barbara Romanowicz, Chair

This dissertation delves into the dynamics of Earth’s interior across varying spatial and temporal scales, using innovative techniques to advance our understanding of the intricate processes that govern our planet’s evolution and structural behavior. It integrates diverse methodologies and datasets within the realm of geophysics, at the intersection of seismology, geodesy, and geodynamics. Following a concise introduction, the subsequent two chapters focus on enhancing computational methods for Earth imaging through seismic tomography. Their objective is to bridge global and regional scales via ”box tomography”, which optimizes computation efficiency for the imaging of target regions in the context of Full-Waveform Inversion. Furthermore, a versatile merging package is introduced, designed to combine multi-scale, multi-resolution georeferenced datasets, which facilitates high-resolution simulations while preserving the global contextual integrity. The exploration of rotational dynamics follows, investigating low-frequency length-of-day oscillations on a pluriannual timescale. These oscillations offer potential insights into the buoyancy structure of the lower mantle. The final chapter expands seismic studies to impact-induced seismic waves, probing potential links between asteroid collisions and volcanic eruptions, notably during the Cretaceous–Paleogene mass extinction. Through systematic sensitivity analyses, computational efforts, and geophysics-based constraints, the dissertation yields insights into Earth’s intricate processes, with implications spanning the fields of seismology and geodynamics.

Résumé en français:

Cette thèse explore la dynamique de l'intérieur de la Terre à différentes échelles spatiales et temporelles, en utilisant des techniques innovantes pour faire progresser notre compréhension des processus complexes qui régissent l'évolution et la structure de notre planète. Nous y intégrons diverses méthodologies et ensembles de données issus de la géophysique, au croisement entre sismologie, géodésie et géodynamique. Après une introduction concise, les deux chapitres suivants se concentrent sur l'amélioration des méthodes de modélisation numérique de propagation des ondes destinées à l'imagerie de la Terre par tomographie sismique. L'objectif est d'améliorer la résolution des modèles de tomographie régionale, tout en utilisant l'information contenue dans les modèles développés à l'échelle globale. En outre, nous proposons une suite de codes, conçue pour combiner des ensembles de données référencées sur la sphère terrestre à différentes échelles spatiales, facilitant les simulations à haute résolution tout en préservant l'intégrité contextuelle à échelle globale. Nous explorons ensuite les oscillations à basse fréquence de la longueur du jour sur une échelle de temps pluriannuelle. Ces oscillations offrent un aperçu potentiel de la structure de densité du manteau inférieur distinct de celui obtenu par imagerie sismique. Enfin, le dernier chapitre étend les études de modélisation de propagation d'onde au contexte où celles-ci sont induites par les impacts majeurs d'astéroïde, en sondant les liens potentiels entre ces collisions et les éruptions volcaniques, en prenant notamment le cas précis de l'extinction de masse ayant eu lieu à la limite du Crétacé et du Paléogène. Grâce à des analyses de sensibilité systématiques, et à des contraintes basées sur la géophysique étayées par la modélisation numérique, cette thèse apporte un aperçu des processus complexes liés à l'évolution de la Terre, avec des implications couvrant les domaines de la sismologie et de la géodynamique.

À Medz Hayrig, Medz Mayrig, et Sofia, pour qui j'ai une pensée chaque jour,
À mes parents et mes sœurs,
À Sacha et Azad.

The capital of knowledge that an individual scholar has to offer is small. Admission of one's shortcomings saves from censure. Kindness from colleagues is hoped for. It is God whom I ask to make our deeds acceptable in His sight. He is a good Protector.

— Ibn Khaldun

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Acknowledgments

As I am leaving California, it is time to write the words that, perhaps, will be the only ones to be read from this work. Time also to close off and reflect on the many years of my life spent on this side of the world. The journey was rich and insightful, and no matter the hardships, I would never trade this defining experience for a more tranquil one, as I am sure it will greatly shape and influence my adult life. Although the Ph.D. experience tends to be a rather solitary adventure, it would have never been possible to reach its end without the many people I have interacted with and benefited from during these long years.

First, I owe to Barbara Romanowicz, my advisor, from whom I learned precious lessons both on a personal and professional, scientific level. I will attempt to keep following the direction you helped me shape and for which you provided me with useful tools and ways of thinking. I would like to thank Michael Manga for his patience and availability with me. His Socratic guidance, which is only possible thanks to his profound understanding of the broadest topics in Earth Sciences and beyond, showed me what a scientific discussion could look like, where ideas are at the center of everything. Finally, I am sincerely grateful to Harriet Lau, without whom I would simply have never completed my Ph.D. Your support, may it be scientific or emotional, is only topped by your deep expertise and knowledge of our field, one which I can only dream to achieve in the future. Your research group has been a great source of comfort during my time at Berkeley.

I learned a tremendous amount from discussions with Yder Masson, and this work would not be the same without him. Same goes for Federico and Dan, whose help has been greatly appreciated. I will not forget it.

Working in McCone Hall was such a fun experience, especially before the Covid years, and it is only the presence of fellow grad students and postdocs to share discussions, scientific or not, that made battling the cold of Office 225 bearable and worth it. Alex, Tushar, Jesse, Manar, Dani, Sarina, Zach, Jiwoon, Claire, Daria, Will, Andrew, Chase, Andy, Chelsea, William H., Nate, Jizhou, and so many others, I have learned from you more than you can imagine.

How to describe all these years without mentioning Chris, Philipp, and Mihai? Had I ever had brothers, I am sure it would have looked like our friendship. I cannot thank you enough for everything you provided, both individually and as the group of four we are forming. Quentin, I feel so happy that you are now representing the French in our department. Your impressive knowledge associated with your kindness and humility truly make you an example for me. Anna, not many people know that you literally saved my life on Mono Lake that day, but I do, and I am forever thankful that you did. French Ben, thank you for playing piano with me, and teaching me that groups of friends last two years in the transient Bay Area. You were right.

Because the Bay Area has a strong French and francophone accent, I cannot fail to mention the "French community", among whom I made friends that I hope to keep beyond our American peregrinations. *Pêle-mêle*, and in no particular order, Valentine, Thomas, Bérénice, Ronan, Heather, Hector, Ahmed, Albert, Olivier, Geoff, Adrien, Solène, Éloïse,

Nico, Adèle, Édouard, Mike, Erin, and all the others who gravitated around this bubble, *merci, mille fois merci* for making this foreign place a bit closer to home. Our cooking nights, games, and other activities were invaluable sources of comfort and joy.

I also think about my geofriends Gaspard and Luc. Even spread across the world, we still managed to finish our Ph.D almost at the same time. One day we will write this paper together. Trust the process. Guillaume D., Martin F., Thomas D. we have not seen each other physically in so many years, but our regular calls during my evenings and your lunches are the perfect example that distance does not alter true friendship. All of you, alongside all the friends in France, from undergrad and the few left from high school: thank you, and we will see each other soon.

I would also like to thank two special persons, who shaped the man I am to an extent they probably do not even realize: Jules Lechanga, and Serguei Markarov. I would not be the same for if you had not taken the time to teach me your passion and your vision of life. Amongst many things, you taught me that rigor and work, when exerted towards achieving an inspiring goal, bring the best out of me, be it in music, sports, or simply in life. You did that in depths and ways that I can still barely comprehend to this day, and you are true role models. I can only hope to transmit these life lessons and that someone else will find them as useful as I did.

This work is dedicated to my family, without whom nothing would be possible. I am nothing without the sacrifice of my parents, their constant support, and the absolute patience of my sisters growing up. Yes, sisters, you taught me how to read, I can admit it now. Medz Hayrig, Medz Mayrig, I still cannot believe you are gone, even after all these years. However, I want to believe you would be proud of me today. I carry your memory and your history as a humbling responsibility, the duty to transmit your heritage with pride. Nothing is ever in vain.

Ivana, meeting you made coming to the Bay Area worth it, and I owe you so much. You do not like to be put on the spot, so I will not say anything more here, but you know all of it. Thank you for being in my life, simply.

Finally, I would like to thank all those who prayed for me, or simply hoped for me. This truly selfless act served as a guiding light when my mind was covered by a numbing fog, the same one that is so characteristic of the Bay Area.

It has been a privilege to be an external observer of this part of the Western world, whose core values vacillate and seem to be tested day after day. Although the journey did not make me particularly hopeful, it participated in redefining my values and priorities, which are worth striving towards and protecting.

For if God is with us, who will be against us? Romans 8:31

Chapter 1

Introduction

The dynamics of the Earth’s mantle drive many of the processes that we observe and experience at Earth’s surface today and over Earth’s 4.5 billion-year history. While the mantle is the single largest constituent of the Earth system, it is comprised of heterogeneity that spans a large range in spatial wavelengths: creep processes that allow the mantle to “flow” are dictated by structural imperfections (or defects and dislocations) at the grain-scale, while features such as plumes and their associated plume heads may span thousands of kilometers. Similarly, while mantle convection operates at timescales that dictate the motion of continents over hundreds of millions of years, it is subject to forces such as earthquakes, which – relative to Earth’s long existence – are near-instantaneous. Accordingly, in order to understand mantle dynamics, and thus the forces that trigger earthquakes, build mountains, produce volcanism, and, as a consequence, set environmental conditions at Earth’s surface, investigations of Earth at all these scales must be met. In this thesis, we take a selection of directions to explore aspects of our multi-scale mantle, developing methods by which to investigate key properties that, by virtue of the underlying physics, must be constrained by the analysis of processes that operate at vastly different spatial and temporal scales. To the end, we present our work in the following order.

In Chapter 2, we begin at the high frequency and short spatial scale end-member of our exploration – namely the seismic band and seismic body waves – where we build on a method that enables the determination of mantle structure, or more specifically, the mantle’s elastic properties, at high resolution. To do so requires vast amounts of computational power, and our goal here is to develop a means to reduce this requirement by *mixing* the spatial scales under consideration. The approach, known as *box tomography*, was introduced in its earliest stage in 2014 [Masson et al., 2014] and seeks to self-consistently calculate wave propagation within a mantle with two designated regions: the region of interest, bounded by a “box” in which resolution is enhanced, and the rest of the mantle domain, where resolution can be reduced. Box tomography has been incrementally developed to test stages within idealized geometries (2D and spherically symmetric 3D mantle models). Here, we take this a stage further and consider a fully 3D mantle and refine aspects of the source-receiver calculations.

In Chapter 3 we continue this theme of scale mixing by introducing a tool that allows the

consistent merging of different fields of interior structure that are constrained in different locations within the mantle and defined at different resolutions. These may come in the form of highly resolved regional models, or smooth global models, whether constrained by data or modeled by geodynamical simulation. And so, patching together several models of Earth’s interior is commonplace in Earth science research and yet presents many difficulties. Regional models have boundaries that when inserted into a global model will result in both a discontinuity within the mantle (imposed by the boundary itself) and artifacts since different resolutions are being mixed. We present a method that, by considering the spectral content of the different models, naturally merges the fields together. This type of methodology need not be limited to seismic tomography models of wave speed variation and in light of this generality, our discussion moves to the opposite end of the spatio-temporal scale.

Chapter 4 is concerned with mantle buoyancy. While seismic body waves are sensitive primarily to Earth’s elastic properties, to constrain buoyancy requires moving to lower frequency processes, and the processes concerned operate at the longest wavelengths within the mantle. Buoyancy within the mantle is a key parameter in governing the dynamics of mantle flow but remains difficult to determine. In this chapter, we explore an observation that operates over years, namely the *six-year oscillation* (SYO) in length-of-day. These subtle variations are in the millisecond range and have been revealed with increasingly precise geodetic measurements made over many decades. Several mechanisms have been proposed to drive the oscillation and we explore one which has explicit dependence on the long wavelength buoyancy structure of the deep mantle. Deep mantle buoyancy structure produces a gravitational force that is imposed on the inner core, deforming its shape as it adjusts to this field. Differential rotation of the mantle and the aspherical inner core produces variations in Earth’s length-of-day. To better elucidate the potential of the SYO as a constraint on mantle buoyancy structure, we explore the sensitivity of this observation to buoyancy within the mantle. We find that the depth distribution of buoyancy sensitivity of the period of the SYO lends itself to potentially providing a new and independent constraint for testing various hypotheses in the current debate in the mantle dynamics community.

Finally, in Chapter 5 we move from constraining properties of the mantle at various wavelengths to applying our knowledge of mantle properties to investigate one facet of the K-Pg mass extinction, an event that ~ 66 million years ago. Two near-synchronous processes have been proposed as causes for this mass extinction: the $\sim M_w 10.5$ impact left behind the Chicxulub crater and the copious eruptions that produced the antipodal Deccan Traps. We explore whether the propagation of seismic waves, triggered by the impact, could generate sufficient dynamic stress upon arrival to the magmatic system underlying the Deccan Traps. As the seismic waves propagate through the mantle, we will use up-to-date seismic tomography models, and investigate the energy deposited within and beneath the Deccan region. Are such stresses sufficient to trigger volcanism? With this investigation, we explore how these short timescale processes of an impact and the subsequent waves potentially are connected to the long-lived eruptions that produced the Deccan Large Igneous Province.

We close with reflections on the collective work that is presented in this dissertation and what future directions may be taken to further these efforts to understanding the minute

and vast time and spatial scales govern important processes that operate on this planet.

Chapter 2

Combining different 3D global and regional seismic wave propagation solvers towards box tomography in the deep Earth

This chapter was published as a journal article in *Geophysical Journal International* in October 2022 under the title *Combining different 3D global and regional seismic wave propagation solvers towards box tomography in the deep Earth*, with co-authors Chao Lyu, Yder Masson, Federico Munch, and Barbara Romanowicz, issued in volume 232.2, pages 1340-1356 [Adourian et al., 2023].

In previous publications, we presented a general framework, which we called "box tomography", that allows the coupling of any two different numerical seismic wave propagation solvers, respectively outside and inside a target region, or "box". The goal of such hybrid wavefield computations is to reduce the cost of computations in the context of full-waveform inversion for structure within the target region, when sources and/or receivers are located at large distances from the box. So far, we had demonstrated this approach with sources and receivers outside the target region in a 2D acoustic spherical earth model, and demonstrated and applied this methodology in the 3D spherical elastic earth in a continental scale inversion in which all stations were inside the target region. Here we extend the implementation of the approach to the case of a 3D global elastic earth model in the case where both sources and stations are outside the box. We couple a global 3D solver, SPEC-FEM3D_GLOBE, for the computation of the wavefield and Green's functions in a reference 3D model, with a regional 3D solver, RegSEM, for the computation of the wavefield within the box, by means of time-reversal mirrors. We briefly review key theoretical aspects, showing in particular how only the displacement is needed to be stored at the boundary of the box, and details of the practical implementation, including the geometrical design of the mirrors, how we deal with different sizes of meshes in the two solvers, and how we address memory-saving through the

use of B-spline compression of the recorded wavefield on the mirror. The proposed approach is numerically efficient but also versatile, since adapting it to other solvers is straightforward and does not require any changes in the solver codes themselves. We present benchmarks of the hybrid computations against direct computations of the wavefield between a source and an array of stations in a realistic geometry centered in the Yellowstone region, with and without a hypothetical plume within the "box", and with a 1D or a 3D background model, down to a period of 20 seconds. The ultimate goal of this development is for applications in the context of imaging of remote target regions in the deep mantle, such as, for example, Ultra Low Velocity Zones.

2.1 Introduction

Full-waveform inversion (FWI) is a promising tool for improving resolution in seismic imaging of the deep earth, as it allows to exploit constraints from waves scattered from both major discontinuities and small scale structures. It is a non-linear problem in which forming the misfit function requires the computation of the seismic wavefield in a 3D earth model. Early FWI global shear-wave velocity models relied on approximate wavefield computations based on normal mode perturbation theory, the validity of which was restricted to weak and long wavelength heterogeneity [e.g., Woodhouse and Dziewonski, 1984, Li and Romanowicz, 1996, Mégnin and Romanowicz, 2000, Panning and Romanowicz, 2006]. Two decades ago, the introduction of the Spectral Element Method (SEM) to earthquake seismology at regional and global scales [Komatitsch and Vilotte, 1998, Komatitsch and Tromp, 2002] opened up new opportunities for accurate computations with few limitations on the strength and size of the heterogeneities in the model, at the expense of computational cost. This resulted in the construction of a new generation of 3D elastic models at the local [e.g., Tape et al., 2007], regional [e.g., Fichtner et al., 2010, Zhu et al., 2015] and global scale [e.g., Lekić and Romanowicz, 2011, French and Romanowicz, 2015, Bozdag et al., 2016, Fichtner et al., 2018, Lei et al., 2020].

Reducing the computational cost of seismic waveform modelling is a major challenge towards further improving resolution in FWI imaging of the deep Earth, particularly when targeting regions of small lateral extent such as Ultra Low Velocity Zones (ULVZ) and the roots of mantle plumes. Importantly, the computational cost for SEM increases approximately as the fourth power of the maximum frequency, limiting the frequency range that can be achieved at reasonable cost, particularly so in the context of global scale, deep earth imaging, with impact on model resolution. In particular, first generation global whole mantle SEM-based FWI models limited their frequency range to periods longer than ~ 30 seconds [French and Romanowicz, 2014, Bozdag et al., 2016]. Recently, Lei et al. [2020] extended the period range for the body wave part of their analysis down to 17s, with considerable development effort and necessitating access to very high performance computing facilities.

To make such computations more affordable, several approaches have been proposed and implemented at the global scale. Capdeville et al. [2003] coupled a 3D SEM solver in the mantle with a normal mode-based solution for the outer and inner core. By taking advantage of the fast 1D mode simulations in the core, the bulk of the intensive computing was reduced to the mantle only. This method was used in the development of models SEMum [Lekić and Romanowicz, 2011], SEMum2 [French et al., 2013] and SEMUCB-WM1 [French and Romanowicz, 2014]. This was later extended to the case of a spherical shell with 3D structure "sandwiched" between two 1D normal mode computations above and below the shell [Capdeville et al., 2003], and applied in forward modeling of Ultra Low Velocity Zones using diffracted S waves (Sdiff) down to 8s period [Cottaar and Romanowicz, 2012, He et al., 2015, Yuan and Romanowicz, 2017].

Meanwhile, Nissen-Meyer et al. [2007] developed a SEM-based solver for seismic wavefield computations in a sphere with axisymmetric structure, allowing the computational domain to be reduced to a 2D disk, enabling teleseismic computations at manageable cost down to 1s period [Nissen-Meyer et al., 2014], and opening the possibility for probabilistic source inversion or cheap and accurate finite frequency tomography [van Driel et al., 2015]. Indeed, Hosseini and Sigloch [2015] imaged the lower mantle using finite frequency travel times of core and diffracted phases, for which the synthetic waveforms were modeled using AxiSEM. Recently, the assumption of axisymmetry was relaxed, introducing asymptotic computations in the direction perpendicular to the great circle plane containing the source and the receiver. Although allowing for a 3D velocity model, it remains that this model needs to be smooth enough in order to be described by low order Fourier coefficients in the azimuthal direction [Leng et al., 2016]. More recently, further theoretical developments allowed them to introduce localized small scale heterogeneities [Leng et al., 2019]. Other approaches are also being explored to take advantage of azimuthal sparsity and introduce adaptive meshing [van Driel et al., 2020]. These approaches make it possible to extend the numerical computation of the 3D wavefield at the global scale to higher frequencies, at the expense of accuracy in the representation of the model structure.

On the other hand, various hybrid methods have also been developed to reduce the heavy computations to a limited, target, volume within the earth, while using either a 1D fast solver or an approximate 2D or 3D solver outside of the target region. These methods were first developed for local and regional applications, in particular for geophysical exploration. The concept, originally proposed by Alterman and Karal Jr [1968], involves computing the seismic wavefield in a reference model in a large region containing all the sources and receivers, and in this process, recording it on the surface of a small "target" subvolume. Secondary sources on that surface are then computed from the recorded wavefield, and subsequent computations and model iterations proceed only within the small subvolume, leading to significant savings in computation time. Most methods to date have considered a target region containing the recording stations, and either 1D, or approximate (2D or 3D) wavefield computations outside of the target region [e.g., Bielak and Christiano, 1984, Moczo et al.,

1997, Robertsson and Chapman, 2000, Chevrot et al., 2004, Roecker et al., 2010, Monteiller et al., 2013, Tong et al., 2014]. Notably, Wen and Helmberger [1998] developed a hybrid 2D methodology, coupling generalized ray theory outside of a small region at the base of the mantle, with finite differences (FD) inside it, to forward model SKS-SPdKS with both sources and stations near the earth’s surface. They applied this approach to the study of ULVZs [e.g., Helmberger et al., 2000].

Several authors proposed hybrid methods that couple 1D solvers outside the target region and SEM inside it, the latter either in 3D (Monteiller et al. [2013], Wang et al. [2016] or in 2D (Tong et al. [2014]. In these studies, stations were located inside the target region. Masson et al. [2014] and Masson and Romanowicz [2017b] proposed a general conceptual framework allowing the coupling of any two solvers inside and outside the target region, that can be applied in any source-station configuration: sources outside and stations inside (“*SORI*”, Fig. 2.1a), sources inside and stations outside (“*SIRO*”, Fig. 2.1b), or both sources and stations outside the target region (“*SORO*”, Fig. 2.1c). This methodology was coined “Box tomography” and was demonstrated in a series of synthetic tomography experiments in a spherical 2D acoustic earth, with the target region at the core-mantle boundary [Masson and Romanowicz, 2017a]. In a recent conceptual study, Lin et al. [2019] validated this approach in a “proof of concept” experiment, using the Spectral Element Method (SEM) in the elastic, spherical 2D case, targeting a structure representing a Large Low Shear Velocity Province (LLSVP) at the base of the mantle. Recently, for the same three configurations, Lyu et al. [2022] proposed a novel hybrid simulation approach by combining physical and numerical representation theorems, and pointed out its high efficiency when a high-order spectral element method is used for the hybrid forward simulation and full waveform inversion [Lyu et al., 2020, 2021], well suited for application to the study of localized 3D structures anywhere within the Earth.

Most recently, Pienkowska et al. [2021] developed a similar methodology, allowing both sources and stations outside of the target region. In this study, a 3D model restricted to a small domain was embedded in a 1D spherically symmetric Earth model. The wavefields were precomputed in the 1D model outside the domain using AxiSEM, and a full 3D numerical solver was used inside the small domain, reaching a maximum frequency of 0.5 Hz, in a global background model and a local domain of size $30 \times 30 \times 30$ km. The authors implemented this methodology in the case where SPECFEM3D Cartesian [Tromp et al., 2008] is used inside the domain. Moreover, their approach requires the explicit computation of the traction at the boundary of the target region, alongside with the surface integrals of the traction vectors to express the mirror excitation force in terms of multiple point sources. However, it also complicates the hybrid implementation because the traction and displacement (or velocity) terms related to the two surface integrations need to be calculated and saved, and then explicitly imposed in the local computation.

Relaxing the axisymmetric constraint of AxiSEM, Leng et al. [2020] used AxiSEM-3D

to generate 3D hybrid seismograms in a global background model that has low complex azimuthal structure, without making any other simplification on the scattered wavefield. However, they used AxiSEM-3D for both the incident and the scattered wavefield, therefore not addressing the difficulties of combining meshes coming from distinct solvers, which is essential for applications that aim to take advantage of using different solvers for the global and regional computations.

Presented in Masson et al. [2014] for the elastic case, the box tomography approach of Masson and Romanowicz [2017b] relies on the implementation of time-reversal mirrors [Fink, 1992] at the boundary of the box. However, these mirrors are used only to reconstruct the wavefield inside the box through an excitation force at this mirror, and not for the more conventional application of refocusing at the source. This methodology was first applied using a 3D global SEM solver outside the target region and a regional SEM solver inside it by Clouzet et al. [2018] to develop a radially anisotropic upper mantle model beneath north-America, albeit with stations inside the target region. Here, we extend it to the case with sources and stations outside the target region ("*SORO*"), in a 3D radially anisotropic spherical earth model, and demonstrate its implementation when coupling two different 3D SEM solvers: SPECFEM3D_globe [Komatitsch and Tromp, 2002], hereafter referred to as SPECFEM3D, outside the target region, and a regional code in spherical geometry, RegSEM [Cupillard et al., 2012], inside the target region, without any assumptions on the smoothness of the 3D models.

Similar approaches have been implemented by other groups [e.g., van Manen et al., 2005, Yuan et al., 2017], but a computation of synthetic seismograms in an Earth model that is 3D both outside and inside the target region in the source outside/receiver outside ("*SORO*") case, using two distinct solvers, and no approximations on the characteristics of the 3D structure, has not yet been presented.

We first review the analytical and numerical framework of "box tomography" in section 2.2, before illustrating the practical implementation of such a methodology in section 2.3. In section 2.4, we present benchmarks performed in a 1D spherically symmetric radially anisotropic model, and in a model containing a plume-like 3D structure within a target region centered on Yellowstone, down to a minimum period of 20 seconds. We also present a benchmark in which the reference global earth model is a 3D radially anisotropic model. Finally, we discuss computational savings and future applications.

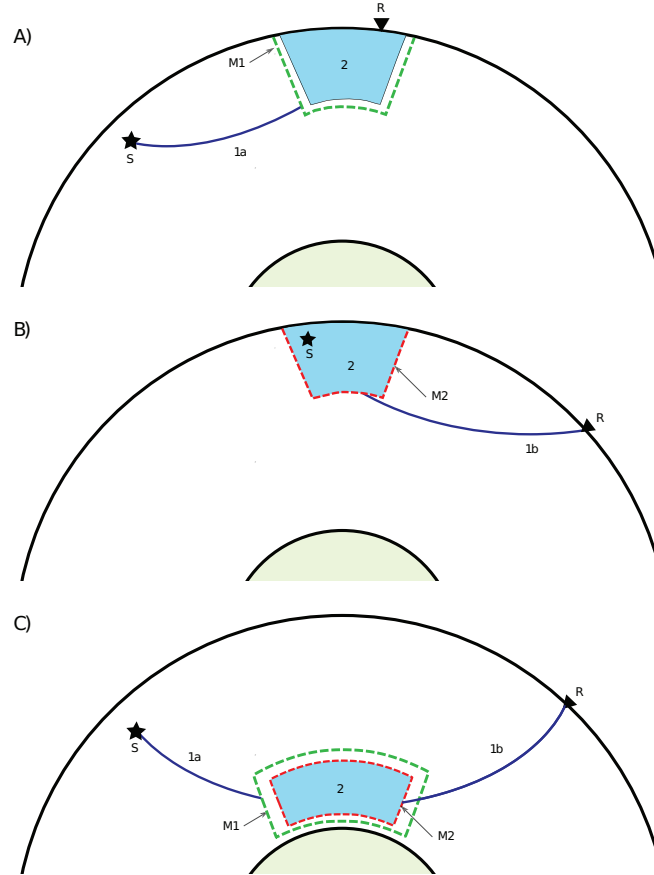


Figure 2.1: A simplified view of the Box Tomography concept, which separates the computation of a synthetic seismogram into three distinct parts (1a,2,1b). (Panel A) and (Panel B): case when the box extends to the earth's surface. (Panel C): case when the box is in the deep mantle. Outside of the target region, the wavefield computation is performed only once in the reference model using a global solver (e.g. SPECFEM3D). (1a): from an earthquake source to mirror M1; (1b): 3-component Green's functions from a distant station to mirror M2. Inside the target region (2, blue), the wavefield is computed using a regional solver that can be different from the global solver. Note that mirror M2 is inside mirror M1. Only one mirror is necessary in cases (A) and (B), when either the source or the station is inside the target region. Mirrors M1 and M2 can coincide if the domain in which the inversion is performed is smaller than the mirror.

2.2 The Box Tomography method

2.2.1 Overview

For the most general case ”*SORO*”, this method is based on breaking down the computation of the seismic wavefield into three distinct steps, as shown in Fig. 2.1c):

1. The wavefield computation from a source located anywhere in the Earth to the boundary of the target region (1a) using the global solver in the reference 3D earth model.
2. The wavefield computation inside the target region (region 2 in Fig. 2.1, hereafter referred to as “the box”) using the regional solver, initially in the starting model and in subsequent iterations of the inversion, in the perturbed model.
3. The extrapolation of the wavefield from the box to a distant receiver outside of the box (1b) using the global solver in the reference 3D earth model.

Step (i) is not required in the ”*SIRO*” case, whereas step (iii) is not necessary in the ”*SORI*” case. If the source and stations are inside the box (”*SIRI*” case, not shown here), neither steps (i) and (iii) are performed.

For applications to FWI within the target region, steps (i) and (iii) need to be performed only once, and at each new iteration of the inversion, the wavefield computation (ii) is performed only inside the box, considerably saving computing time, especially when both sources and/or receivers are far from the box, and thus enabling computations to higher frequencies at accessible cost.

2.2.2 Theoretical considerations

Theoretical expressions

We recall the elastic wave equation, expressed in the space and frequency domain, valid for any bounded domain V_{tot} :

$$\rho \omega^2 u_n + \partial_j (C_{njkl} \partial_k u_l) = f_n \quad (2.1)$$

where u_n and f_n are respectively the displacement and external force in the n^{th} spatial direction, ω is the frequency, ρ is the density of the medium, C_{njkl} is the fourth order elasticity tensor. The ∂_j derivative represents the partial differentiation along the j^{th} direction. The Einstein summation convention is used.

Following Masson et al. [2014], we wish to construct a mirror that regenerates the wavefield within a subvolume V of V_{tot} , bounded by a closed surface ∂V . Let us define a window function $w(\mathbf{x})$ as:

$$w(\mathbf{x}) = \begin{cases} 1 & \forall x \in V \\ 0 & \forall x \notin V \end{cases} \quad (2.2)$$

We also define $u^V(\mathbf{x}, t)$ the displacement field restricted to the volume V :

$$u^V(\mathbf{x}, t) = w(\mathbf{x}) \cdot u(\mathbf{x}, t) \quad (2.3)$$

$$= \begin{cases} u(\mathbf{x}, t) & \forall x \in V \\ 0 & \forall x \notin V \end{cases} \quad (2.4)$$

The displacement field u^V can be obtained by solving eq. (2.1) using a specific source term. We have:

$$\rho \omega^2 u_n^V + \partial_j (C_{njkl} \partial_k u_l^V) = f_n^V \quad (2.5)$$

where f_n^V is the force needed to generate the local displacement u_n^V . Replacing the local wavefield by its expression from eq. (2.1) in terms of the global wavefield and the window function, we obtain the following expression for the source term:

$$f_n^V = w f_n + \partial_j (C_{njkl} \partial_k w u_l) - w \partial_j (C_{njkl} \partial_k u_l). \quad (2.6)$$

Thus, the local wavefield is obtained by successively solving eq. (2.1) to obtain the global wavefield $u(\mathbf{x}, t)$, evaluating the source term in eq. (2.6) and solving eq. (2.5) to obtain $u^V(\mathbf{x}, t)$ [for further details, refer to Masson et al., 2014]. When the Green's function $\mathbf{G}(\mathbf{x}, \mathbf{s})$ of the reference medium is known, instead of using eq. (2.5), we may obtain the local wavefield directly using the convolution integral:

$$u^V(\mathbf{s}, t) = \int_0^t \int_{V_{tot}} \mathbf{G}(\mathbf{x}, \mathbf{s}, t - \tau) \times f_n^V(\mathbf{x}, \tau) dV_{tot} d\tau. \quad (2.7)$$

In the present study, eq. (2.5) is solved numerically to obtain the local wavefield inside the box, while an equation similar to eq. (2.7) is used to evaluate the wavefield outside the box. More precisely, the wavefield $u^{V_{ext}}$ measured by receivers outside the box:

$$u^{V_{ext}}(\mathbf{x}, t) = (1 - w(\mathbf{x})) \cdot u(\mathbf{x}, t) \quad (2.8)$$

$$= \begin{cases} 0 & \forall x \in V \\ u(\mathbf{x}, t) & \forall x \notin V \end{cases}, \quad (2.9)$$

is evaluated using:

$$u^{V_{ext}}(\mathbf{s}, t) = \int_0^t \int_{V_{tot}} \mathbf{G}(\mathbf{x}, \mathbf{s}, t - \tau) \times f_n^{V_{ext}}(\mathbf{x}, \tau) dV_{tot} d\tau, \quad (2.10)$$

where:

$$f_n^{V_{ext}} = (1 - w) f_n + \partial_j (C_{njkl} \partial_k (1 - w) u_l) - (1 - w) \partial_j (C_{njkl} \partial_k u_l). \quad (2.11)$$

There are two distinct contribution to the outer wavefield $u^{V_{ext}}(\mathbf{s}, t)$. The first one is associated with the first term on the R.H.S. of eq. (2.11), it accounts for the wavefield

generated by sources located outside the box that is measured at the receivers. The second one is associated with the last two terms on the R.H.S. of eq. (2.11), it is the wavefield measured on the surface ∂V that is extrapolated to the receivers and accounts for the sources inside the box. The latter contribution vanishes when no sources nor perturbation are present within the box. Practically, the seismograms recorded by receivers located outside the box are obtained by first computing the local wavefield in the perturbed medium using eq. (2.5). Then, the computed wavefield is used to evaluate the source term in eq. (2.11) and is extrapolated to the receivers using eq. (2.10). Notice that the reference wavefield computed in the unperturbed medium at the distant receiver needs to be added to the result of the convolution on ∂V only when the source is located outside the box.

Numerical expression

The numerical equivalent of the window function $w(\mathbf{x})$ is a matrix $\bar{\mathbf{W}}$ such that the displacement field $\bar{\mathbf{u}}^V$ in the subvolume V is equal to $\bar{\mathbf{W}} \cdot \bar{\mathbf{u}}$. The bar denotes a discrete variable. $\bar{\mathbf{W}}$ is a diagonal matrix, and its elements are values of the window function at interpolation nodes of the numerical solver. It is a bi-valued matrix, with elements on the diagonal equal to 1 for nodes that belong to the subvolume V , and 0 elsewhere.

Eq. (2.1) then takes the form [Fichtner, 2010]:

$$\mathbf{M} \cdot \ddot{\mathbf{u}} + \mathbf{K} \cdot \bar{\mathbf{u}} = \bar{\mathbf{f}} \quad (2.12)$$

where $\mathbf{M}$ and $\mathbf{K}$ represent the *mass matrix* and the *stiffness matrix*, respectively.

Following the same approach as in the previous section, substituting $\bar{\mathbf{u}}$ by $\bar{\mathbf{u}}^V$, we obtain the discretized mirror excitation $\bar{\mathbf{f}}^V$, necessary to regenerate the wavefield inside V :

$$\mathbf{M} \cdot \ddot{\bar{\mathbf{u}}^V} + \mathbf{K} \cdot \bar{\mathbf{u}}^V = \bar{\mathbf{f}}^V \quad (2.13)$$

Replacing $\bar{\mathbf{u}}^V$ by its expression in terms of the window function and the global wavefield, we obtain the equation for the mirror excitation force:

$$\bar{\mathbf{f}}^V = \mathbf{M} \cdot (\bar{\mathbf{W}} \cdot \ddot{\bar{\mathbf{u}}}) + \mathbf{K} \cdot (\bar{\mathbf{W}} \cdot \bar{\mathbf{u}}) \quad (2.14)$$

Now, substituting the product $\mathbf{M} \cdot \ddot{\bar{\mathbf{u}}}$ by its expression from eq. (2.12), we obtain:

$$\bar{\mathbf{f}}^V = \bar{\mathbf{W}} \cdot (\bar{\mathbf{f}} - \mathbf{K} \cdot \bar{\mathbf{u}}) + \mathbf{K} \cdot (\bar{\mathbf{W}} \cdot \bar{\mathbf{u}}) \quad (2.15)$$

However, keeping all this information at all the interpolation nodes of the solver (either inside or outside V) is inefficient and unnecessary. Indeed, for the sake of clarity, let's now assume that we are working with finite elements (spectral or not). Inside one such element, we have the local wave equation, based on eq. (2.12), where the subscript “e” indicates that we are inside the element e :

$$\bar{\mathbf{f}}_e = \mathbf{M}_e \cdot \ddot{\bar{\mathbf{u}}}_e + \mathbf{K}_e \cdot \bar{\mathbf{u}}_e \quad (2.16)$$

In this case, the window matrix $\bar{\mathbf{W}}_e$ is a diagonal matrix containing values of the window function at each interpolation node within the element e . In the case of the SEM, these nodes are also the integration points for Gauss-Lobatto-Legendre (GLL) quadrature.

Following the same steps as previously, we obtain the local mirror excitation force within the element e :

$$\bar{\mathbf{f}}_e^M = \mathbf{M}_e \cdot [\bar{\mathbf{W}}_e \cdot \ddot{\mathbf{u}}_e] + \mathbf{K}_e \cdot [\bar{\mathbf{W}}_e \cdot \bar{\mathbf{u}}_e] \quad (2.17)$$

$$= \bar{\mathbf{W}}_e \cdot \mathbf{M}_e \cdot \ddot{\mathbf{u}}_e + \mathbf{K}_e \cdot [\bar{\mathbf{W}}_e \cdot \bar{\mathbf{u}}_e] \quad (2.18)$$

$$= \bar{\mathbf{W}}_e [\bar{\mathbf{f}}_e - \mathbf{K}_e \cdot \bar{\mathbf{u}}_e] + \mathbf{K}_e \cdot [\bar{\mathbf{W}}_e \cdot \ddot{\mathbf{u}}_e] \quad (2.19)$$

Assuming no external force on this element ($\bar{\mathbf{f}}_e = 0$), we obtain the equation to express the mirror excitation force:

$$\bar{\mathbf{f}}_e^M = -\bar{\mathbf{W}}_e \cdot [\mathbf{K}_e \cdot \bar{\mathbf{u}}_e] + \mathbf{K}_e \cdot [\bar{\mathbf{W}}_e \cdot \ddot{\mathbf{u}}_e] \quad (2.20)$$

Now, let's impose that $\bar{\mathbf{W}}_e = \alpha_e \cdot \mathbf{I}$, where α_e is a scalar coefficient, with $\alpha_e = 0$ if the whole element is outside the volume V , $\alpha_e = 1$ if the whole element is inside V and $0 < \alpha_e < 1$ if part of the element is outside and part inside V .

From eq. (2.20), it becomes clear that only the elements that are neither fully inside or fully outside V will contribute to the mirror excitation force.

Since most of the elements of the mesh do not contain the boundary of the box, this property considerably reduces the number of values one needs to store in order to regenerate the wavefield inside V .

Using the discrete representation theorem in the elastic case, one can express the displacement field u for component k at any point $\mathbf{x}$, and at any time t as the equivalent of eq. (2.10):

$$\bar{\mathbf{u}}_n(\mathbf{x}, k) = \sum_{i=1}^3 \sum_{l=0}^t \sum_j \bar{\mathbf{G}}_n^0|_{\mathbf{x},i}(j, k-l) \cdot \bar{\mathbf{f}}_i(j, l) \quad (2.21)$$

where $\bar{G}_n^0|_{\mathbf{x},i}$ denotes the n^{th} component of the Green's function calculated at $\mathbf{x}$ for an impulse force in the direction i ($I = 1, 2, 3$), located at point j on $M2$, and $\bar{\mathbf{f}}_i$ is the corresponding mirror force excitation, as computed in eq. (2.20). The summation in j corresponds to the summation on all the points of $M2$ and the summation in l to time.

The approach presented here allows us to couple any two wave propagation solvers, one used inside and the other one outside the target region V . The model outside the target region V , i.e. the "reference model" is fixed, so the computations outside V are performed only once using the "global solver". Wave propagation inside V is computed using the regional solver, and may evolve as a function of iteration in the context of a Box

Tomography application. Importantly, the global and regional solvers may require different meshes. In what follows, we consider two fully 3D spectral element solvers, for which the relevant discretization points are the GLL points inside each element [e.g., Komatitsch and Tromp, 2002]. However, this approach can be applied to the coupling of any two numerical wave propagation solvers.

2.3 Practical implementation

Following Masson and Romanowicz [2017b], we introduce two mirrors $M1$ and $M2$ around the target region within which we plan to perturb the 3D model. A zoomed view of this geometry is shown in a 2D cross-section in Fig. 2.2. The mirror $M1$ is introduced inside the boundary of the computational domain (V_c) for the regional solver and serves for the reinjection of the global wavefield into this computational domain, as needed in cases *SORI* and *SORO* (Fig. 2.1). The mirror $M2$, located within the volume spanned by $M1$, serves to record the information needed for extrapolation of the wavefield from inside the box to external stations (i.e. into the extrapolation volume V_e in Fig. 2 of Masson and Romanowicz [2017b], as needed in cases *SIRO* and *SORO*). The Green's functions representing the propagation from mirror $M2$ to external station R in the reference medium are also stored on $M2$.

The workflow for computing the wavefield (Fig. 2.3) is slightly different for the 3 cases considered in Fig. 2.1. In each case, the source S is defined by its location, moment-tensor and a frequency band.

For the case *SORI*, only one mirror ($M1$) is necessary, and the workflow is as follows:

1. Define the geometry of mirror $M1$ and the coordinates of each of the GLL points on this mirror using the regional solver mesh.
2. Compute the seismic wavefield generated by the external seismic source at S in the reference model using the global solver, and store the displacement on each point of the mirror $M1$ defined in step (i).
3. Propagate the wavefield inside the box V_c using the reinjection of the secondary sources computed in step (ii) from mirror $M1$ and record the wavefield at station S .

For the case *SIRO*, only one mirror is needed ($M2$) and the workflow is as follows:

1. Define the geometry of mirror $M2$ and the coordinates of each of the GLL points on this mirror using the regional solver mesh.
2. Compute the wavefield from the source S to the mirror $M2$ using the regional solver and record it at the GLL points defined in step (i)
3. Calculate the three Green's functions from each point of mirror $M2$ to the distant receiver R in the reference model

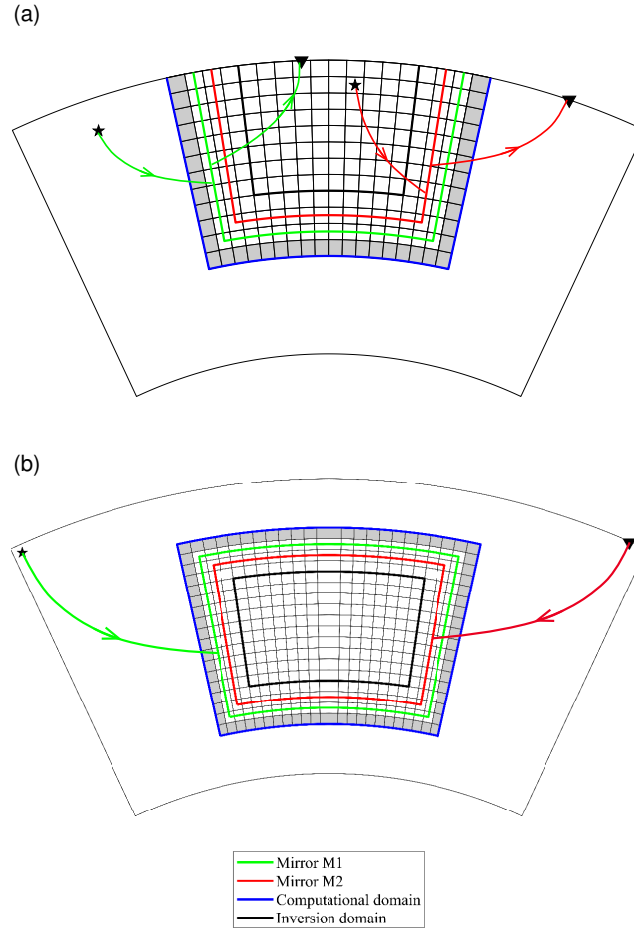


Figure 2.2: A zoomed view of the Box Tomography concept including three cases of interest: (a) (“*SORI*” and “*SIRO*”) and (b) (“*SORO*”). The methodology is fully 3D but the sketch is presented in 2D for simplicity. In each case, the locations of the sources and receivers are indicated by black stars and reverse triangles, respectively. The blue and black solid lines are the boundaries of the modeling and inversion domains, respectively. The mesh shown is the regional solver mesh. The grey elements are those used for the absorbing boundaries in the regional solver. A “layer” of elements separates the internal mirror from the domain in which model updates will be performed, and is used to smoothly connect the reference model to the evolving regional model. Mirror forces and Green’s functions are summed over the points of mirror M2.

4. At each point on $M2$, convolve the mirror forces computed from the wavefield on $M2$ with the corresponding Green's function computed in step (iii) and sum over all the points on $M2$ to obtain the complete wavefield at station R .

For the case *SORO*, where the wavefield is computed from a distant source to a distant receiver located outside of the box, the workflow is as follows:

1. Define the geometry of mirrors $M1$ and $M2$ and the coordinates of each of the GLL points on these mirrors in the regional solver meshing.
2. Calculate the seismic wavefield generated by the external seismic source at S in the reference model using the global solver, and store the displacement on each point of the mirror $M1$, as well as the reference wavefield at all stations R located outside of the box.
3. Calculate the three Green's functions from each point of mirror $M2$ to the distant receiver R in the reference model.
4. Propagate the wavefield inside the box V_c using the reinjection of the secondary sources computed in step (ii) from mirror $M1$ and record the wavefield at the GLL points on mirror $M2$ using the regional solver.
5. At each point on $M2$, convolve the mirror forces computed from the wavefield on $M2$ with the corresponding Green's function computed in step (iv) and sum over all the points on $M2$.
6. Add the time series obtained in step (v) to the reference seismograms computed in step (ii) to obtain the complete wavefield at external receiver R .

We note that in the case *SIRO*, the convolution performed in the corresponding step (iv) produces the complete wavefield. This is not the case when the source is outside V_c (*SORO*). In this case, the result of the operation performed in step (v) is the perturbation to the reference wavefield recorded at R due to a perturbation in the model inside V_c . This contribution, which is non-zero only in the case when the model inside V_c has been perturbed, needs to be added to the reference wavefield to obtain the total wavefield at station R .

We also note that in the cases *SIRO* and *SORO*, instead of computing Green's functions from mirror $M2$ to the external station R , which would involve as many SPECFEM computations as there are GLL points on the mirror, we invoke the reciprocity theorem, which allows us to compute only 3 Green's functions, one for each component of motion, from the station R to mirror $M2$.

2.3.1 Global simulations

Here, we use SPECFEM3D [Komatitsch and Tromp, 2002] as our global solver to compute the secondary sources at the boundary $M1$ of the target region in the reference 3D model, as well as the Green’s functions that are necessary for the extrapolation from the box (Mirror $M2$) to the external receiver. As the coordinates of the points on both mirrors correspond to the location of the GLL points in the regional solver (see below), it is necessary to perform a spatial interpolation when recording the displacement or the force in order to match the GLL point locations imposed by the regional solver. These GLL points are not exactly the same as those of the code SPECFEM3D, due to the different spatial meshes in the two solvers.

In SEM, spatial Lagrange interpolation is used to obtain the values at points that are inside the element but not exactly on the GLL points. We adapt the same spatial Lagrange interpolation to evaluate the mirror forces on $M1$ and the Green’s functions on $M2$. However, this Lagrange interpolation can introduce significant errors for the subsequent computation of the wavefield inside the target region if SPECFEM3D is used with a polynomial order of 4, as commonly done (125 GLL points per element) (Lyu et al., 2022 under review). To reduce this error, we use a finer mesh than is theoretically required for computations down to a period of 20s (as presented in the benchmarks that follow), one which would be accurate for computation with a minimum period of ≈ 11.5 s.

2.3.2 Regional or local simulations

RegSEM is a regional numerical solver for the elasto-dynamic equation, appropriate for region sizes ranging from a few squared kilometers to 90° by 90° [Cupillard et al., 2012]. The vertical extent of the region is also user-defined, and does not have to extend to the Core-Mantle boundary (CMB). RegSEM is used to compute the wavefield propagation within the box. It is with the mesh constructed in RegSEM that we define the points that belong to the mirrors $M1$ and $M2$ prior to any simulation, at which the Green’s functions, the mirror force excitation on $M1$ and the secondary sources on $M2$ will be computed.

In order to avoid the artificial reflections that would arise at the borders of the region, Perfectly Matched Layers [PML; Festa and Vilotte, 2005] are implemented in RegSEM at the boundary of the computational domain. In RegSEM, the PMLs are isotropic, but the elements composing them are described with a much higher polynomial order in the damping direction, which ensures satisfactory results even in the case where the simulation is performed in an anisotropic medium.

In the context of Box Tomography, RegSEM is used to perform all the regional simulations, that are performed at each iteration of the inversion for structure in the target

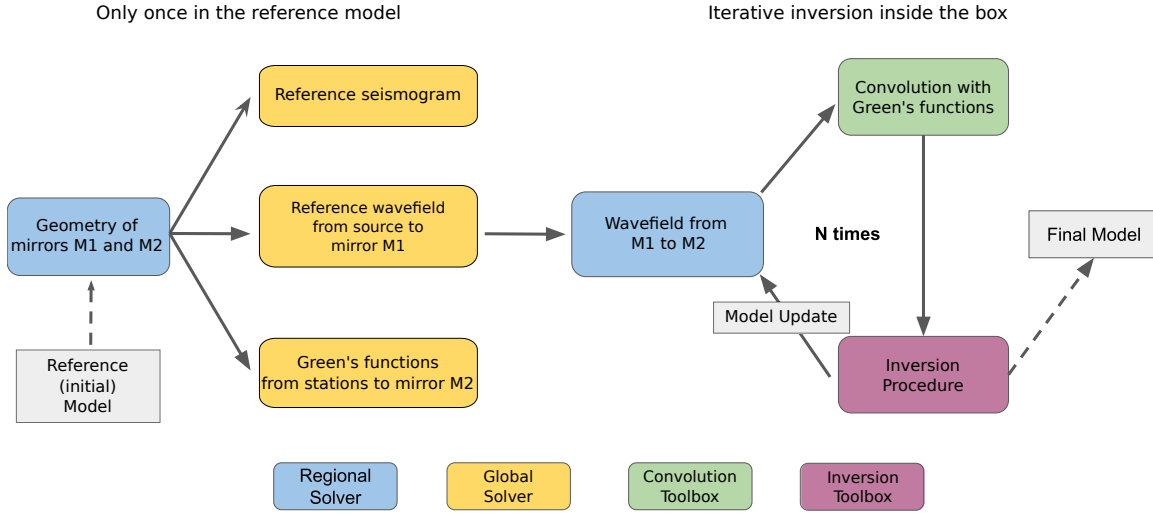


Figure 2.3: A schematic description of the workflow in order to perform regional tomography using the Box Tomography framework for the direct problem.

region. It is the only part of the workflow (Fig. 2.3) that needs to be computed each time the regional model is updated.

2.3.3 Convolution: extrapolation to a distant receiver

In order to match the Green's function time series with those obtained after propagation inside the box using the regional solver for the purpose of computing the convolutions in the cases *SIRO* and *SORO*, we have designed a meta-indexing scheme valid for all types of solvers, with the goal to ensure that each point of the mirror *M2* has the same meta-index in the global and regional solvers. To compute it, we sort the coordinates of the mirror points in a Cartesian reference coordinate system. Since the Cartesian reference frame is global and common to all used solvers, it has the advantage of being mesh independent.

The size of the mirror represents a numerical challenge in terms of storage and input/output (I/O) access. In order to avoid the highly inefficient swapping with the hard drive memory, and the convolution of very long time series, it is essential to try and reduce the size of those files as much as possible. First, we decimate the time series: in order to ensure the stability of the numerical wave equation solver, the synthetic seismograms are computed at a high-sampling rate, much higher than the Nyquist frequency of the waveform itself. It is hence possible to downsample all the time series to keep a sampling rate equal to four times the maximum frequency of our simulation, in order to keep a comfortable margin with respect to the Nyquist frequency.

Second, we have implemented a compression algorithm on all our recorded time series (mirror forces and Green’s functions). For this, we use a projection on a B-spline basis (see Appendix B for more implementation details), which further reduces the size of the files that need to be read in order to perform the convolution and summation in steps (iii) and (iv) for *SIRO* and steps (v) and (vi) for *SORO*. An interpolation of the time-series is here chosen in order to save only a certain number of coefficients needed to expand this time-series at a frequency that will still be higher than the minimal period we will be interested in. In practice, we then store spline coefficients. In order to evaluate the signal at any given time, one needs to know $N + 1$ coefficients, where N is the order of the polynomial. For this study, we have used a typical value of $N = 4$. However, even though the spline interpolation is a piecewise polynomial fit between two consecutive knots, we only update one coefficient per time step. Reconstructing the signal at a given time requires search for the N nearest coefficients (i.e. those that correspond to basis functions that are non zero at the interpolation time), multiplying them by the basis function values at interpolation time, and summing over the non-zero basis functions. Although Pienkowska et al. [2021] have used a higher-order Lanczos resampling, Monteiller et al. [2021] have used a similar strategy to decimate their computed velocity and traction fields, allowing them to reconstruct the time-series on the fly.

To further increase the computational efficiency of the convolution step, at the end of step (iv), we transform the files that contain all the compressed recordings from being ”snapshot ordered”, which is the natural order obtained as the numerical simulation is progressing in time, to being ”time-series ordered”. This way, each mirror point will have their time-series stored contiguously, which ensures easy access without substantial jumps across the files. In practice, this requires transposing the arrays contained in the files recorded at steps (iii) and (iv) (for *SORO*), which can be easily handled by dedicated libraries. The convolutions to be computed for each point on mirror $M2$ are performed on their compressed representations in the B-spline domain (See Appendix C).

To obtain the complete seismograms, we sum the contributions of all the mirror points to the convolution. It is possible to distribute the convolution computation over multiple cores, making our algorithm naturally scalable, if the size of the mirror increases due to a larger region or a finer mesh for higher frequency simulations. Furthermore, we made this code naturally cache-friendly thanks to the meta-indexing introduced earlier for matching two distinct grids. Each processor then only stores the relevant coefficients associated with the points for which it computes the discrete convolution, without having to read and store the whole files where Green’s functions and mirror force excitation are stored, for an increased efficiency at runtime.

2.3.4 Post-processing

We note that, numerically, the Green’s functions sources are not perfect Dirac delta functions in time, so that the reconstructed hybrid seismogram is, in fact, convolved by the

effective source time function used to compute the Green's functions. In order to compare it with real waveform data corresponding to propagation between the source S and the receiver R , it is necessary to convolve the latter by the pseudo-Green's function source time function. In practice, it is sufficient to define the bandwidth of the pseudo-Green's function so that its corner frequencies are outside of the cut-off frequencies of the seismic source S . In order to account for the acausality of the Green's function, one only needs to appropriately shift the resulting signal in the time domain. This is also the case when benchmarking the results of the hybrid computation against a reference wavefield computed between S and R without the box - in our case using SPECFEM3D.

2.4 Validation

We tested our implementation of the forward hybrid wavefield computation in 3D for different setups, taking advantage of the versatility of the solvers we use. In each case, we compared the results of the hybrid computation with the solution obtained by computing the wavefield from the source to the station using the 3D global solver SPECFEM3D, without mirrors.

For simplicity, in what follows, we only focus on the elastic case, not including anelastic attenuation nor ellipticity corrections. We considered flat surface topography and a 1D crust, with a fixed Moho discontinuity, in order to avoid the potential discrepancies that could arise from the element distortion needed to accommodate such features in the regional and global solvers. This is however not an issue for the SORO case with a remote target region in the deep earth.

First, we validated our implementation in a simple case, in which both the model inside and outside the target region is a 1D spherically symmetric radially anisotropic Earth model. For the purpose of the comparisons shown here, this model is based on PREM [Dziewonski and Anderson, 1981], in which we have replaced the ocean by continuation of the structure at the top of the crust to the earth's surface. In a second test, we introduced a 3D perturbation in the target region. Finally, we considered a recent global 3D Earth model as the reference model and, as in the second test, added a 3D perturbation in the target region.

For all these tests, we used the same target region V , centered on the Yellowstone area, with a size of 20° in longitude by 20° in latitude, extending from the surface down to 1000 km depth. The event S is located to the north of the target region, and three lines of stations are considered at different azimuths, and at epicentral distances ranging from 3000 to 5500 km. In each line, the furthest station is located outside the box ("SORO"), while other stations are inside the box (case "SORI"). The geometry of this setup is shown in Fig. 2.4.

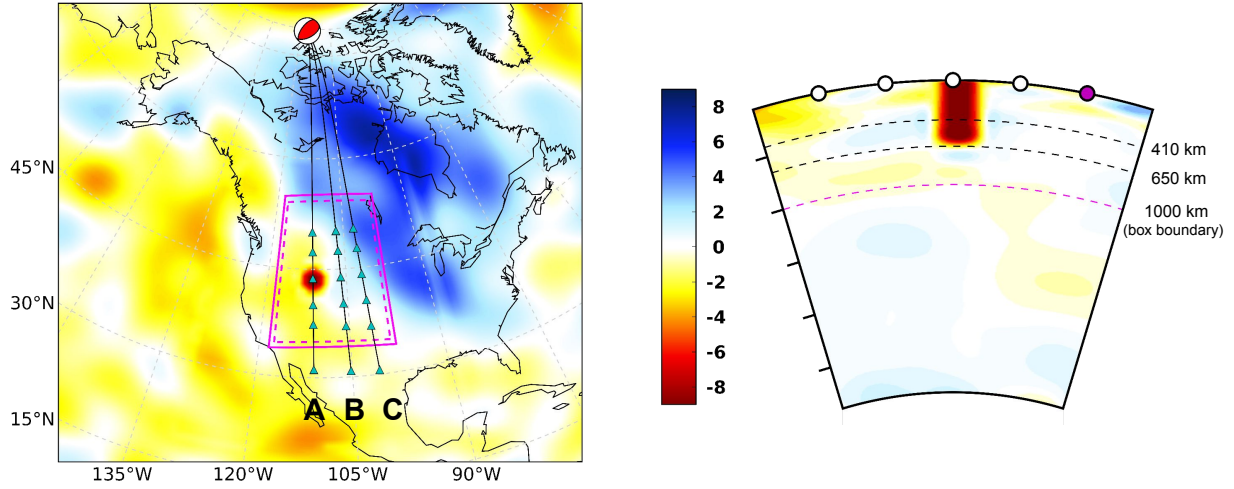


Figure 2.4: Design of the benchmarks. *Left panel:* A map view of the background 3D velocity model (SEMUCB_WM1) used in some of the benchmarks, with a focus on the target region in which we input a 3D plume-like perturbation, indicated by the red disk, in the Yellowstone area. The color scale to the right of this panel corresponds to the velocity perturbation distribution with respect to the 1D average, in percent. The boundaries of the region are plotted in magenta, with the solid lines representing mirror $M1$ and the dashed lines representing mirror $M2$. The fictitious stations used to record the synthetic wavefield for all benchmarks are indicated by triangles. They are aligned along 3 lines (arrays) A, B and C, sampling the plume (array A), and at increasing distance from it (arrays B,C). The source, which is the same for all the benchmarks, is represented by a beach ball. We used the source parameters from the "global CMT" catalog [Ekström et al., 2012] for a real event of $M_w = 4.8$, which occurred on 17/11/2017) in northern Canada. *Right panel:* Depth cross section of the velocity model used in the 3D/3D benchmark. The synthetic plume extends from the surface to 650 km depth, with a velocity perturbation of 8%, and a lateral extent of 500 kilometers.

We computed 60 minutes (3600 seconds) long time-series, starting from the origin time, filtered with corners at 30 and 250 seconds, and cut-offs at 20 and 400 seconds.

2.4.1 Benchmark for a radially anisotropic 1D model both inside and outside the box

We first performed a simulation in the 1D model. This simple test is necessary to understand where the mesh differences can be of importance when coupling two different 3D

solvers, as well as the efficiency of the B-spline compression.

In our setup, the mirror at the boundary of the target region has over 540,000 points, which is still relatively small but already allows us to take advantage of our cache-friendly and optimized convolution algorithm to keep the convolution insignificant compared to the computational cost of the numerical waveform simulation (see Table 2.1).

In Fig. 2.5, we compare the velocity seismograms obtained in the reference solver without the box to those reconstructed using the hybrid approach, ordered as a function of epicentral distance for each of the 3 lines of stations considered (A,B,C, in Fig. 2.4).

We note an excellent agreement between the two computations. The error, as computed by the sum of absolute differences (L1-norm) between the hybrid seismogram and the reference seismogram, is of the same order of magnitude ($\sim 2.0\%$) as the difference between the SPECFEM3D seismogram and a RegSEM seismogram computed without the box.

The level of agreement shown at the stations located inside the box was obtained thanks to the effort to match the grids of our two solvers in order to minimize numerical dispersion error. In this context, the interpolation of each point of $M1$ from the RegSEM grid to the SPECFEM3D grid can accumulate a few percent error between the reference synthetic seismogram and the hybrid one. For the purpose of this benchmark, we have used more elements in order to increase the numerical stability and reduce this interpolation error, that mainly impacts the amplitude of the signal. However, when applied in the context of real data, this source of error is below the noise level from any instrument, and will not seriously influence the velocity structure obtained after inversion.

2.4.2 Benchmark with 1D structure outside and 3D inside the box

In the second test, we added a 3D plume-like heterogeneity to the 1D background model inside the target region, and recomputed both the reference and the hybrid seismograms in this model. We kept the same experimental set-up. The low-velocity anomaly is designed such that it keeps a constant radius with depth, with a maximum perturbation located at the center of this radius, in order to avoid ringing phenomena when projecting the synthetic plume on the spherical spline basis we use to describe 3D models.

In Fig. 2.6, we show the differences between the case with the 3D anomaly inside the box and the case without it. Here again, we find a very good agreement between the reference computation in SPECFEM3D and the hybrid computation, which further confirms the success of our implementation of both the wavefield reinjection and its extrapolation to a distant receiver.

As expected, both the hybrid seismogram and the 3D SPECFEM seismogram show signifi-

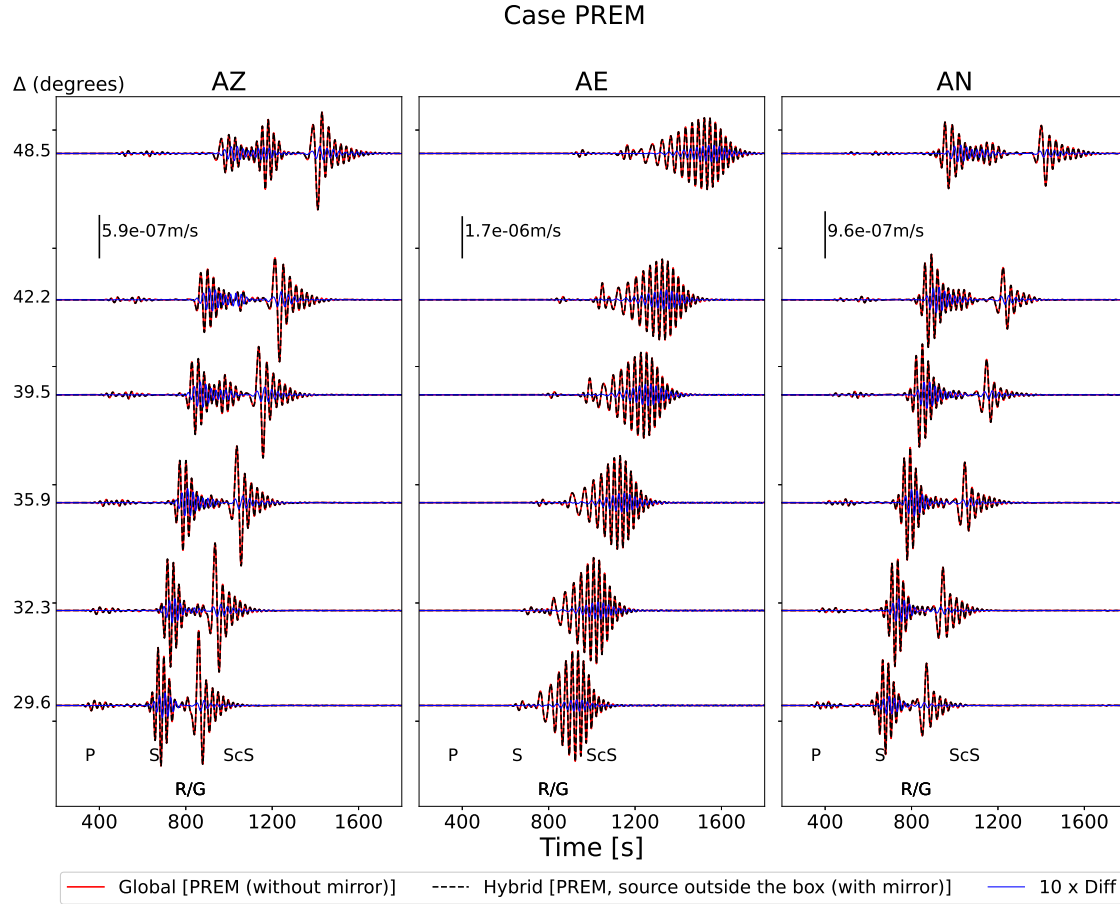


Figure 2.5: Benchmark results in the PREM model (without ocean or attenuation) for line A as presented on Fig. 2.4. The reference SPECfEM3D solution (thick continuous red line), is compared to the hybrid seismogram obtained with the methodology described in this paper (black dashed line). The difference between the two time-series (blue) is shown blown-up by a factor of 10. *Left panel*: Vertical component of the velocity wavefield, arranged with distance from the epicenter. *Center panel*: East component of the velocity wavefield. *Right panel*: North component of the velocity wavefield.

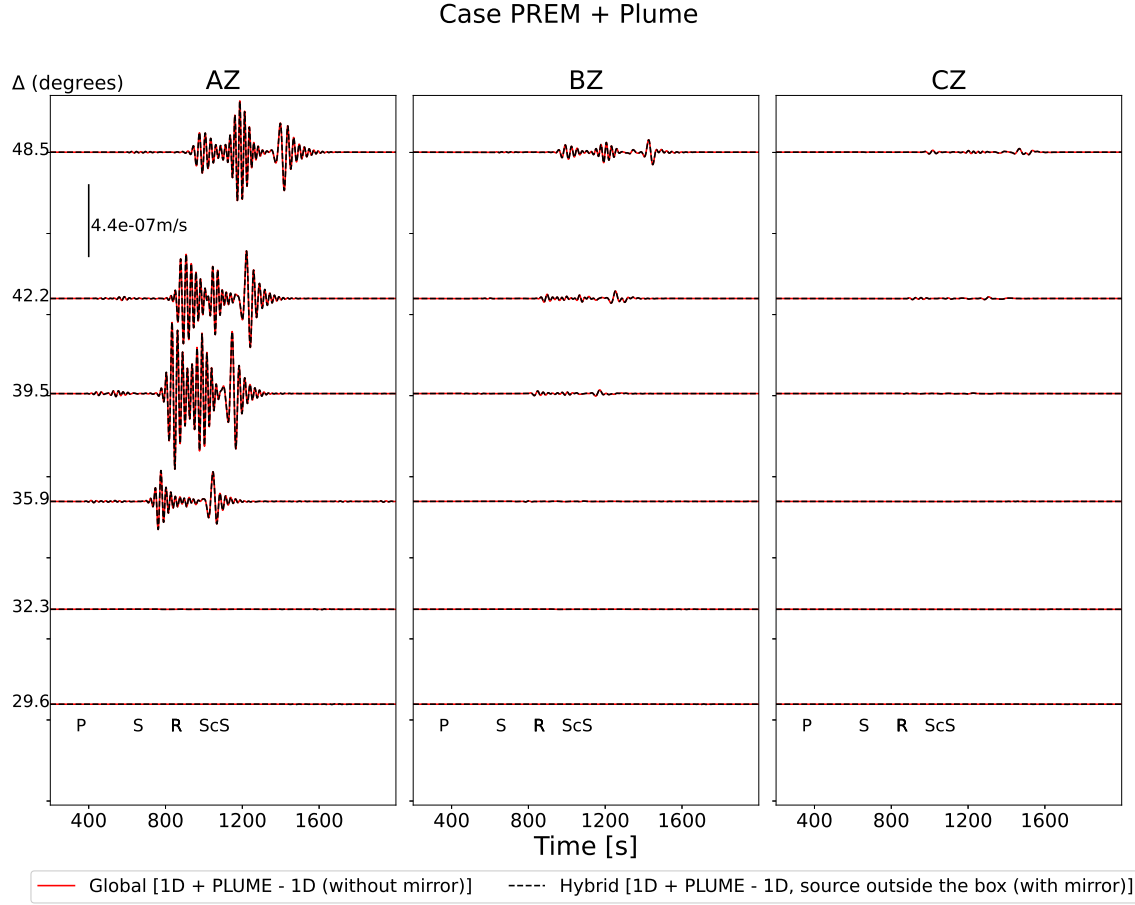


Figure 2.6: Benchmark results in the 1D-PREM background model with a plume-like 3D anomaly in the target region for all stations. The results are shown on the same scale, visible at the top left corner of the left panel. Plotted here are the differences between the computation with and without the 3D plume anomaly. The reference SPEC-FEM3D solution (thick continuous red line) shows a good agreement with the hybrid seismograms (dashed black lines) obtained with the methodology described in this paper. *Left panel*: Vertical component of the velocity wavefield, for line A. *Center panel*: Vertical component of the velocity wavefield, for line B. *Right panel*: Vertical component of the velocity wavefield, for the line C. See Figs. S2 and S3 in Supplementary Material for the corresponding plots on the East and North components, respectively. Note that receivers have been placed intentionally in front and away from the plume, in order to verify that the hybrid modeling process does not introduce unrealistic energy due to theoretical or interpolation errors in the code. Hence the many zero traces in this figure and in 2.7.

cant differences compared to the 1D seismogram for paths that are directly affected by the anomaly, which confirms that both methods capture the effect of the 3D anomaly on the resulting wavefield.

The slight discrepancies between these two calculations do not impact the phase arrival but only the amplitude of the signal, compared to the previous test, and could be explained by round-off errors, interpolation errors from the global mesh to the regional mesh, the different spatial and temporal dispersion errors, and the way the two different meshes handle the discretization of the 3D perturbation.

Interestingly, while the maximum difference between the 1D and 3D cases is observed on the paths that directly sample the center of the anomaly, waves that travel on great-circle paths that miss the anomaly by about a minimum wavelength (i.e. line B) are also impacted by the perturbation in the velocity model. This highlights the importance of FWI in the context of tomography, in order to take advantage of the information contained in the scattered wavefield, which travel time tomography does not include.

It is also worth noting that the hybrid method accurately includes seismic phases that bounce between the surface and a reflecting discontinuity located below the lower boundary of the box (including core phases). This would not be the case if the regional code was used by itself, without coupling to a global code. When the model is updated in the target region, the subsequent reinjection of the secondary sources into the box includes such phases.

2.4.3 Benchmark with 3D structure both outside and inside the box

In our final benchmark, we replaced the 1D isotropic reference model by a 3D radially anisotropic model with a 24.4 km thick 1D crust, modified from SEMUCB_WM1 [French and Romanowicz, 2014]. The resulting differences between the seismograms computed in this background model with and without the added plume-like structure in the box are shown in Fig. 2.7 and the corresponding errors between the reference and hybrid computations are shown in Fig. 2.8 for the Z component on line A. For the corresponding East and North components, please refer to Figs. S4 and S5, respectively in Supplementary Material. For completeness, we also present in Fig. S1 (Supplementary Material) the benchmark results in the 3D SEMUCB_WM1 background model without any anomaly superimposed in the target region (the equivalent of the Fig. 2.5 in a 3D model), and the corresponding errors between the reference and hybrid computations, same as the Fig. 2.8, but for the East and North components on line A are also displayed in Figs. S6 and S7.

2.4.4 Computational cost

The highest computational cost in the generation of hybrid seismograms is for the global simulations, i.e. steps (ii) and (iii) in section (2.3) for the case SORO.

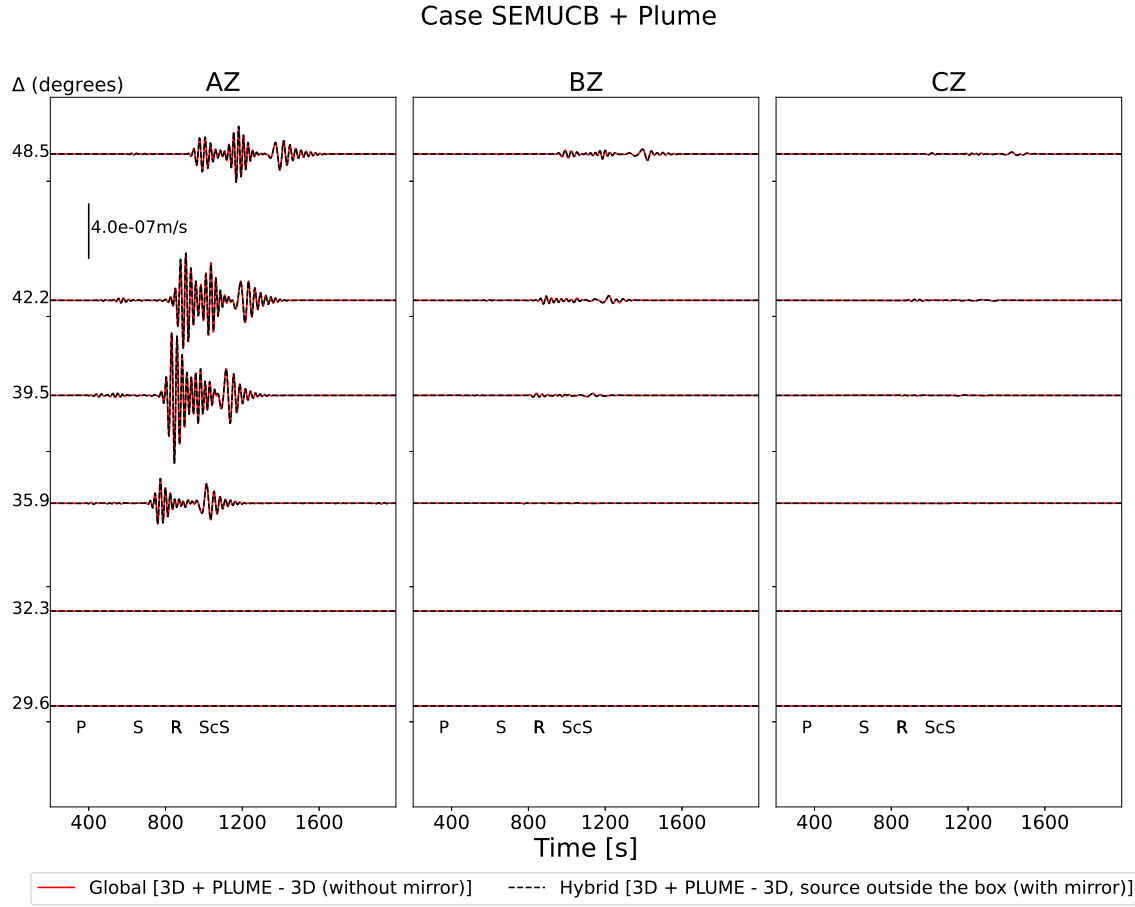


Figure 2.7: Same as Fig. 2.6 but for the benchmark performed in the 3D SEMUCB background model with a plume-like anomaly in the target region for all stations of our setup. *left panel*: Vertical component of the velocity wavefield, for line A. *center panel*: Vertical component of the velocity wavefield, for line B. *right panel*: Vertical component of the velocity wavefield, for line C. For the corresponding East and North components please refer to Figs. S2 and S3, respectively, in the supplementary material.

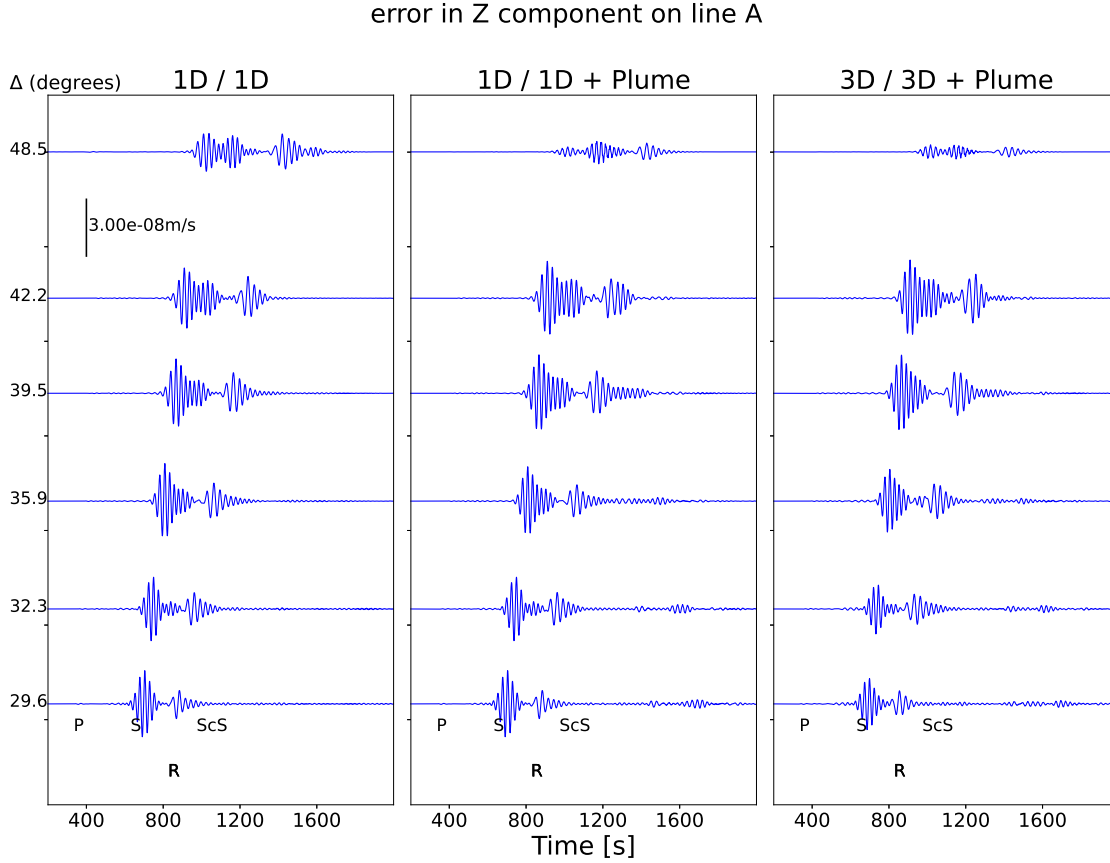


Figure 2.8: Differences between the reference and hybrid seismograms, computed for all three benchmarks for all stations in array A (passing through the synthetic plume). We refer to them as "errors". Note the amplitude scale, which is 40 times smaller than in previous figures. The amplitude of the error obtained is consistently below 3.6%, for all the cases considered. *Left panel:* Errors for the 1D case. *Center panel:* Errors for the case with 1D PREM in the background, and a 3D low-velocity plume-like anomaly in the target region. *Right panel:* Errors for the case where the background model is 3D (SEMUCB.WM1), with a low-velocity plume-like anomaly located in the target region.

However, these computations need to be performed only once in box tomography, as the model outside the box does not change during iterations of the inversion. Once they are done and stored, the remaining computational cost for the regional wave propagation and the convolution is significantly smaller.

For each run of our benchmark, the various costs of wavefield reinjection and extrapolation are summarized in Table 2.1. Once the initial iteration synthetic seismograms are computed in the reference model, obtaining seismograms for a single event costs at least an order of magnitude less than if we were to use a global 3D solver such as SPECFEM3D.

The computational cost associated with N_{ITER} iterations of a "box-tomography" inversion, assuming an adjoint-based formalism using the hybrid methodology, is equal to:

$$T_{hyb} = T_G \times (3 \times N_R + N_S) + 2 \times (T_R \times N_S) \times N_{ITER} \quad (2.22)$$

where T_{hyb} is the total computational cost of the forward modeling using the hybrid methodology, in CPUh, T_G and T_R are the computational costs of one run of the global and regional solver respectively, N_S , N_R and N_{ITER} correspond to the number of external sources, stations, and model inversion iterations respectively. Here we assume a single source time function for the earthquake source. The wavefield at any station located inside the target region can be computed at no additional cost. The factor of 2 assumes that in an adjoint formalism, two wavefield computations are necessary at each iteration, the second one to compute the first-order Fréchet kernel.

In a conventional approach, where all synthetic seismograms are computed using a global solver, the total computational cost for the same inversion is:

$$T_c = 2 \times T_G \times N_S \times N_{ITER} \quad (2.23)$$

Let us consider an example study with a target region surrounded by 50 external stations and 50 external sources. Let $R = \frac{T_c}{T_{hyb}}$ be the gain in computational time achieved with the hybrid approach for N_{ITER} iterations of inversion of structure within the target region. We have:

$$\frac{1}{R} = \frac{3 \times N_R + N_S}{2 \times N_S \times N_{ITER}} + \frac{T_R}{T_G} \quad (2.24)$$

The gain R is shown in Fig. 2.9a as a function of number of iterations and size of the mirror. This figure shows that the efficiency of box tomography consistently increases with the number of iterations. Depending on the relative performance of the two solvers, the computational time can be divided by an order of magnitude or more in our current setup compared to a conventional approach (black dashed line shows the theoretical limit). With our current regional solver RegSEM, which has not been optimized, we achieve an efficiency gain of 10 after about 20 iterations.

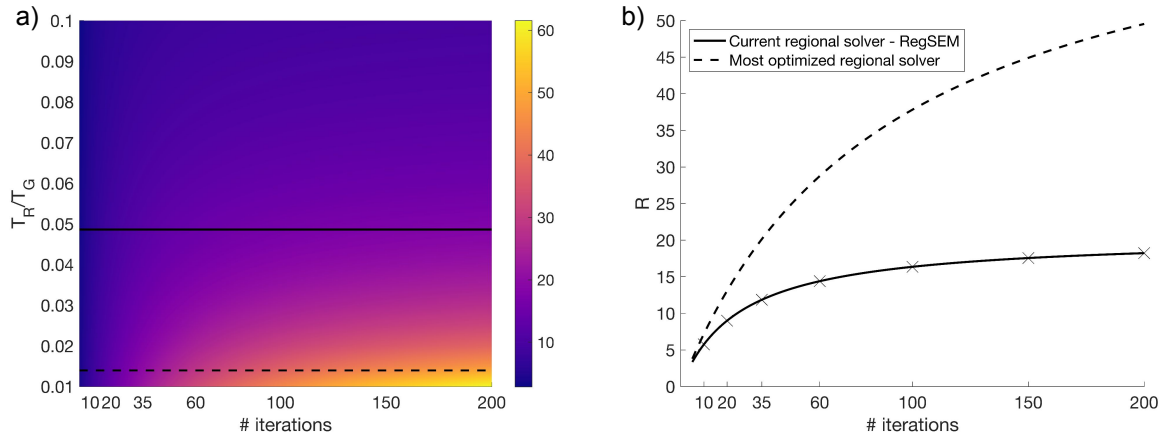


Figure 2.9: Gain R in total computational time, as expressed by the ratio between the computational time using the conventional and hybrid approach and defined in eq. (2.24), for the case with 50 stations and 50 sources all outside the target region. *Left panel:* Visualization of R as a function of the number of iterations and the ratio between the computing time of the regional solver (T_R) and the global solver (T_G). This ratio can be interpreted in two different ways: when the size of the box increases, T_R/T_G increases as well. However, when the optimization of the regional solver increases, T_R/T_G decreases. The solid black line represents the efficiency gain for our current regional solver and the dashed black line represents the efficiency gain for our size of the box if the regional solver was as optimized as the global solver. *Right panel:* R as a function of the number of iterations for our size of the box. The dashed black line (equivalent to Fig. 2.9a) represents the theoretical efficiency gain we would obtain if the regional solver was as optimized as the global solver. The solid black line (equivalent to Fig. 2.9a) represents the efficiency gain for our current regional solver RegSEM.

2.5 Discussion

We have shown that the full 3D hybrid forward modelling part of the box tomography approach can provide a gain in computational time of at least an order of magnitude compared to a conventional approach where complete synthetics need to be recomputed at each iteration of an adjoint-based inversion, regardless of the maximum frequency of computation. This is particularly interesting for applications where one would want to bury the target region and, for example, image an ULVZ at the base of the mantle. In that case, sources and stations are always at large distance from the target region and the structure requires observations at relatively short period (5s or less), and the vertical extent of the target region would be small, making the hybrid computations more efficient.

Table 2.1: Computational costs of the different tests presented in this paper. The size of the mirror remained the same for all tests, with 540,725 points on the $M2$ mirror. All time-series have been computed for an equal length of 3600 s. Computations were performed on NERSC facilities, using Intel Xeon Processor E5-2698 v3. dt indicates the sampling rate of the computation for the global and regional solver, respectively. Final dt (in the 4th column) corresponds to the sampling of the output of convolution. It is much larger than the dt for the solvers due to the decimation we have applied on the input signals.

Test type	Global dt	Regional dt	Final dt	Global CPUh	Regional CPUh	Convol3D CPUh	Total CPUh
1D/1D	0.1045s	0.0464s	4.7361s	4608×4	224	0.2	≈ 18656.2
1D/3D	0.1045s	0.0464s	4.9218s	4608×4	224	0.2	≈ 18656.2
3D/3D	0.1045s	0.0462s	4.9439s	4608×4	224	0.2	≈ 18656.2

Given our implementation of the method, and in particular how the extrapolation from the box to external stations is performed using the convolution step, the method is practically "solver independent": changing solvers would only require updating the way the displacement time-series obtained from the two solvers are read, when recording the wavefields on the mirrors. In many similar approaches, where integration over mirror points is done on-the-fly using the instaseis database [Pienkowska et al., 2021], it is necessary to modify the corresponding solver source code to perform this integration.

It is however important to consider the limitations of this approach. While we decrease computational time considerably, we require significant storage for the mirror files, which depends on the mirror size and on the maximum frequency. For our $24^\circ \times 24^\circ$ box and for a target minimum period of 20 seconds, each mirror file (three Green's functions file for each external receiver and one secondary sources file per external source) has a size of 4.9 Gb. For an application such as imaging of a ULVZ at the root of a mantle plume [e.g., Yuan and Romanowicz, 2017], where the target region would extend $1500\text{km} \times 1500\text{km}$ laterally and a 500km vertically above the core-mantle boundary, and for a target maximum frequency of 0.2Hz, we estimate that there would be at least $\approx 650,000$ points on the mirror, that is about two times more (including the mirror points in the outer core) than the current setup we have tested in this benchmark. The increase in frequency also implies a finer time sampling, and we would need 4 times more points in each time series, which would further increase the size of the mirror file by a factor of 4. In total, each mirror file would be ≈ 8 times larger than the ones we generated for this benchmark, i.e. ≈ 40 Gb.

We also note that, in the hybrid approach as described here, any strong scatterer located outside of the target region but close to its boundary will not be able to interact multiple times with a scatterer located inside the target region. That is, only the Born approximation

would be used for this specific scatterer. Keeping this in mind, in practical applications, it is important to verify that no strong scatterers are present outside of the box, in its immediate vicinity. It is also important to choose the 3D background model optimally, since the model will not be updated outside of the box. So far, the imperfection of the global reference model has been shown to not be important in a 2D synthetic experiment [Masson and Romanowicz, 2017a]. It will need to be verified in the 3D elastic case. In order to avoid repeated global simulations, it is also important to design the mirrors and the maximum frequency of computation carefully in advance.

The 3D benchmarks shown here have been performed in the purely elastic (radially anisotropic) case with a 1D crust. For application to real data, the following capabilities need to be included: a 3D crust, an ocean, ellipticity corrections and anelastic attenuation. Because the two solvers considered treat these effects slightly differently, we did not present this here, in order to focus on the coupling of the two codes. However, including them should not have any incidence on the performance of the mirror implementation.

Finally, in the present paper, we have shown benchmarks with a regional solver that could be significantly optimized (e.g. Fig. 2.9). We could have used a regional version of SpecFEM3d cartesian, however, we wanted to demonstrate the coupling of two 3D SEM codes developed independently, with different meshing strategies.

2.6 Conclusions

In this study, we have successfully coupled two 3D elasto-dynamic wave propagation solvers developed by different groups, one global and one regional, in order to reconstruct displacement wavefield between sources and stations that may be either inside or outside a target region for tomographic inversion. The proposed methodology relies on the introduction of time-reversal mirrors, on which only the displacement from a distant or internal source, and the displacement Green’s function from a distant station need to be recorded. These computations only need to be done once using the global solver for a given set of sources and stations and a target maximum frequency. Model iterations are obtained by propagating the wavefield inside the target region and coupling it to the global wavefield by means of secondary sources on the one hand, and convolution with the Green’s functions on the other.

Our methodology is not meant to replace efficient global 3D wave propagation solvers for the purpose of forward simulations only. It is suitable for applications to full waveform inversion in the case of remote target regions, in which case it can provide at least an order of magnitude reduction in computational cost compared to a conventional approach using a global solver, independently of frequency, and may obtain even higher order reduction in cost when using an optimized local solver. It can be ported easily to different solvers and is well suited for various structure and seismic applications. It is particularly promising in

the case of a deeply buried target region of small dimensions, such as ULVZs, sampled by teleseismic body waves.

Chapter 3

A merging package for multi-scale, multi-resolution geo-referenced datasets

This paper introduces a new package designed to merge multiscale, multi-resolution geo-referenced datasets. The package is flexible, efficient, and user-friendly, providing a simple and effective way to combine global and regional datasets, which can be both observations or models. The merging process relies on a binary mask and a window function defined on a sphere as a sum of spherical harmonics. The package takes advantage of the versatility of the netCDF format although it can also handle other formats, including plain ASCII files. The merging process is demonstrated in the example of blending a regional tomographic model within a global tomographic model in the context of full waveform inversion for seismic tomography. The paper presents the different stages of the merging process, including pre-processing of the geolocated datasets, spherical harmonics decomposition, and windowing. The package is a valuable tool for researchers who work with geo-referenced datasets and want to perform high-resolution simulations while keeping the information coming from a global background. We show a significant improvement in terms of picked wavepackets for the test case of a seismic event synthetic computation confronted with real data.

3.1 Introduction

3.1.1 Multiscale georeferenced datasets

Geo-referenced datasets are of utmost importance in various scientific disciplines, such as climate modeling, deep Earth geophysics, or even satellite imaging and remote sensing. Associating data obtained in the field, or models retrieved using them, to their geographical location is crucial for processing, visualizing, or comparing said data or models. Efficiently storing and effectively managing these datasets hence becomes essential due to their extensive

size and complex file structures. Geo-referenced datasets can encompass global-scale studies, or focus on specific regions that warrant a more detailed examination to gain deeper insights into localized physical or chemical processes that drive these datasets.

To this end, the netCDF format [Rew and Davis, 1990] has emerged as a standardized and widely adopted solution for handling geo-referenced datasets, offering an interface to a library of data access functions for efficient storage and retrieval of data in the form of arrays. Its ability to store data along with metadata, encompassing location, time, and other relevant information facilitates seamless access, manipulation, and analysis of the stored fields.

However, it is sometimes necessary to use data coming from different datasets to extract their essence and answer scientific questions, whether it is because different instruments were used to acquire the data, or because one wants to focus on a specific region without ignoring a global background field, sometimes with a coarser resolution. Datasets acquired during different campaigns, at different resolutions, and with distinct geographical interests may need to be combined, ensuring both the preservation of global-scale information and the integration of high-resolution localized details. Creating a consistent representation that seamlessly blends global and regional information becomes essential for performing higher-resolution simulations without sacrificing the global context. This also holds for patching multiple satellite images together and creating a smooth global image that contains all the spectral information without introducing any artificial sharp boundaries at the border of the different pictures. The same problem arises when one wants to merge models coming from regional inversions, which allow a finer grid description, and global inversions, which are often described at a coarser resolution due to computing and data availability issues. In geophysics, the issues of multiple scales are important in adaptive mesh refinement (e.g., in the case of mantle convection, see Kronbichler et al. [2012], or seismic tomography [Thrustarson et al., 2020]) and have also been seen increasingly used in patching regional and global models of viscosity variations in studies of glacial isostatic adjustment [e.g., Goldberg et al., 2016, Powell et al., 2021].

In these situations, it is therefore essential to create a tool that accurately performs this type of merging, in order, for example, to perform higher resolution simulations without losing the global information or introducing significant artifacts that would lead to numerical imprecision.

In this paper, we introduce a new package that merges multiscale, multi-resolution geo-referenced datasets. Our package is designed to be flexible, efficient, and user-friendly, providing a simple and effective way to combine global and regional datasets, which can be both observations or models. It relies on the SHTools package [Wieczorek and Meschede, 2018] and the pySHtools wrapper, a Fortran 95/Python library interface that is used for representing geo-referenced datasets in spherical harmonics and performing further manipulation on them, in both the spatial or the spectral domain. To blend smoothly the regional model in the global model, it is necessary to form a localized binary mask associated with a window function that is defined on the sphere. As the traditional spherical harmonic analysis can

suffer from spectral leakage and poor spatial localization, it is therefore challenging to accurately analyze or express data with localized features. PySHtools is specifically implemented to deal with those issues, building on the work which proposed a new framework that combines the benefits of spherical harmonics with a localization mechanism, allowing for precise spatio-spectral concentration [e.g. Wieczorek and Simons, 2005, Simons et al., 2006]. By implementing the "Slepian functions on the sphere" introduced by Slepian [1983], Wieczorek and Simons [2005], it becomes possible to successfully achieve localized spectral analysis, enabling the extraction of detailed information from data on the sphere with improved accuracy and spatial localization [Simons et al., 2006], compared to the approach of boxcar windows introduced by Simons and Hager [1997], which does not optimally concentrate the energy in the window and introduces spectral leakage. This has been used extensively in geodesy, for example in order to address the issue of the polar gap, which refers to the missing data near the poles when representing the Earth's gravitational field using spherical harmonic expansions [Simons and Dahlen, 2006].

Our package relies on this efficient optimization method implemented in pySHtools to build localized, concentrated windows on the sphere, and we believe that it can be a valuable tool for researchers who work with geo-referenced datasets and want to perform high-resolution simulations while keeping the information coming from a global background. We demonstrate the effectiveness and efficiency of the package by merging different datasets at different resolutions and scales.

3.1.2 The case of seismic tomography

The ability to understand the structure of the Earth's interior is crucial for a variety of fields, including geology, geophysics, and natural resources exploration. Since its inception in the 1970s [e.g., Aki et al., 1977, Dziewonski et al., 1977], seismic tomography has evolved into various specialized forms targeting specific aspects of Earth's structure. These include traveltime tomography, surface wave tomography, normal-mode inversions, and their combinations [Romanowicz, 2003]. These tomographic techniques have provided valuable insights into the convective nature of our planet and the large-scale velocity perturbations. Recently, most efforts to obtain such models have been deployed for Full waveform inversion (FWI), which aims to utilize the complete information contained within seismic traces to extract physical parameters of the medium sampled by seismic waves (see Romanowicz [2023] for a recent and complete review on FWI). Each unexplained residual data sample at receivers, originating from a single seismic source, is attributed to a perturbation from an initial model, which can be associated with any point within the medium. By summing the contributions from various sources and receivers, the anomalies in the medium properties can be located, irrespective of the involved phase, via a non-linear optimization problem involving the computation of both the gradient vector and the Hessian matrix [e.g., Pratt et al., 1998].

In this context of FWI, forward wavefield simulations are an essential component for computing the misfit between observed and synthetic wavefields. To this end, Spectral El-

ement Method (SEM) has been the latest preferred way to compute synthetic wavefields for any source, recorded at any receiver (see Chapter 2 for appropriate references) which will be later compared with real data recorded by seismometers. One extremely convenient advantage of SEM is the versatile use of meshing, which allows computing a synthetic wavefield in any geometry, and in any model, regardless of the smoothness of said model and the discontinuities, granted that they are matched by the element boundaries. By embracing the capabilities of SEM, researchers were able to conduct more accurate and comprehensive computations, empowering the creation of sophisticated 3D elastic models across different scales. This breakthrough revolutionized FWI and paved the way for improved resolution in seismic imaging, enabling a more detailed understanding of the deep Earth structure.

In recent years, with a goal of reducing the computational costs of the simulations, hybrid methodologies have been developed to compute forward wavefields in the context of FWI for regional-scale problems using decoupled stations and receivers, as developed in Chapter 2 [e.g., Monteiller et al., 2013, Pienkowska et al., 2021]. However, since regional tomographic models are often obtained at higher frequencies than the surrounding global models, it becomes necessary to find a way to blend these new iterations of regional models within global tomographic models. Furthermore, a naive "cut and paste" approach can introduce velocity jumps at the boundary between the regional and the global model, leading to numerical artifacts in the resulting computed synthetic waveforms.

Recently, Afanasiev et al. [2016] established a computational framework that can effectively integrate seismic data across various spatial scales and a wide frequency range, facilitating the creation of a comprehensive Collaborative Seismic Earth Model (CSEM) that captures Earth's structure at multiple scales. The model's construction involves iterative refinements within subregions and the assimilation of diverse seismic data using a combination of tomographic techniques. Based on the combination of interpolation techniques and neighboring algorithms, the background model, S20RTS [Ritsema et al., 1999] expressed as perturbation with respect to the 1D PREM model, and the different regional models are expanded on an arbitrarily refined mesh. No explicit attempt is made to neither reconcile the different models at the boundaries of each region nor combine the different spectral content. This methodology works within the framework of the resolution of the inverse problem and the global improvement of this composite model is obtained through global scale updates, using long-period data. As the global distribution of seismic data improves on land, it is possible that the future of global models resides in combining multiple, higher-resolution regional models in a global background model. Thus, accurately addressing the merging problems briefly described in the previous paragraph and largely discussed in this paper becomes crucial for the seismic tomography community.

With this in mind, we decided to design this merging package to address those caveats while being independent of both forward and inverse problems, in order to make it as versatile as possible, and potentially use it beyond the scope of seismic tomography. In this specific case though, it can integrate any regional tomographic model within any global background

model in a way that effectively solves the spectral and boundary discrepancies. The resulting model will contain both the longer and shorter period features of the two models, while smoothing the differences that can arise at the boundaries due to the different methods used to obtain those models, making it suitable for use as a starting model for full waveform inversion.

3.1.3 Objectives and outlines

In this paper, we present the implementation of our merging package. We first describe the different stages of the merging process, including pre-processing of the geolocated datasets, spherical harmonics decomposition, and windowing. We show an example in the case of two regional models merged with a global model. We also quantify the errors introduced by the naive "cut and paste" approach and show that our approach results in more accurate synthetic wavefields for use in the context of FWI.

3.2 Package implementation

In this section, we provide the different stages that are necessary to merge a regional model within a global model to perform higher-resolution simulations without losing global information. Our package is implemented in Python and relies on the pySHtools wrapper around the SHTools package [Wieczorek and Meschede, 2018] to perform standard operations around spherical harmonic transforms. It takes the most advantage of the versatility of the netCDF format, but it can also take other formats to store datasets, including plain ASCII files.

3.2.1 Pre-processing of the geolocated datasets

Both the regional and global models can be provided on geolocated reference frames with grids that may not be evenly spaced and could differ in their latitude and longitude definitions. The regional model might span the entire grid with zeros filling areas outside its defined domain, or it may be confined to its specific region. Our first crucial step involves resampling this data onto a sphere in an even manner while considering Earth's geometry. To achieve this, we employ a bivariate spline interpolation method (for more details, see appendix D). This representation allows us to express both the global and regional models on a uniformly sampled grid in latitude and longitude, where longitudes range from $[0, 2\pi]$. The spacing can be different for both models, as long as they are expressed on an even grid, as this grid uniformity is essential for performing the spherical harmonic decomposition of both models. It is to note that if both models are already expressed using a global basis, or if they both already are expressed on regular grids, the resampling step is not necessary. Nevertheless, for utmost versatility, we demonstrate in section 3.3 an example of building a merged model that combines a global model expressed with splines (already decomposed on

a global basis) with a regional model expressed on an irregular grid, thus highlighting the importance of the interpolation step.

To ensure consistency and ease of reconstruction at any depth, we opt to use a B-spline basis to express the radial dimension of our 3D fields. This approach employs the same co-location knots for both regional and global models, ensuring smooth integration across all depths. In cases where the regional model does not cover the same radial extent as the global model, our merging algorithm focuses on the common depth layers, while using the global model for depths where the regional model is not defined. This guarantees a coherent and continuous representation of the merged model.

In the context of regional and global models defined as perturbations relative to a 1D model, ensuring consistency in the constant part of the combined models is crucial. Extracting a 1D model from a region may not yield the same profile as a global 1D model, due to potentially higher velocities in the region compared to the entire surface. To reconcile the constant part (degree 0) of both models, it is necessary to express them as perturbations with respect to the same 1D model. There are two possible approaches here, both requiring the expression of all fields as absolute values rather than perturbations with respect to a 1D model. In the context of seismic tomography, this translates to computing absolute wave velocities.

The first method involves computing absolute velocities only for the regional model and then converting those values into perturbations with respect to the global model. However, if the average velocity in the region is different than the global average velocity at a given depth, the new average of perturbations will not be equal to 0, when integrated on the surface at this given depth. To circumvent this potential issue, the second method requires computing absolute velocities for both the global and regional models and extracting an updated 1D model in such a way that the perturbation integrated and averaged at each depth layer is 0. When the region is relatively small, and the updated 1D model closely resembles the global 1D model, the first method is typically preferred.

3.2.2 Construction of the window function

We first generate a binary mask $M(\theta, \phi)$ that takes the value 1 inside a certain region R on the sphere and 0 outside that region R , such that:

$$M(\theta, \phi) = \begin{cases} 1 & \text{if } r(\theta, \phi) \in R, \\ 0 & \text{if } r(\theta, \phi) \notin R \end{cases} \quad (3.1)$$

Let $W(\theta, \phi)$ be the window function, defined on the sphere.

We assume that the function is band-limited to some maximum degree L . That is, we can express the function as a sum of spherical harmonics up to degree L :

$$W(\theta, \phi) = \sum_{l=0}^L \sum_{m=-l}^l c_{l,m}^W Y_{l,m}(\theta, \phi) \quad (3.2)$$

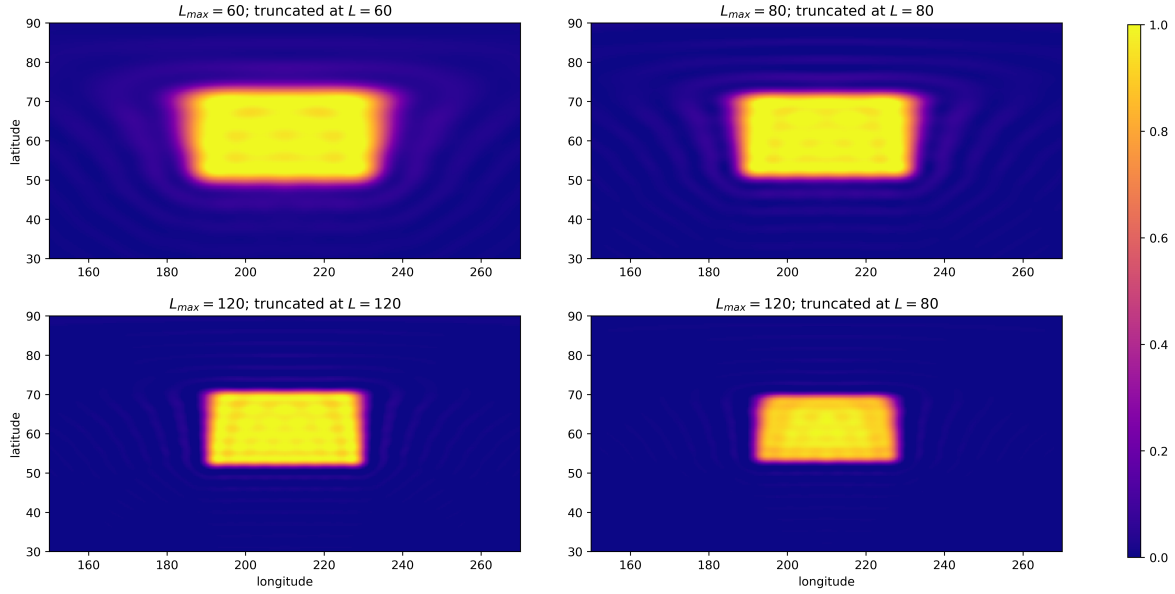


Figure 3.1: Amplitude of the window function W , as we vary the maximum value of expansion of the window function. On the top left, we choose a maximum degree of $L_{max} = 60$, and we represent it as a sum all the way to $L_{eff} = 60$. This yields a very blurred area, and we can observe a lot of ringing outside our region of interest. On the top right, we represent the same thing for $L_{max} = 80$ and $L_{eff} = 80$. The ringing can still be observed, and the window is more concentrated around our region of interest. On the bottom right, we chose $L_{max} = 120$, and $L_{eff} = 120$, which makes the ringing disappear almost completely. However, the values jump from 0 to 1 in a very short spatial area, which will generate sharp jumps at the border between the global and regional models, and nullify the purpose of the smoothing. On the bottom right panel, we chose $L_{max} = 120$, and $L_{eff} = 80$, which has the advantage of keeping a very controlled ringing, while blurring the border between the global and regional models.

where $c_{l,m}^W$ are the spherical harmonic coefficients associated with the window function W , and $Y_{l,m}(\theta, \phi)$ are the spherical harmonics of degree l and order m .

We can compute the spherical harmonic coefficients $c_{l,m}$ using the spherical harmonic transform, as part of the pySHtools package:

$$c_{l,m}^W = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi M(\theta, \phi) Y_{l,m}(\theta, \phi) \sin \theta d\theta d\phi \quad (3.3)$$

However, unlike in the global case, where the data is assumed to be stationary and isotropic, localized regions exhibit varying spectral properties, making traditional global spectral analysis techniques inadequate. Therefore, obtaining the power spectrum estimation of a function, or a field, defined locally on the sphere needs a specific treatment and can not simply consist of multiplying a window function with the spectrum obtained on a global basis. Indeed, a windowed spectral estimate is not only smoothed due to the reduction of high-frequency components but might also be biased because of the interaction between the window function and the data's spectral content. The relationship between an unbiased global spectrum and a regional spectrum can be expressed with a coupling matrix, which relates the power spectrum obtained in the global sphere basis to the power spectrum obtained after applying a windowing or tapering function to obtain a localized estimate. The matrix encodes the influence of windowing on the spectral properties, and it can be asymmetric, leading to biases and distortions in the localized spectrum.

The coupling matrix, denoted as $\mathbf{K}$, is defined as the linear transformation that relates the coefficients of the localized spectrum coefficient $\mathbf{c}^{\text{loc}}$ to the coefficients computed in a global basis $\mathbf{c}$ via the window coefficients $\mathbf{c}^W$ and the triple spherical harmonic product [Meschede and Romanowicz [2015] (see appendix B for exact derivation details)]

$$\mathbf{c}^{\text{loc}} = \mathbf{K} \mathbf{c} \quad (3.4)$$

where the elements of the coupling matrix $K_{l_1, l_3}^{m_1, m_3}$ are given by

$$K_{l_1, l_3}^{m_1, m_3} = \sum_{l_2, m_2} c_{l_2, m_2}^W \int Y_{l_1, m_1} Y_{l_2, m_2} Y_{l_3, m_3}^* d\Omega \quad (3.5)$$

Here, $d\Omega$ denotes the solid angle element on the sphere. l and m correspond to the degree and order of the spherical harmonic coefficients, with 1, 2, and 3 referring respectively to the localized spectrum, window spectrum, and the biased spectrum computed on the global basis.

The coupling matrix $\mathbf{K}$ plays a crucial role in understanding the effect of the windowing and addressing potential biases introduced by that process. Minimizing the coupling in $\mathbf{K}$ becomes essential for accurate and meaningful localized spectral analysis on the sphere and can be achieved by selecting appropriate window functions in order to focus on specific regions of interest while preserving local spectral information.

As proposed by Wieczorek and Simons [2005], we use multitaper windows in order to mitigate the bias introduced by a single window function. Each taper provides an independent estimate of the power spectrum, and their combination reduces the overall bias and improves the spectral resolution. The averaging of multiple tapers reduces the impact of window-induced biases, and the resulting spectrum tends to have a more accurate representation of the underlying spectral content, therefore minimizing the impact of the coupling matrix $\mathbf{K}$.

Defining such a window function is particularly efficient for two datasets whose amplitude does not match at all the boundary, as this might be the case if the regional model and global model were obtained using very different methods. The window function $W(\lambda, \theta)$ applies a smoothing or tapering function to the mask $M(\lambda, \theta)$ to gradually transition between regions with weights close to 0 and regions with weights close to 1. The exact form of the smoothing function depends on the chosen window type and its maximum degree of spherical harmonic expansion. To illustrate this, we show in figure 3.1 how the choice of the maximum expansion degree of the window function L impacts the smoothing at the edges of the region of interest.

As we increase the value of L , the boundaries of the window function in the spatial domain get sharper, making the transition between the global and regional model to be happening on a shorter spatial scale, therefore increasing the possibility of getting sharp jumps. On the other hand, choosing a low value of L and truncating a spherical harmonics expansion at a low degree can lead to the apparition of spectral leakage [Wieczorek and Simons, 2005], which is characterized by overshoots or oscillations near discontinuities or sharp changes in the function. Choosing such parameters would introduce artifacts in the final model, and eventually affect the overall quality of the merging. Another advantage of the multitapered window is that it gradually reduces the amplitude of the window function towards its boundaries, replacing the abrupt truncation with a smoother transition in the spectral domain. This effectively reduces the high-frequency components that would cause spectral leakage.

One way to obtain a smoothed geographical transition, without introducing Gibbs phenomena is to initially expand our mask M to a higher degree L_{max} , typically equal to 120, and then use this expansion to a degree $L_{eff} < L$ in order to generate a geographical smoothing of our choice, while keeping the high accuracy of the localized spectra. This is what we show on the lower right panel of Figure 3.1. This way, the window function is effectively designed to attenuate the contributions of the regional model gradually as we move away from the region of interest, eventually reaching zero influence in regions outside the defined domain. We can also observe how the energy of the window function is effectively contained within the region of interest, thanks to the spectro-spatial localization [Simons and Dahlen, 2006], and does not leak uniformly on the rest of the sphere. Overall, the values of the regional model are left untouched within our target region, while the global background model does not experience significant changes, should L_{max} and L_{eff} be chosen wisely.

3.2.3 Application of the window function

Once the windowing coefficients are computed, we transform them back to the spatial domain to obtain the window function. To preserve the amplitude of the data when applying the window function as described in the next section, it is important to normalize the window function's values and divide by the maximum energy across all the degrees and orders. We then multiply that function by the regional dataset in the spatial domain. Finally, we compute the "unbiased" multitapered spectrum of the resulting product [Meschede and Romanowicz, 2015, Wiecek and Simons, 2005]. In the spectral domain, we add the spectrum of the global model in which we wish to merge the regional model. As shown in Figure 3.4, the rapid decay of the global model combined with the low energy in the low degrees of the regional model allows us simply sum the two contributions, without the need to further smooth their connection.

Outside of the region of interest should be the unchanged global model, unless the window function expansion parameters are not chosen optimally in order to minimize spectral leakage.

3.2.4 Implementation details

To summarize, the implementation is as follows:

- Reading a parameter file that specifies the geolocated files containing the datasets, the variables to merge, the region's location, and the degree of smoothing at the edge of the window.
- Reading in the regional and global model, either from a netCDF format or another user-defined format.
- Pre-processing the fields by re-interpolating them on an evenly spaced grid in latitude and longitude.
- Reconcile degree 0 of both models by expressing the chosen fields as perturbations of a common 1D model (typically the 1D model of the global dataset).
- Computing the Spherical Harmonics expansion of both fields, respectively $c_{l,m}^{glo}$ and $c_{l,m}^{reg}$.
- Constructing a mask using a specified longitude/latitude region.
- Computing the multitaper windows, and their corresponding Spherical Harmonics coefficients $c_{l,m}^W$ from the geographical mask, with a maximum expansion degree L_{max} .
- Normalizing W from 0 to 1, in order to conserve the energy of the system.
- Expanding the window function in spatial coordinates and applying it to the regional model by multiplying both fields in the spatial domain.

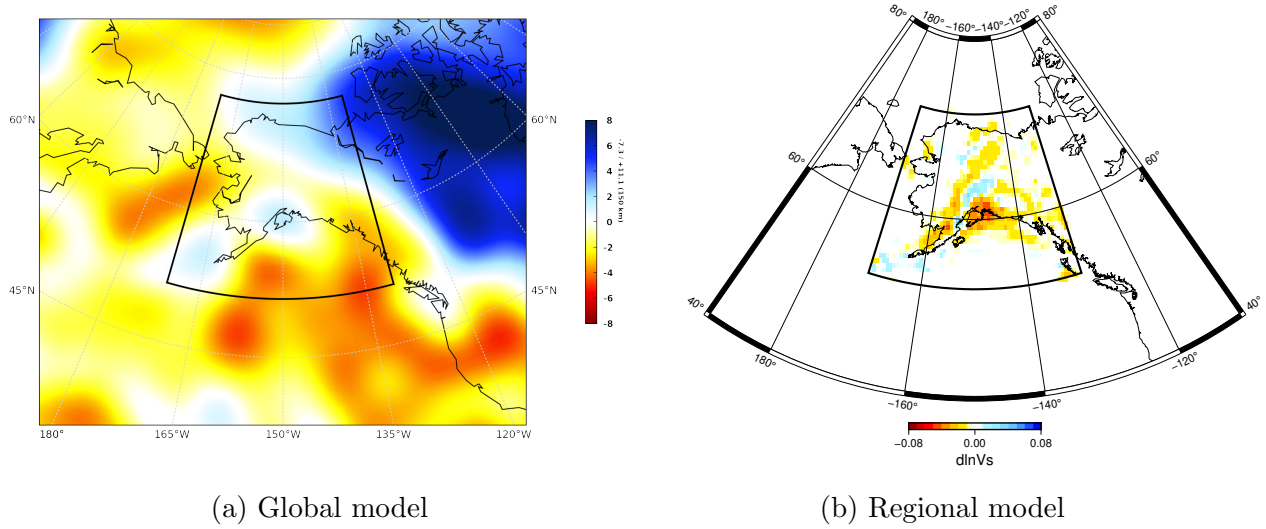


Figure 3.2: Alaska initial model at 150km depth. On the left panel a slice of SEMUCB at 150km depth, centered around Alaska. On the right panel the regional model of Alaska as described in section 3.3.1. The regional model has much more sensitivity than the global model, as expected, and we note that the slab in our image appears more sharply defined than on the global model. we also observe the low velocities associated with the Yakutat terrane, which can only be guessed on the global model at this depth.

- Computing the multitaper-ed estimation of the unbiased spectrum of the windowed regional model and summing the obtained spectrum with the global model spectrum.
- Expanding the merged model in the spatial domain and writing it out for this depth.
- Iterating over all the depths.

Since each depth layer is independent of the other, the code is executed in an embarrassingly parallel fashion to generate a complete merged model in the same amount of time it takes to compute just one layer. The computation time will vary depending on the sharpness of the window, and the shortest wavelengths in your regional model, although the order of magnitude of computing time necessary to produce a full mantle model never exceeds a few minutes.

3.3 Results

3.3.1 Models setup

We apply this method in the context of seismic tomography, to merge a regional model of shear wave velocity of Alaska [Roecker et al., 2018] in a global tomographic model SEMUCB [French and Romanowicz, 2014], in order to run synthetic seismogram computations. For illustrative purposes, we later present a merged model of the regional CANVAS model [Doody et al., 2022], a model of shear wave velocity of California and Nevada, into SEMUCB as well.

Regional model

Alaska The Alaska regional model [Roecker et al., 2018] has been constructed using travel-time tomography to constrain V_p and V_p/V_s models in a region that extends from $52^\circ N$ to $71^\circ N$ in latitude and $130^\circ W$ to $170^\circ W$ in longitude. The inversion was carried out using arrival times of locally and teleseismically recorded body waves. 3500 local events with reported magnitudes $M > 2$ and 269 teleseisms with $M > 6$ (Fig. 3) were used which resulted in 347,682 P and 136,898 S wave arrival times. In setting up the joint inversion, we parameterized the subsurface by specifying P and S velocities on a 3D grid of nodes with a resolution in all dimensions of $\sim 10\text{km}$. A slice at 150km depth of this model is shown in Figure 3.2b.

Western US CANVAS [Doody et al., 2022] is an adjoint waveform tomography model focused on California and Nevada, with an emphasis on resolving the uppermost mantle below this region. The model utilizes a dataset of 103 events, whose magnitude is comprised between $M_w = 4.5-6.5$, recorded by over 1300 unique stations over a 20-year period. CANVAS iteratively refines the model over 6 period bands, gradually reducing the minimum period from 30 seconds to 10 seconds.

Global model

SEMUCB-WM1 [French and Romanowicz, 2014] is an FWI model constraining V_s and radial anisotropy for the full mantle. It uses a spectral element method solver to compute accurate synthetic seismograms up to 32s period, and a method based on perturbation theory of normal modes to compute the partial derivatives (see French and Romanowicz [2014] for full implementation details). A slice of SEMUCB, centered around the Alaska region is shown in Figure 3.2a

The methodologies employed to obtain those models are all distinct, involving the use of dissimilar wavepackets, frequency bands, and techniques (travel time and full waveform). This yields different lateral and vertical parametrizations, and 1D background models (degree 0 of the spherical harmonic expansion), which need to be taken into account in the subsequent

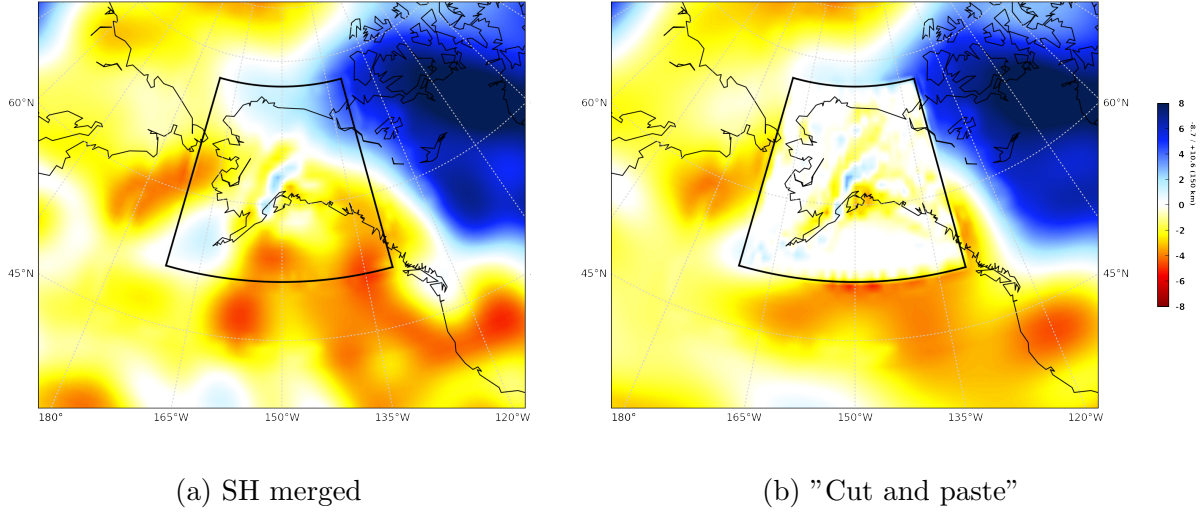


Figure 3.3: Merged models for the Alaska region of interest. On the left panel, a slice of the SH merged model at 150km depth, centered around Alaska. On the right panel is CP merged model, centered on Alaska at 150km depth. We note that the SH model visually contains both the long wavelength information from the global model and the higher resolution highlighted by the regional model. On the boundaries, no sharp jumps are observed. The slab in the SH figure still appears more sharply defined than in the global model, and the features of the Yakutat terrane are visible as well. The CP model contains a lot of sharp jumps at the boundaries of the region of interest, and there is visually no continuity outside the target region and inside of it. For the SH model, the regional model was re-expanded as absolute wave velocities, before expressing those absolute velocities as perturbations with respect to the global 1D model.

merging. Furthermore, given the different frequency content of regional and global models, substituting in the regional model would also cause frequency discrepancies. Consequently, if the regional model were substituted for the global model, there would be no direct correlation at the boundaries, neither in the spatial nor in the spherical domains.

Merged models

The first merged model involves directly inserting the regional model into the global model, replacing the information in the global model at those locations without any specific adjustments at the border (we call it the "cut and paste" (CP) merging style), for which a slice at 150km depth is shown in Figure 3.3b. We then create a model that is merged according to the spherical harmonics methodology described in this paper (designated hereafter by "SH"), for which a slice at 150km depth is shown in Figure 3.3a. We can observe how the

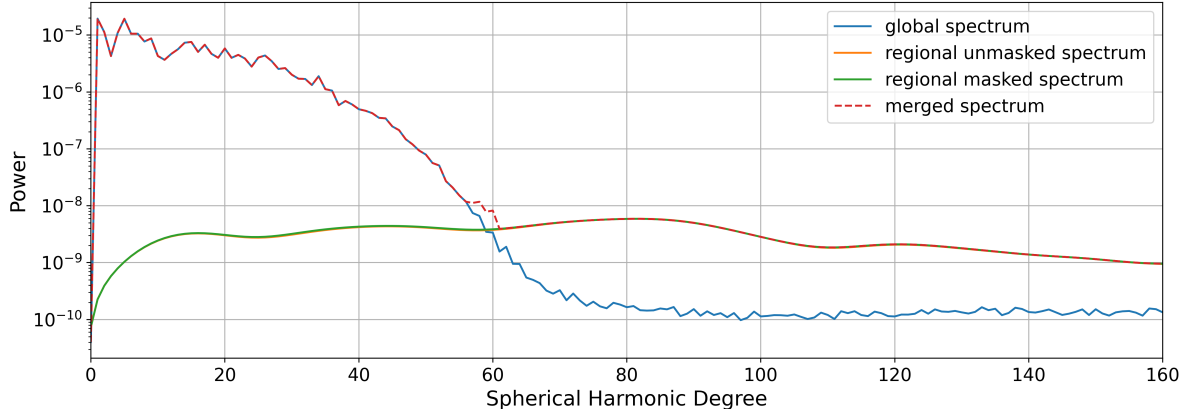


Figure 3.4: Power amplitude as a function of spherical harmonic degree for merged, global, regional models, and the window function are denoted by the blue, orange, green, and red solid lines, respectively. Those spectra were computed for the region of interest, at a depth of 150km.

CP model presents sharp boundaries at the border of the region, where the SH model is completely smooth, transitioning to the higher resolution part of the model without any velocity jumps. Also, the CP model is completely oblivious to the long-wavelength structure of the global model, for example, the high-velocity structure in the North-East of the region, or the low-velocity structure in the South-East of the target region. This is illustrated by the spectra of all models represented in Figure 3.4. This figure shows that the merged power spectrum contains the spectral information of the global model at the lower degrees (long wavelength) until the regional model’s spectral content picks up more amplitude and is incorporated in the resulting merged model around degree 60.

In the next section, we assess the efficacy of the merging process, by first selecting an event and a distribution of synthetic stations to achieve an ideal azimuthal and distance coverage. This enables us to investigate any differences that arise due to the merging process and whether any spurious wavepackets emerge due to artificial velocity jumps at the boundary of the region. We set the event and the stations outside the region and allow the wavefield to propagate through the region to study its effects. The setup of this first experiment is shown Figure 3.5. We then use a real event and a realistic distribution of stations to assess the performance of our merging algorithm in the context of realistic seismic inversion.

3.3.2 Synthetic test

We are utilizing the wave propagation solver SPECFEM3D_Globe [Komatitsch and Vilotte, 1998, Komatitsch and Tromp, 2002] to compute the acceleration wavefield (as the second

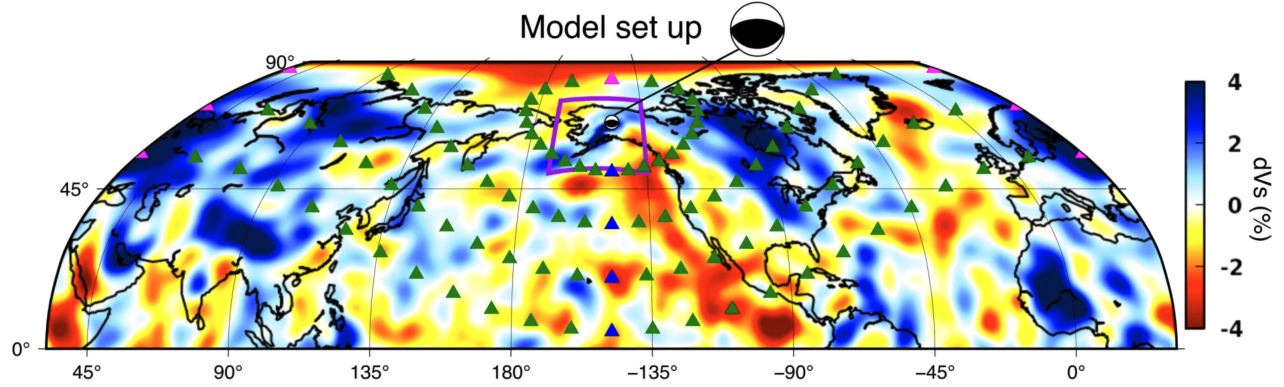


Figure 3.5: Test setup in merged models, with a synthetic source in Alaska and synthetic stations regularly placed at 15, 30, 45, and 60° source-receiver distances for a range of azimuths. The source is located inside the region of interest, represented by its beach-ball diagram. Stations at azimuths of 0 and 180° are colored pink and blue, respectively, while all other stations are green. The target region is represented here by the purple box. The background represent the velocity perturbation in the merged model at 250 km depth.

derivative of the displacement field, with respect to time) from our remote source to the distant receivers in three distinct models: (1) CP (2) SH (3) Global SEMUCB. We consider ellipticity, topography, and a 3D crust, in order to achieve the highest possible simulation accuracy. The seismograms of the synthetic data were generated for a bandpass between 16 and 400 seconds. All simulations were conducted under the same settings, with the only difference being the 3D velocity model.

The synthetic seismograms obtained from the three distinct models exhibit little variation in body waves, except for very short distances ($\Delta \approx 15^\circ$), as depicted in Figure 3.6. However, synthetic seismograms computed in the CP model demonstrate significant differences in phase and amplitude at later arrivals, particularly surface waves, sometimes resulting in anti-correlated signals, as compared to the global model or the SH merged model. On the other hand, the global model and the SH merged model remain consistent throughout all distances and azimuths.

Furthermore, we observed the emergence of new phases in the traces propagating through the CP model, such as at 2000 seconds for $\Delta \approx 60^\circ$. These additional phases are due to the sharp velocity discontinuities at the boundary of the region, which scatter the wavefield energy, generating spurious wavepackets that are not associated with any physical signal.

Additionally, it appears that there is a strong resonance with surface waves, as the amplitude of the coda waves greatly differs for larger distances.

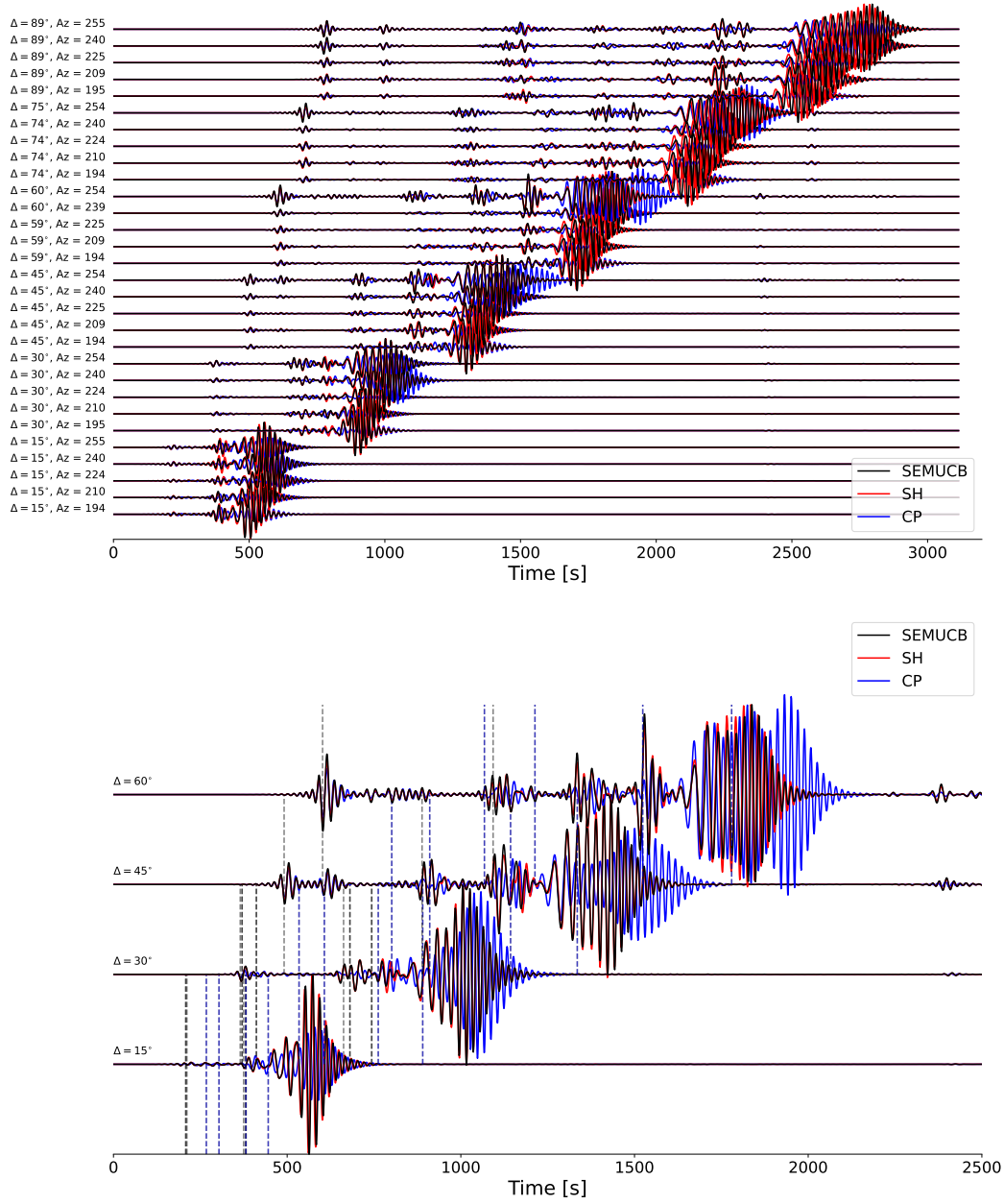


Figure 3.6: Synthetic seismograms calculated using SPECFEM3D Globe, comparing the global model (black) to the CP model (in blue) and the SH model (in red). They are displayed as a function of distance from source to receiver. The upper panel shows them at different azimuths, at distances ranging from 15° to 90° . The lower panel shows specific examples at 4 distinct distances, to display the discrepancies introduced by the "cut and paste" model, compared to simulations in a global model or merged with our methodology. Simulations are run at a minimum period of 16s.

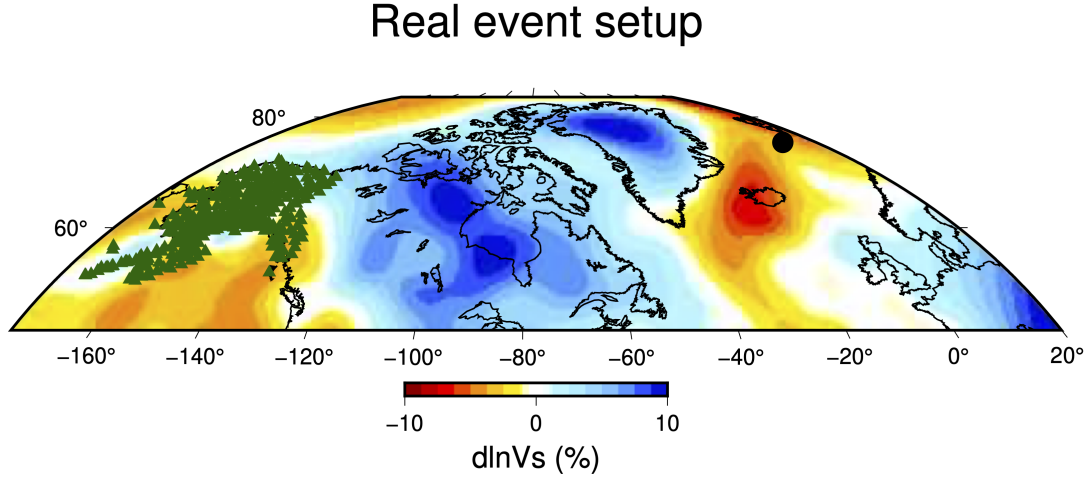


Figure 3.7: Real setup for merged models, with a real source in the Greenland Sea and existing stations located in Alaska. The source is located far from the region of interest and is represented by the black circle. Stations are depicted in dark green. The background shows the velocity perturbation model at 250 depth.

3.3.3 Test with real data

In the next stage of our study, we evaluate the effectiveness of the merging code by applying it to a real event with a corresponding distribution of seismic stations. Specifically, we compare the observed data against two models: the CP model and the SH model. The aim is to assess the impact of computing combined spectra in cases where the models roughly agree at the border. For this evaluation, we utilize data from a real earthquake event with a magnitude of $M_w = 5.7$ that occurred in the Greenland Sea in August 2018. The seismic data were recorded at stations suitable for tomographic inversion of the mantle structure beneath Alaska. Synthetic seismograms are computed at a minimum period of 25 seconds to maintain a reasonable computational cost for future tomographic inversion, although additional earthquakes and iterations would be required.”

We then subject the resulting synthetic waveforms from this event to an automatic picking algorithm, which relies on arrival time predictions and energy analysis around these arrival times. The picking, which automatically determines the starting and ending point of various wavepackets considers a few metrics to compare data and synthetic seismograms, such as the correlation coefficient, and the quality of the data by evaluating a signal-to-noise ratio. This process also ensures that the phase of the synthetic wavepackets is close enough to the phase of the real data, in order to avoid cycle-skipping issues. Therefore, comparing the picked data from the SH or the CP model allows us to determine whether the merging process alone was sufficient to pick more data that can be used for inversion. The results, summarized in Table

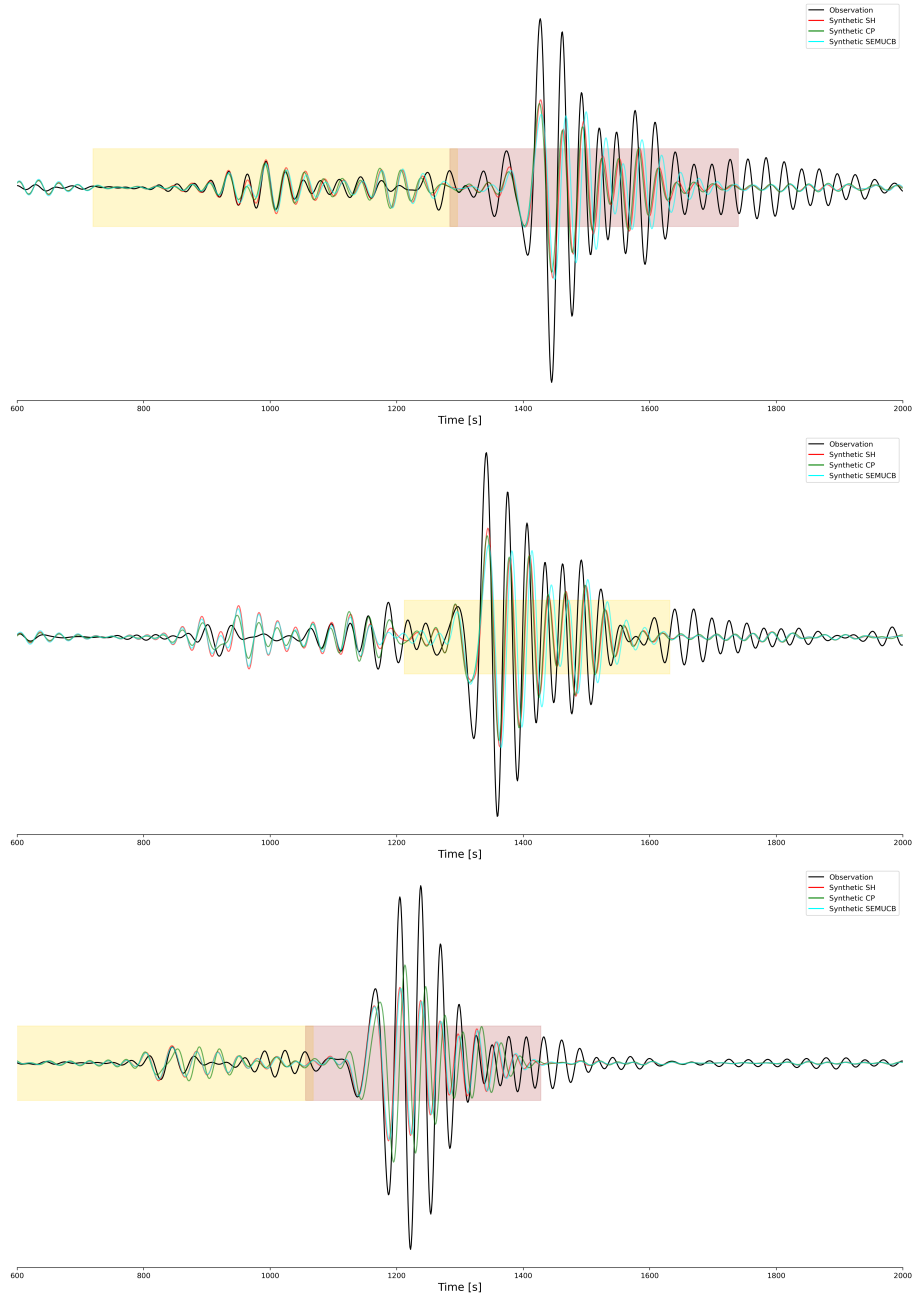


Figure 3.8: Three examples of wavepackets that were picked in the SH model, and which were not in other models. All synthetic seismograms calculated using SPECFEM3D Globe ran at a minimum period of 25s. (*Continued on the following page.*)

Figure 3.8: In all of these figures, we look at the Z component, the black line corresponds to the real data, the red, green, and cyan traces are the synthetic waveforms computed in SH, CP, SEMUCB, respectively. The colored boxes correspond to the extent of the wavepackets picked by the algorithm. All wavepackets considered here are surface waves, with the later arrival being the fundamental mode, and the earlier arrival being an overtone. The distances between the source and receiver are 49° , 46° , and 41° for the upper, middle and lower panel, respectively.

3.1, reveal a significant increase (around 15%) in the wavepackets picked by the automatic algorithm for this event, across all three components, with the most substantial improvement observed in the vertical component. This increase in picked waveforms indicates that without altering the starting models, the SH merged model better explains the "true Earth" compared to a naive approach. The increase number of picked wavepackets is accompanied by a slight increase in the average correlation between the synthetic wavepackets and their real data counterpart. Moreover, the absence of spurious wavelets generated by sharp boundaries suggests that the signal is not contaminated, and future inversions will not optimize to accommodate these artifacts, leading to faster convergence.

Table 3.1: Number of wavepackets picked in models computed with different methods of merging, in the three different components of the computed seismograms. R stands for the radial component of the ground acceleration, T stands for the transverse component of the ground acceleration, and Z corresponds to the vertical component of the recorded acceleration. The last three lines of the table show the average correlation coefficient between the synthetic seismogram computed in a given model with the data in the picked wavepackets.

Model	# R picks	# T picks	# Z picks	Total
SEMUCB	510	449	519	1469
CP	495	506	557	1558
SH	550	531	625	1706
Difference SH/CP (%)	+11.1	+4.9	+12.2	+9.5
Difference SH/SEMUCB (%)	+7.8	+18.3	+20.4	+16.1
Average correlation SEMUCB	0.66	0.63	0.62	0.64
Average correlation CP	0.68	0.65	0.61	0.65
Average correlation SH	0.69	0.68	0.62	0.66

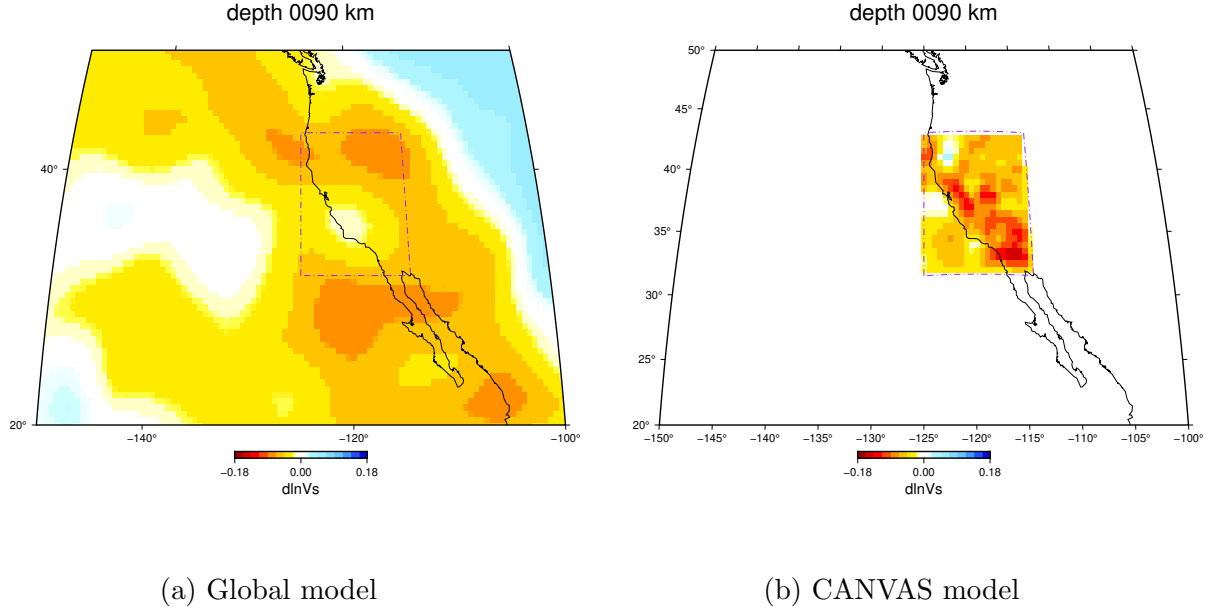


Figure 3.9: Map view of the initial models for a test around California and Nevada at 90km depth. On the left panel a slice of SEMUCB at 90km depth, centered around California and Nevada. The boundaries of the target region are shown on both panels as the purple dashed line. On the right panel is the same slice for the CANVAS model. The regional model has much more sensitivity than the global model, just like the Alaska example in Figure 3.2.

3.4 Discussion and Perspectives

We have illustrated here the importance of merging a global and a regional model in the context of seismic tomography. In the case where multiscale models are to be used, we have shown that the way of merging them can introduce significant biases, independent of the inversion process. A naive and direct way to do so leads to, at best, fewer wavepackets being used for the inversion, and at worst, spurious wavelets that can be interpreted in terms of seismic structure which can change the overall interpretation of the model. This is particularly important in the case of FWI, which uses the entire signal contained in the seismograms, including the coda, which we observed to be ringing in the case of the model being poorly merged, as shown in Figure 3.6. In the case of Alaska, we see that the CP model introduces significant ringing in the coda, but also on the body waves, especially at larger distances, which would, without a doubt become problematic in the context of inversion, since the inversion will attempt to introduce velocity structure into the model that fits these artifacts. Consequently, by using a merging approach that retains information across wavelengths and does not impart sharp boundaries, it is possible to accelerate the convergence of the inversion process and save computational time, without changing anything to the inversion methodology.

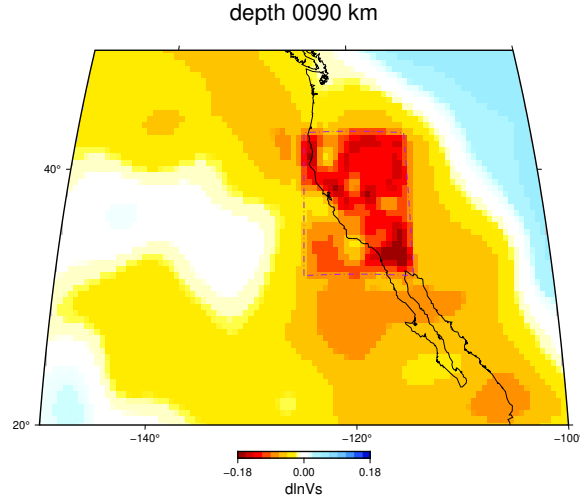


Figure 3.10: Merged models for California/Nevada target region. Map view of a slice of the SH merged model at 90km depth, with the boundaries of the target region being depicted in a purple dashed line. We note that the SH model visually contains both the long wavelength information from the global model and the higher resolution highlighted by the regional model. On the boundaries, the sharp jumps are smoothed by the window function, but the difference in amplitude between the global and regional model makes the transition between the regional and global model rougher, especially on the West end of the region. The transition is better handled in the East boundary. The absence of a long-wavelength structure from the global model in the target region did not generate any artifacts.

Merging models in the spectral domain allows to smooth the transition at the border between the global and regional model, as we have seen in Figure 3.3a. This is valid, independent of the method used to construct it. However, if the amplitudes are too different between the two models that are to be merged together, the contrast can still be too sharp to be smoothed over spherical harmonic windowing. This is the case where we merge the CANVAS regional model 3.9b, centered on California, with SEMUCB, shown centered on California and a depth of 90km in Figure 3.9a. The high number of iterations, combined with the large dataset of local and regional earthquakes used to construct it led to a much higher amplitude of velocity perturbations than in the global model (there is a ratio of 2 between the highest amplitudes in absolute value between the two models). Combined with the absence of structure in the same region in the global model, it becomes difficult to ensure the absence of a velocity jump, as we can see on the West boundary of the merged region, in Figure 3.10. In this case, the region is relatively tiny ($\approx 10^\circ \times 10^\circ$), and lowering the spherical harmonic expansion of the window function, which would have the effect of blending the sharpness of the regional model on a larger spatial distance, could have the unintended consequence

of smoothing the high-resolution structure of the regional model to the point where the advantage of using a better-defined model could be lost. It is possible to overcome it, by choosing a more judicious location for the target region, or a bigger one. In such cases, where the regional model might incorporate information and energy in the lower degrees using a priori information such as an initial global model, it might be useful to treat the summation of the global with the regional spectrum, which works in our Alaska case, differently. For instance, it could be interesting to consider the model that shows the maximum amplitude at such low Spherical Harmonic degrees or taper out the long wavelength information from the regional model in the same way we have defined our window function.

Recently, more hybrid methodologies have been developed in order to lower the computational cost of forward modeling [e.g. Pienkowska et al., 2021, Leng et al., 2020, Adourian et al., 2023], which consist of discriminating the wave propagation between inside the target region and outside of it, in order to further refine the regional model. This package is a good tool to generate the initial model in which to compute the first iteration of synthetic seismograms. Furthermore, the development of more finely resolved regional models, following the CSEM initiative [Afanasiev et al., 2016, Fichtner et al., 2018] could benefit from using this package, as one can use as many windowing functions as one wants, thus enabling the merging of multiple regional models within a global model, at no significant computational cost.

More generally, we have shown that merging models in the frequency model not only takes care of the sharp discontinuities that could arise at the boundaries between the regional and global model but also smoothly incorporates the longer wavelength structure of the global model into the region of interest. This goes beyond the interest of seismic tomography alone. Climate sciences often use multiscale grids to study a localized or regionalized phenomenon [see for example Fildier et al., 2021], and this package could also be useful for the community of atmospheric and climate science. Finally, all data acquired on a grid, either at surface or not, could also benefit from using this package, in order to accurately and smoothly concatenate the data from multiple acquisition campaigns.

3.5 Conclusion

We have presented the usefulness of a user-friendly, computationally inexpensive, merging procedure for multiscale, multiresolution, geo-referenced datasets. We believe that this package could be of good use outside the context of which it was developed, which was seismic tomography. The versatile implementation allows to take as an input netCDF, or ascii gridded formats, but adding any type of format would not be an immense task. It is freely available at <https://github.com/SevanAdourian/TomoMergeModel>.

Chapter 4

The sensitivity of the Six-Year length-of-day oscillation to the “geoid-at-the-CMB”

Large Low-Shear Velocity Provinces (LLSVPs), as revealed by global tomographic models, correspond to two large-scale ($\sim 10,000$ km) slow velocity anomalies in the deep mantle, rooted at the Core Mantle Boundary (CMB), one beneath Africa and the other beneath the Pacific Ocean. Their lateral extent is relatively well-constrained and consistent across many studies [Lekic et al., 2012]. However, seismic waves are relatively insensitive to the buoyancy structure in the deep Earth, and it is, to this day, unclear if the LLSVPs are produced by a purely thermal effect, or a compositional effect, both resulting in opposite buoyancy fields. In order to understand the full force balance of the mantle, the buoyancy of the LLSVPs must be constrained.

Recently, geodetic constraints on small fluctuations in the length-of-day (LOD) that occur over a period of ~ 6 years have been improved [Ding and Chao, 2018]. This six-year oscillation (SYO) in LOD has been suggested to be produced by a gravitational coupling between the inner core and lower mantle [Buffett, 1996]. Buffett [1996] introduced this process and estimated variations in LOD of approximately 3 years, based on buoyancy structure of the mantle was based on the assumption of purely thermal heterogeneity Forte et al. [1994]. Since, new constraints of Earth’s deep mantle buoyancy have been made and in light of this, we revisit this mechanism to understand if these new constraints yield an oscillation period that is closer to the observed data and conduct a systematic sensitivity analysis of this process. In addition, we extend the theory so that the oscillation period may be predicted based on perturbations in CMB topography. Within the framework of Buffett [1996], we compute 1D, depth-dependent sensitivity kernels for the SYO relative to long wavelength density anomalies. We show that this sensitivity is broad across the mantle but peaks at the CMB. It also holds a unique sensitivity to CMB topography. Unlike other observations used to probe deep mantle buoyancy (e.g., seismic normal modes [Ishii and Tromp, 1999,

Moulik and Ekström, 2016] or body tides [Lau et al., 2017]), there are no trade-offs with elastic properties of the Earth. Therefore, we conclude that the SYO may be an additional constraint to evaluate whether the inferred LLSVPs models derived from seismic tomography or global geodynamics are consistent with this independent geodetic observation. In the discussion, we explore the possibility to reconcile the different hypotheses on the cause of the SYO and the potential effect of the mantle inner core gravitational coupling exciting torsional waves in the outer core.

4.1 Introduction

Geodynamics seeks to understand the underlying physical processes that govern the evolution of the Earth’s interior, including its heat budget, the dynamics of mantle convection, and the formation and evolution of its deep-seated structures. One class of these structures is the Large Low-Shear Velocity Provinces (LLSVPs), or Large Low-Velocity Provinces (LLVP) [Koelemeijer, 2021], which represent two of the largest and most enigmatic features in the Earth’s mantle. In global shear-wave tomography models, the LLSVPs robustly imaged regions of the deep mantle characterized by anomalously slow seismic wave velocities compared to the surrounding mantle [McNamara, 2019, Lekic et al., 2012, Garnero et al., 2016]. They extend from the CMB up to approximately 1000 km above and have been observed beneath Africa and the Pacific Ocean. Given their velocity properties, they were first discovered with shear wave tomography models.

While their existence is observed throughout many tomographic models [Lekic et al., 2012], the nature of LLSVPs remains uncertain, and multiple competing hypotheses have been proposed to explain their characteristics. Key observations include their distinct boundaries in terms of elastic properties [Ni et al., 2002], the anti-correlation between shear-wave and bulk sound velocities [Masters et al., 2000, To et al., 2005], and the presence of numerous hotspots above them have even led to the idea that mantle plumes could be originating from LLSVPs [e.g., Garnero and McNamara, 2008, Davaille et al., 2002]. While the former two might point to a thermochemical origin, e.g., in an enrichment of iron [e.g., Kellogg et al., 1999], and thus a negative buoyancy, the latter, with might point to a thermal origin, whereby hot anomalies produce the slow-down in seismic wavespeed [e.g., Davies et al., 2012]. Both result in conflicting pictures of mantle buoyancy.

As such, hypotheses for the source of LLSVPs can be broadly categorized by two endmember scenarios, though realistically, the LLSVPs likely fall somewhere in between: thermal (or effectively isochemical) and thermochemical. Effectively isochemical models assume that convection is driven solely by thermal buoyancy, while compositional heterogeneity may exist but does not actively drive convection [Bunge et al., 1998]. Under this assumption, the resulting mantle plumes are thought to be characterized by thin and clustered conduits but appear larger when imaged due to smoothing introduced by seismic tomography [Davies et al., 2012].

Thermochemical models, on the other hand, propose that both thermal and compositional buoyancy contribute to convection, leading to a range of dynamic possibilities [Garnero and McNamara, 2008]. These hypotheses suggest that LLSVPs have distinct compositions from the surrounding mantle and can be further categorized based on their time-averaged buoyancy and the extent to which they interact with the surrounding mantle. Such hypotheses tend to be favored by geochemical analyses of mantle-derived rocks which consistently shows long-lived heterogeneity within the mantle [e.g., Hofmann, 1997].

By employing tidal tomography techniques and applying Global Positioning System (GPS)-based measurements of semi-diurnal body tide deformation, Lau et al. [2017] constrained the deep-mantle buoyancy through a probabilistic approach, revealing that the lower two-thirds of the LLSVPs are characterized by negative buoyancy with values of excess density $\mathcal{O}$ 0.5 %. On the other hand, Koelemeijer et al. [2017] have analyzed the splitting of Stoneley modes, highly sensitive to the lower mantle, and concluded that the observed pattern was better explained by a lighter-than-average overall density of the LLSVPs. It is important to note that, splitting functions of Stoneley modes, when treated in the context of single coupling as is the case for their study, can lead to significant errors in the interpretation of the results [Robson et al., 2022]. Romanowicz [2017] suggested that the reduced sensitivity of Stoneley modes coinciding with the CMB may be where the excess density required to fit tidal data lies. Subsequently, Richards et al. [2023] tested this idea and found that such a confined configuration of excess density in the lowermost 100 km of the mantle was able to reconcile a variety of geodynamic, Stoneley mode, and tidal data. Thus, it is clear that the distribution of density within the LLSVPs is now at the heart of what must be further explored.

Another way to investigate the buoyancy structure of the LLSVPs is to examine their effects on the Earth’s rotation, manifested in changes in LOD [Chao et al., 2014]. These fluctuations, spanning time scales from days to years, now exhibit variations on the order of milliseconds, with current values reaching a precision of 0.02 ms [Abarca del Rio et al., 2000]. These LOD variations, particularly on interannual timescales, are of significant interest here as they may reflect changes in the rotation rate and angular momentum of the Earth’s mantle. While LOD variations at different frequencies have been correlated with atmospheric angular momentum at various frequencies, an observed LOD oscillation with a period of approximately 6 years [e.g., Ding and Chao, 2018] remains unexplained by known angular momentum exchanges with the atmosphere, oceans, and continental water reservoirs [Mound and Buffett, 2006]. Two hypotheses, the Mantle-Inner-Core Gravitational coupling (MICG) [Buffett, 1996, Mound and Buffett, 2006] and the torsional mode in the fluid outer core [Dumberry and Bloxham, 2006], have been proposed to explain the six-year oscillation (SYO). The MICG mechanism, associated with inner-core superrotation, has been a subject of debate due to the required strength to transfer angular momentum between the core and mantle through gravitational coupling. Recent developments in the MICG dynamics have further explored the sectorial quadrupoles of the MICG system, contributing to the Axial Torsional Libration (ATL) of the inner core [Chao, 2017]. In their proposed mechanism, the

precise period of the SYO is directly affected by spherical harmonic degree two and order two variations in the gravitational potential at the CMB. As the LLSVPs have strong degree 2 and degree 3 components [Lekic et al., 2012], the precise SYO period could be used as an independent geodetic observation to provide insights into the LLSVPs.

In this chapter, motivated by both more precise constraints on the period of the SYO [Ding and Chao, 2018] and new ideas on LLSVP buoyancy [Lau et al., 2017, Koelemeijer et al., 2017, Richards et al., 2023], we conduct a sensitivity analysis of the SYO period under the assumption of the MICG mechanism to evaluate whether they hold any promise as a tool to constraining LLSVP buoyancy structure. We show that the period of the SYO is directly sensitive to long wavelength density anomalies that peak at the base of the mantle and to long wavelength CMB topography. Thus, we believe that this observation may be used as a complementary constraint that any long wavelength buoyancy model of Earth’s deep mantle must conform to.

4.2 A Conceptual Description of the MICG Mechanism

Before describing the theory used to predict the precise period of the SYO, as driven by the MICG mechanism, we briefly describe the mechanism conceptually. The solid components of the Earth, i.e., the mantle and the inner core, approximately rotate synchronously. However, the presence of the fluid outer core provides a strong means to decouple their rotation. The MICG mechanism is one means by which a coupling between the mantle and the inner core could be enhanced. In this scenario, Buffett [1996] proposes that lateral buoyancy structure at the base of the mantle imposes a gravitational force down to the inner core. If the inner core viscosity is low enough, which Buffett [1996] argues is the case, the inner core’s shape would adjust to the perturbed potential on time scales that are short enough for the SYO. In the following, we focus on the spherical harmonic degree-two order-two density structure of the mantle, as Buffett [1996] did, but augment this with core-mantle boundary perturbations in the same harmonic. If the potential projected down to the inner core boundary is sufficient to produce a large enough change in the inner core’s shape, then such an elongation could produce a redistribution of angular momentum such that Earth’s length of day is slightly modulated.

4.3 Theory

In this section, we derive kernels associated with the SYO period that are caused by the gravitational coupling of the inner core (IC) and the mantle. Buffett [1996] defines the

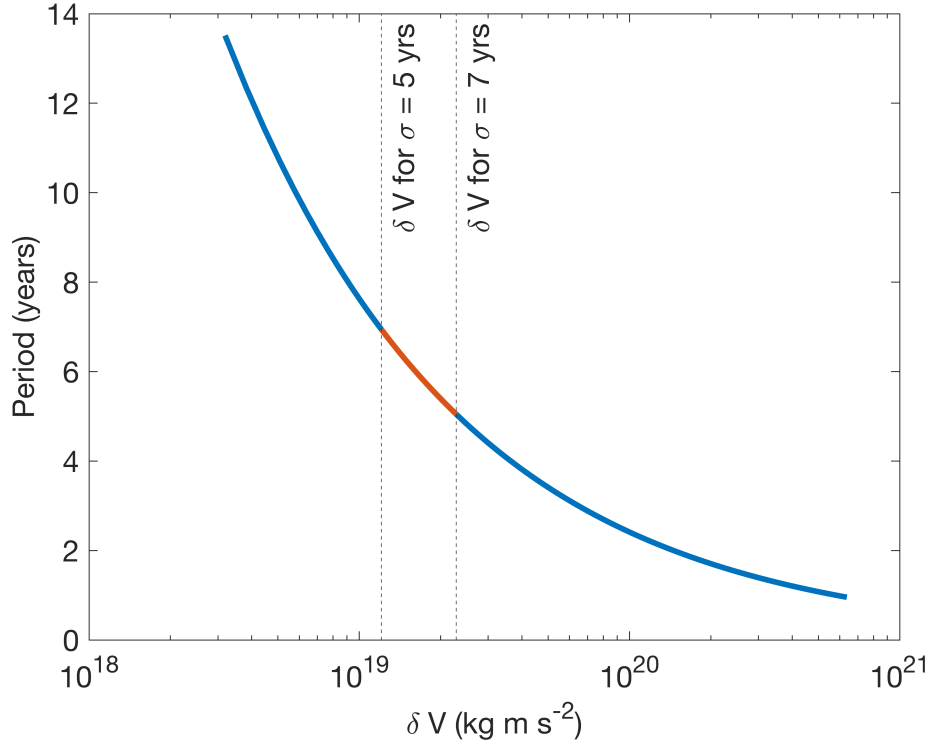


Figure 4.1: Changes in LOD period associated with MICG mechanism as a function of δV . The line segment in red corresponds to the values of δV that would result in SYO periods of 5 to 7 years, within the observation range of Ding and Chao [2018]

oscillation period, σ , as

$$\sigma^2 = 4 \delta V C_s^{-1} \left(1 + \frac{C_s}{C_m} \right), \quad (4.1)$$

where V is the gravitational energy, C_s and C_m are the polar moment of inertia for the inner core and the mantle, respectively. Their values are considered well-constrained, given our understanding of the 1D model of the Earth [Sikdar and Dumberry, 2023], and computed in PREM [Mathews et al., 1991]. δV corresponds to the perturbation to the gravitational energy due to structural lateral variations of density. Under these assumptions, δV is the only unknown variable in the computation of σ , we can compute the acceptable range for δV such that σ has a period between 5 and 7 years (Fig. 4.1)

Our goal is to relate δV to density perturbations within the lower mantle. We express such variations in spherical harmonics. In contrast, we consider the inner core to be radially stratified, i.e. that the core does not present lateral density perturbations. This assumption is largely valid since 1D profiles of seismic wave velocity and density throughout the core

are consistent with well-mixed iron and lighter element structures Olson [2015]. With this approximation, δV associated with the inner and outer core (IC) is equal to zero. After Jeffreys [1924], it is possible to define a surface on which the gravitational potential is constant as follows

$$r(\theta, \phi) = a' \left(1 + \sum_{s,t} \epsilon_{s,t} Y_{s,t}(\theta, \phi) \right) \quad (4.2)$$

where a' is the mean radius of this surface. The summation within the parentheses is the variation about this mean surface expressed in spherical harmonics, where $\epsilon_{s,t}$ is the spherical harmonic coefficient of degree $s \geq 1$ and order t and $Y_{s,t}$ is the spherical harmonic. For $a' = r_{\text{CMB}}$, ϵ may be considered as the “geoid at the Core Mantle Boundary”, i.e. ϵ is the spherical harmonic description of the equipotential which has an average radius equal to the radius of the core in a 1D model. As a consequence of defining equipotential surfaces, it is possible to express the perturbation to the gravitational potential at a given radius r as a function of ϵ is given by [Jeffreys, 1924]

$$\delta\Phi_{s,t}(r) = \frac{4\pi G}{2s+1} \rho r^{2-s} a'^s \epsilon_{s,t}, \quad (4.3)$$

where G is the gravitational constant and ρ is the density at the radius r .

The goal of the following section is to describe ϵ as a function of the parameters which control the gravitational potential. Here we will focus on the density perturbations and the topography on this discontinuity, which both influence the shape of ϵ .

To this end, we begin by expressing the perturbation of the gravitational potential as a function of the density perturbation. As an extension to Buffett [1996], we also include the effect of topography at major discontinuities d . Following Ishii and Tromp [1999], it can be described within the Earth at a location $\mathbf{r}$ as

$$\delta\Phi(\mathbf{r}) = -G \int_V \frac{\delta\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' + G \sum_d \int_S \frac{[\rho]_-^+ \delta d(\hat{\mathbf{r}}')}{|\mathbf{r} - \mathbf{r}'|} d^2\mathbf{r}'. \quad (4.4)$$

The first term on the right-hand side is associated with volumetric density perturbations, $\delta\rho$, defined as perturbations to the 1D, radially symmetric, background profile (for instance PREM) within the mantle. The choice of the 1D model here has no influence on the computation since only the perturbations around it generate a perturbation in the gravitational potential, and the degree 0 becomes non-important. The second term is associated with topography at discontinuities, δd (e.g., the 660 km discontinuity or the CMB), which describes the relative radius perturbation of the radius at a discontinuity d , at an average radius r_d . We evaluate $\delta\Phi$ at a radial point r , a is the radius at the surface of the Earth, d is the

sum over all discontinuities, and $[\rho]_-^+$ is the density contrast at a given discontinuity. This, together with the relationship [Dahlen and Tromp, 1998]

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{s=0}^{\infty} \frac{4\pi}{2s+1} \frac{[\min(r, r')]^s}{[\max(r, r')]^{(s+1)}} \sum_{t=-s}^s Y_{st}(\hat{\mathbf{r}}) Y_{st}^*(\hat{\mathbf{r}}'), \quad (4.5)$$

(where the asterisk denotes complex conjugation), yields

$$\delta\Phi_{s,t}(r) = \begin{cases} -\frac{4\pi G}{2s+1} \left(\int_0^r \delta\rho_{s,t}(r') \frac{r'^s}{r^{s+1}} r'^2 dr' + \int_r^a \delta\rho_{s,t}(r') \frac{r^s}{r'^{s+1}} r'^2 dr' \right. \\ \quad \left. + \sum_d [\rho]_-^+ \frac{r_d^s}{r^{s+1}} \delta d_{s,t} \right) & \text{when } r < r_d \\ -\frac{4\pi G}{2s+1} \left(\int_0^r \delta\rho_{s,t}(r') \frac{r'^s}{r^{s+1}} r'^2 dr' + \int_r^a \delta\rho_{s,t}(r') \frac{r^s}{r'^{s+1}} r'^2 dr' \right. \\ \quad \left. + \sum_d [\rho]_-^+ \frac{r^s}{r_d^{s+1}} \delta d_{s,t} \right) & \text{when } r > r_d \end{cases} \quad (4.6)$$

Once again, the first term on the right-hand side is associated with volumetric density perturbations within the mantle and the second term with discontinuities. Here, r_d corresponds to the mean radius of the discontinuity d , $\delta\rho_{s,t}$ and $\delta d_{s,t}$ are the spherical harmonics coefficients of variations in density and topography of the d -th discontinuity, respectively, both relative to the background profile. We evaluate $\delta\Phi$ at a radial point r , a is the radius at the surface of the Earth, d is the sum over all discontinuities, and $[\rho]_-^+$ is the density contrast at a given discontinuity.

Equating eq. 4.3 and eq. 4.6, we arrive at

$$\epsilon_{s,t}(r) = \begin{cases} \frac{a^{s-2}}{r^s} \left(\int_0^r \delta\rho_{s,t}(r') \frac{r'^s}{r^{s+1}} r'^2 dr' + \int_r^a \delta\rho_{s,t}(r') \frac{r^s}{r'^{s+1}} r'^2 dr' \right. \\ \quad \left. + \sum_d [\rho]_-^+ \frac{r_d^s}{r^{s+1}} \delta d_{s,t} \right) & \text{when } r < r_d \\ \frac{a^{s-2}}{r^s} \left(\int_0^r \delta\rho_{s,t}(r') \frac{r'^s}{r^{s+1}} r'^2 dr' + \int_r^a \delta\rho_{s,t}(r') \frac{r^s}{r'^{s+1}} r'^2 dr' \right. \\ \quad \left. + \sum_d [\rho]_-^+ \frac{r^s}{r_d^{s+1}} \delta d_{s,t} \right) & \text{when } r > r_d \end{cases} \quad (4.7)$$

We focus on a single spherical harmonic, degree and order two (i.e., $s = t = 2$) since this will have the greatest effect on the MICG [Buffett, 1996]. Fortunately, it is also the single most dominant harmonic in global tomography models in the deep mantle [Lekic et al., 2012], and essentially best describes the LLSVP contribution to the spherical harmonic spectrum.

Extracting this single harmonic, we have

$$\epsilon_{2,2} = \frac{1}{\rho(r)} \frac{1}{r^2} \left[\int_0^r \delta\rho_{2,2}(r') \frac{r'^4}{r^3} dr' + \int_r^a \delta\rho_{2,2}(r') \frac{r^2}{r'} dr' + \sum_d [\rho]_-^+ \frac{r_d^2}{r^3} \delta d_{2,2} \right] \quad (4.8)$$

where $\delta\rho_{2,2}(r) = \rho(r)\partial \ln \rho_{2,2}$. Once more, we note the two distinct contributions from the volumetric density perturbations and from the topography at the interfaces.

Having now expressed ϵ as a function of $\delta\rho$ and δd , we use this to determine the period of the LOD oscillation (Eq. 4.1). In the following, we determine how ϵ gravitationally couples to the inner core. Intuitively, these perturbations in potential may be downward continued onto the inner core and thus impose a force that deforms the inner core. Following Buffett [1996], the perturbation in gravitational energy due to the presence of the rotating inner core, as a function of ϵ is given by

$$\delta V = \frac{4\pi G}{5} |\bar{\rho}\epsilon + \rho_f \epsilon(a_s)| |(B_s - A_s) - (B'_s - A'_s)| \quad (4.9)$$

where ρ_f is the density of the fluid at the CMB, a_s is the radius of the inner core, and A_s and B_s are the equatorial moments of inertia of the inner core. Thus, $B_s - A_s$ corresponds to their difference. Without coupling from ϵ , since we do not consider lateral heterogeneity within the inner core, this difference would be zero. Projecting the effect of ϵ onto the inner core surface means that their difference becomes

$$B_s - A_s = \frac{8\pi}{15} \int_0^{a_s} \rho(a') \frac{\partial}{\partial a'} (\epsilon(a') a^5) da'. \quad (4.10)$$

$B'_s - A'_s$ corresponds to the difference in equatorial moments of inertia for a core whose density is constant and equal to ρ_f .

Substituting Eq. 4.9 in Eq. 4.1, and using Eq. 4.8, we arrive at an expression for the period of the SYO, given degree-2 and order-2 buoyancy distribution in the mantle and topography at the CMB. We assess each of these contributions to the σ separately and use this outlined theory to conduct a sensitivity analysis of the SYO period.

4.4 Results and Discussion

4.4.1 Depth Sensitivity of the SYO Period to Mantle Buoyancy Structure

We present our results on the 1D sensitivity analysis of the two key parameters that affect the SYO period, the perturbed gravitational potential energy, δV , and the long wavelength “geoid at the CMB”, $\epsilon_{2,2}(r = \text{CMB})$. In Fig. 4.2a, these are shown relative to perturbations in degree-two, order-two buoyancy structure throughout the mantle. To obtain these sensitivity

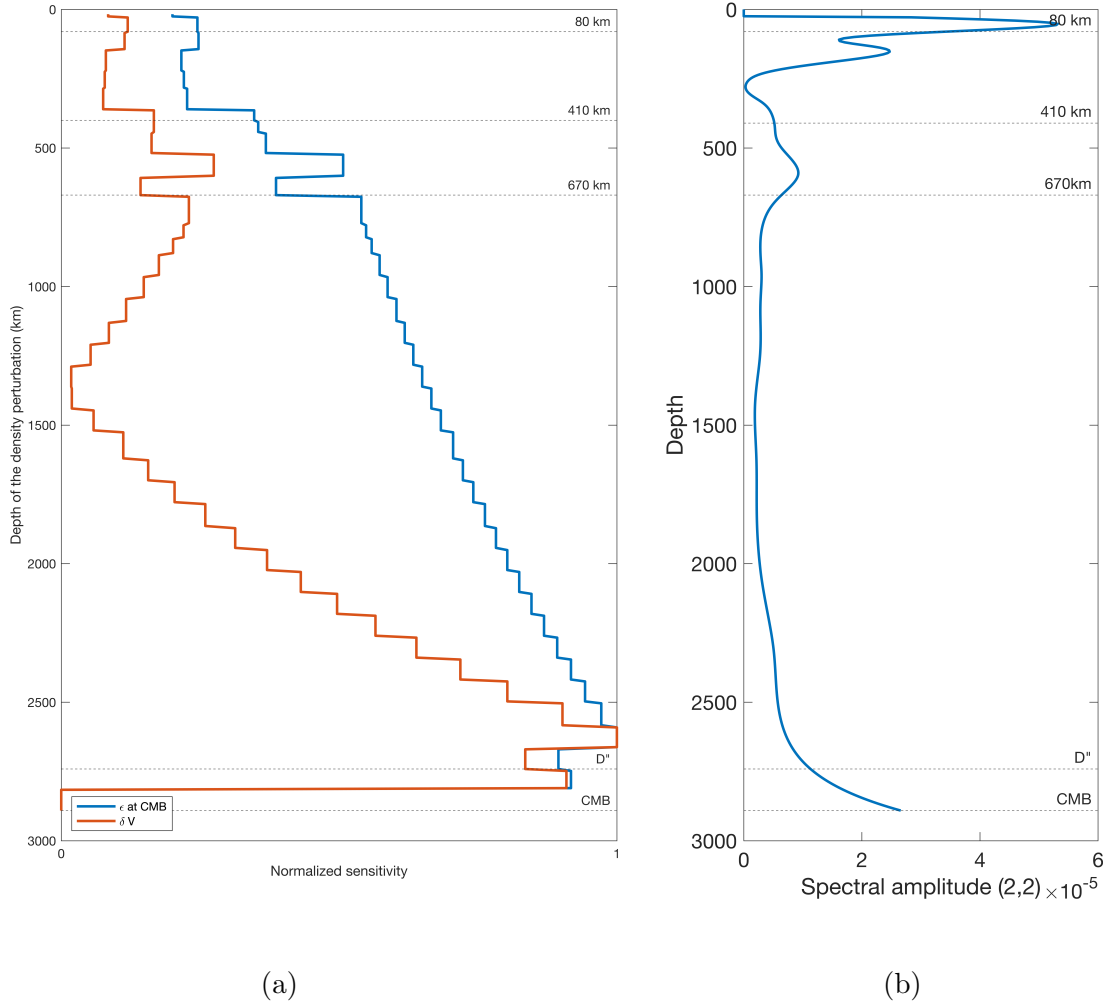


Figure 4.2: On the left panel, the depth-dependent sensitivities of the perturbed gravitational potential energy, δV (Eq. 4.9, orange line), and the long wavelength “geoid at the CMB”, $\epsilon_{2,2}(r = \text{CMB})$ (Eq. 4.8, blue line) to degree-two, order-two (i.e., $s = t = 2$) density perturbations throughout the mantle. The sensitivities are normalized to 1 to aid comparison. The right panel shows the depth-dependent amplitude of the degree-two, order-two (i.e., $s = t = 2$) spherical harmonic component of global shear-wave tomography model S40RTS [Ritsema et al., 2011]

kernels, we began with the 1D density structure from the Preliminary Reference Earth Model [Dziewonski and Anderson, 1981]. We then introduced a perturbation to the $s = t = 2$ buoyancy structure of a single discretized layer in the mantle. The discretization of each layer is readily visible with the staircase appearance of the sensitivity profiles in Fig. 4.2a. We then calculated the associated values of δV and $\epsilon(r_{2,2}(r = \text{CMB}))$. We repeated the same perturbation for each layer in the mantle and plot these perturbations across the mantle.

Our computations show that both δV and $\epsilon(r_{\text{CMB}})$ have sensitivities to degree-2 order-2 buoyancy perturbations that gradually increase to reach their maximum at the CMB, indicating that the SYO periods will be most impacted by changes in the buoyancy structure at this depth. This significance of the enhancement of sensitivity at the base of the mantle in both these measures is emphasized by comparing these profiles to how the $s = t = 2$ structure varies with depth (Fig. 4.2b). The panel shows how the signal of $s = t = 2$ in shear wave speed variations, as in global tomography model S40RTS [Ritsema et al., 2011], varies. Note, that $s = t = 2$ in the base of the mantle is dominated by the LLSVPs. As can be seen, this signal also peaks at the base of the mantle. The very signal we wish to explore is the very signal the SYO period is most sensitive to. In addition, we see that there is relatively little sensitivity to the surface, where there is also a strong degree-two signal in Earth’s structure (Fig. 4.2b), stemming from Earth’s ocean-continent distribution, and surface tectonics. With the muted sensitivity at shallow depths, it follows that the period of the SYO is not sensitive to shallow structure and thus will not be contaminated by this.

Moreover, since the MICG mechanism is entirely gravitational, no trade-off with elastic parameters or viscosity structure is present, as in seismic and body tide studies for the former [e.g., Koelemeijer et al., 2017, Lau et al., 2017], or geodynamical studies for the latter [e.g., Kellogg et al., 1999, Forte and Mitrovica, 2001, Richards et al., 2023]. Thus, we conclude that our sensitivity analysis can provide a complementary, independent constraint on LLSVP buoyancy.

4.4.2 Parameter Space Exploration for Discontinuity Topography and Buoyancy Structure

In the previous section, we focused on the sensitivity of the SYO period to volumetric perturbations in density. We turn our attention to consider its sensitivity to CMB topography and the trade-offs between these two types of perturbations. To do this, we conducted a thorough exploration of the parameter space in density and topography perturbations and their resulting periods of SYO. As its period only takes into account the perturbations to the 1D model, the influence of its choice is rather limited and our conclusions hold for any background radial model. In this case, we choose PREM for the 1D reference.

We consider a uniform, 300 km-thick layer of $s = t = 2$ density perturbation at the base of the mantle. This is chosen since it lies in the middle of the range of expected density excess within the LLSVP, as suggested by Lau et al. [2017]. We further explore a range of density perturbations, varying from ± 1 – ± 5 % anomalies as well as topography variations

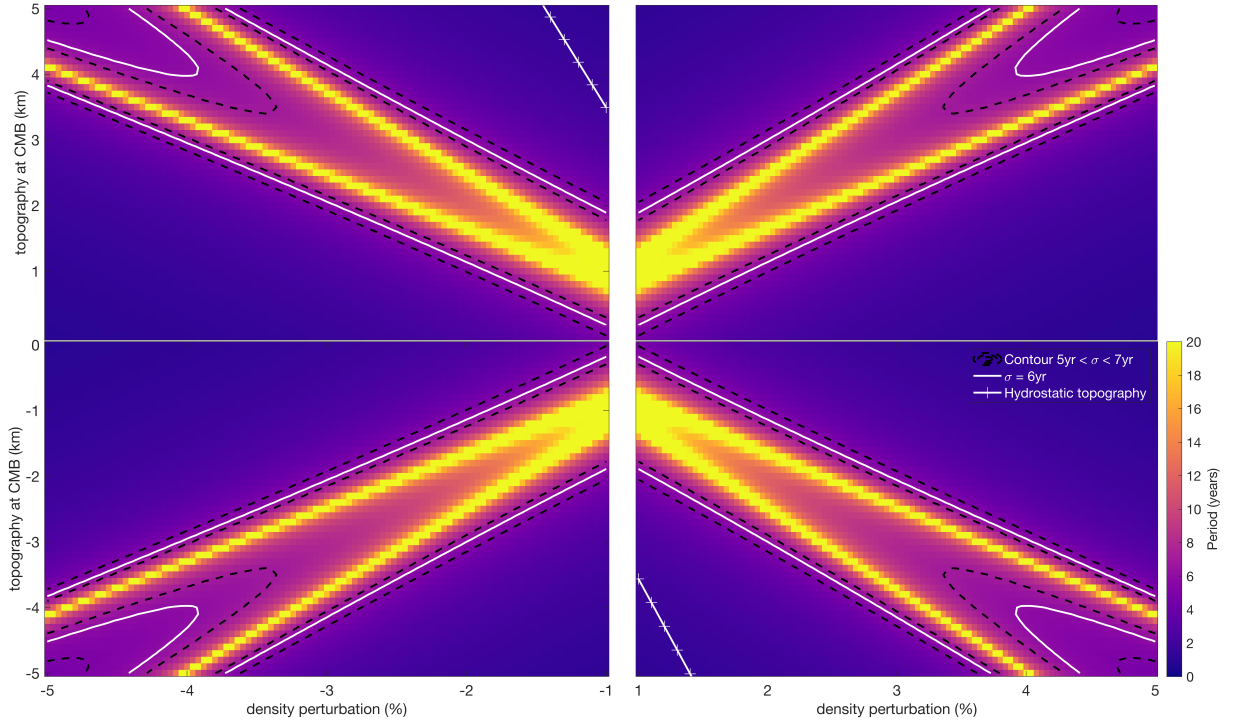


Figure 4.3: The SYO period, σ (Eq. 4.1), as a function of degree-two and order-two ($s = t = 2$) CMB topography and density perturbations, where the perturbation is applied to a uniform layer of 300 km thickness situated at the base of the mantle. The black dashed lines bracket a region within which the period is 5–7 years (constrained by observation). The white line marks isostatically balanced topography given the density perturbation.

with amplitudes from ± 0 – ± 5 km for the $s = t = 2$ spherical harmonic structure. The latter values are within the upper range of possible values as described by Koelemeijer [2021]. For every single combination of $\delta\rho_{2,2}$ and $\delta d_{s,t}$ perturbations, we calculate the period of the SYO, σ (Eq. 4.1). It is important to note that our study involves an exploration of the sensitivity of the SYO to a wide range of parameter values, including those beyond what has been constrained by observational studies. This approach allows us to better understand the potential effects of extreme scenarios on the SYO and gain insights into the system’s behavior under various conditions.

The result of this grid search is a 2D map of oscillation periods in the parameter space of topography and density perturbation (Fig. 4.3). We note, by virtue of the symmetry of the $\epsilon_{2,2}$ structure, each quadrant of perturbations is symmetrical. Of course, emphasis should be given to regions across which the SYO is within the observational range. The predicted period range of 5–7 years is bounded by black dashed lines in Fig. 4.3, where

the white line marks the 6-year period. Within this region, the topography and density structure had contrasting effects. Fixing the density perturbation and traversing along the topography axis shows that even slight changes in topography may move the SYO period out of realistic values. A similar conclusion may be made with density perturbations. As such, within the vicinity of the observed SYO period, there exists a strong sensitivity to both CMB topography and excess density. We note, however, that we have considered a single thickness of $s = t = 2$ structure and more tests may be undertaken to explore this sensitivity further.

A density perturbation at the CMB and CMB topography are not independent of one another. If no viscous stresses exist at the base of the mantle, imparted by the convective flow of the mantle, then any density perturbation at the base of the mantle must be isostatically compensated by the topography. While it is well known that degree-two CMB topography is not in hydrostatic equilibrium [Mathews et al., 2002], any density perturbations and CMB topographies that are not in hydrostatic equilibrium have implications for the dynamic topography at the CMB and therefore the viscosity structure of the mantle around this region. In order to assess the degree of non-hydrostatic topography within our grid search, we estimate the isostatic compensation required for our 300 km-thick perturbed density layer, using a compensation depth located within the outer core. Specifically, we used the equation

$$\delta d_{\text{iso}} = \frac{H_m \times \delta \rho}{\rho_{\text{LLSVP}} - \rho_{\text{OC}}}, \quad (4.11)$$

where δd_{iso} is the static topography necessary to compensate the $\delta \rho$ imposed in the LLSVP, H_m is the thickness of the LLSVP, ρ_{LLSVP} is the density of the LLSVP, and ρ_{OC} is the density of the outer core (considered fixed for this simple case). The values for which $\delta \rho_{2,2}$ and $\delta d_{2,2}$ correspond to isostatic equilibrium are approximately shown by the white crossed line in Fig. 4.3. As can be seen, if our uniform layered model here were realistic, in order to satisfy the observed SYO periods, topography on the CMB must be dynamically supported by both core and mantle flow, since none of the hydrostatically equilibrated lines are anywhere near the region bounded by the dashed black lines.

4.5 Other Explanations for the Six-Year Oscillations

Buffett [1996] originally introduced the MICG mechanism to drive the SYO, and it has been subsequently explored by Mound and Buffett [2006] and Davies et al. [2014]. In the latter study, they found the MICG mechanism to be too insignificant to drive the SYO but were using much earlier ideas of mantle buoyancy variations. Ding and Chao [2018], in light of revised ideas of LLSVP buoyancy have revived the idea of the MICG mechanism for the SYO oscillation. Nevertheless, our study shows that reaching a period close to 6 years with MICG coupling requires strong perturbations, both on the buoyancy structure and on the dynamic topography, and other mechanisms have been proposed. Multi-year hydrological

forcing at Earth’s surface has been proposed [Rosat et al., 2021], Alfvén waves have been thought to have characteristic periods of 6 years and thus may cause exchange of Earth’s angular momentum from the outer core and the solid Earth [Gillet et al., 2010, Rosat and Gillet, 2023], and flow-drive pressure changes within the outer core have also been proposed [e.g., Dumberry and Bloxham, 2006]. Each of these processes holds large uncertainties in how they affect Earth’s LOD since our understanding of outer core flow dynamics remains incomplete [e.g., Dumberry and Mandea, 2022]. However, it is clear that each of these processes needs further investigation in order to understand their role in the SYO.

4.6 Conclusions

Our investigation focused on the coupling between the inner core and the mantle, which is hypothesized to cause the SYO through the perturbation in the gravitational potential. We computed 1D density sensitivity kernels for the SYO, which allowed us to directly analyze the sensitivity of the oscillation to the buoyancy anomalies in the deep mantle and the topography at the CMB, and concluded that, in the context of MICG coupling, the SYO is sensitive to both the buoyancy structure and the topography in the lowermost mantle. By examining the period associated with the SYO for different combinations of buoyancy perturbations and topography, we generated a 2D map of the SYO period in the parameter space. Our findings revealed that the sensitivity of the SYO to the LLSVP structure is highly dependent on both the topography and the density perturbation. We observed that the topography and density structure have opposing effects on the SYO period.

In our parameter space exploration, we identified regions corresponding to a characteristic period of six years for the SYO. The contrasting effects of topography and density structure revealed valuable insights into the behavior of the SYO with respect to the LLSVP structure. The results of this exploration, along with the isostatic compensation analysis, contribute to a better understanding of the SYO and its relationship with the LLSVPs. As our study focused on establishing a sensitivity analysis to the resolution of the parameters of the LLSVPs, it is clear that the values for dynamic topography necessary to get to a period close to 6 years are unrealistically large. This could be due to the simplistic model used to model the LLSVPs, which by no means we deemed to be realistic. This exercise was to emphasize the concurrent effect of the topography at the CMB and the density structure of the lower mantle. This could also be due to the fact that the MICG has too small of an influence to drive the oscillations visible in the LOD data.

In fact, our study provides an argument to use the SYO period as an independent geodetic observation that can be used to evaluate and validate already established density LLSVP models, derived from seismic tomography or global geodynamics. By examining the sensitivity of the SYO to the mantle’s buoyancy structure and topography at the CMB, we gain insights into the origin and nature of the LLSVPs and their potential role in the dynamics and evolution of the deep Earth.

Although this test was realized in a rather simple setting given the sensitivity to the large

scale, degree two density perturbation, our analysis provides valuable insight into what the SYO is able to resolve of the structure in the lowermost mantle of the Earth. Thanks to ever-improving, longer, geodetic measurements, many oscillations, once buried under the noise and the dominating signal, come into light, which are the results of complex interactions between the different layers that comprise the Earth. Because of the nature of the SYO measurement, it is unthinkable to imagine building an LLSVP model uniquely based on this single data point. However, as it is an entirely new and independent constraint, it is possible to test hypotheses on LLSVPs and confront it with what it would mean for the period associated with the inner core interaction with the lower mantle.

Chapter 5

Influence of a Hydrophysics-derived Source Time Function on the Wave Propagation through a Large Magma Body: a Study of the Potential Link between the Chicxulub Impact and the Deccan Traps

The relationship between seismic activity and volcanic eruptions has long captured the interest of the scientific community throughout history. With the earliest reference from Pliny, documenting the eruption of Vesuvius that soon overwhelmed Pompeii in volcanic output (79 AD), there have been many observations of distant earthquakes mobilizing fluids in the Earth's crust and triggering magmatic volcanic eruptions. While the phenomenon has been well-documented, the underlying mechanisms behind the intricate triggering process remain enigmatic. This research proposes an extension of earthquake studies to large impact-induced seismic waves from asteroid collisions, using seismic modeling to assess their effects on volcanic systems worldwide. Specifically, the study focuses on the Deccan Traps Large Igneous Province (LIP) in Central India, which is associated with the Cretaceous–Paleogene (K-Pg) extinction event. The synchronous timing of the Deccan Traps formation and the Chicxulub meteorite impact raises questions about possible connections, akin to those observed between earthquakes and volcanic activity Brusatte et al. [2015].

5.1 Introduction

Volcanic eruptions are among the most geologically significant events on our planet as they not only shape landscapes but also influence climate and ecosystems. Understanding

the factors that lead to volcanic eruptions is crucial for hazard assessment and mitigation strategies. Among the numerous triggers of volcanic activity, another catastrophic hazard has emerged as a key mechanism that can induce and/or influence eruptions: earthquakes.

Volcanic eruptions are complex phenomena governed by a multitude of factors, including magma composition, pressure, temperature, and volatile content. Seismic activity, particularly earthquakes, has been suggested as one such trigger of volcanic eruptions, both within hours to days and, in some cases, delayed by longer periods after the seismic event [Linde and Sacks, 1998]. However, the mechanisms behind these triggers are still an open question.

Over the course of millennia, historical accounts have revealed instances where remote earthquakes have accompanied volcanic activity, with Pliny’s account of the eruption of Vesuvius in 79 AD serving as one of the earliest descriptions of this phenomenon Jerram et al. [2017]. Additionally, evidence has emerged pointing towards the intriguing prospect of widespread and even global increases in volcanic activity following significant earthquakes [e.g. Madonia et al., 2013, Delle Donne et al., 2010, Eggert and Walter, 2009].

Static stress changes and dynamic stress changes are two potential mechanisms for the initiation of eruptions. Static stress changes involve compression or expansion of magma reservoirs due to seismic events [e.g. Barrientos, 1994, La Femina et al., 2004, Diez et al., 2005, Walter and Amelung, 2007]. On the other hand, dynamic stress changes produced by seismic waves have a larger impact and may influence subsurface conditions over greater distances from the epicenter [Kilb et al., 2000]. Unlike static stress changes, seismic waves should not produce permanent stress changes unless they alter the mechanical and/or transport properties of the crust. Dynamic stresses, arising from the passage of seismic waves, have been identified as potential key players in the triggering process [Hill et al., 2002]. The larger amplitude of dynamic stress changes compared to static stress changes further accentuates their potential impact on magma reservoirs and volcanic systems [Watt et al., 2009].

It is postulated that dynamic stress changes may affect eruptions by influencing permeability, nucleating or mobilizing bubbles, and mobilizing magma [e.g. Walter et al., 2009, Manga et al., 2012, Hill et al., 2002, Sumita and Manga, 2008]. Nonetheless, the significance of bubble growth through rectified diffusion or bubble motion-induced overpressure has been questioned [e.g. Ichihara and Brodsky, 2006, Sahagian and Proussevitch, 1992, Bagdassarov, 1994].

While the number of documented magmatic eruptions triggered by earthquakes is relatively small [Linde and Sacks, 1998], there is mounting evidence suggesting widespread and possibly global increases in volcanic activity following significant earthquakes [e.g. Madonia et al., 2013, Delle Donne et al., 2010, Eggert and Walter, 2009]. To further investigate this phenomenon, we propose to extend the study of earthquakes to the large impact-induced seismic waves that result from the collision of a large asteroid on the planet.

One of the most famous catastrophic volcanic episodes captured in the geological record resulted in the formation of the Deccan Traps Large Igneous Province (LIP) in Central

India. The formation of the Deccan Traps raises particular interest since its timing occurred concurrently with one of the five mass extinctions known in our fossil record: the Cretaceous–Paleogene (K-Pg) extinction event, during which $\approx 70\%$ of species went extinct Brusatte et al. [2015]. The Deccan Traps, which formed over the course of 5 Ma [Renne et al., 2013], are possibly linked to the catastrophic event through cooling and/or acid rain associated with sulfate aerosols injected into the atmosphere during the intense volcanism period [Courtillot et al., 1986]. Another catastrophic event related to the same mass extinction is the meteorite impact of Chicxulub [Alvarez et al., 1980]. According to recent dating of the impact ejecta and lava samples from the Deccan Traps [Renne et al., 2013], the two events happened effectively synchronously, at $66.04 \text{ Ma} \pm 32 \text{ ka}$. This coincidence in timing could be completely unrelated, or, just like with earthquakes and volcanism, there may exist links that should be studied in depth.

It has been shown with seismic modeling that long-period, large-amplitude Rayleigh waves likely generated stresses sufficient to trigger volcanic systems worldwide [Wang and Manga, 2010]. To establish a more direct link between these stresses and volcanic triggering, in this chapter we model the propagation of seismic waves generated by a realistic consideration of the impact dynamics. In particular, we focus our attention on how energy evolution of the seismic wavefield within the low-velocity, low- Q , plume-head region beneath the Indian plate. We hope to consider whether the presence of the plume might cause focusing of the arriving seismic waves and thus amplify the deformation within the volcanic source of the Deccan Traps. If these amplifications are sufficient, it is then possible that the Chicxulub impactor is the single trigger of the entire extinction, with direct and indirect consequences.

To this end, we combine a hydrophysics-based impact simulation of the Chicxulub impact with a wave propagation modeling code in order to simulate the associated wavefield and its evolution within the vicinity of the Deccan Traps. iSALE-2D [Wünnemann et al., 2006] is a numerical code that simulates impact cratering. We will use iSALE-2D in order to estimate the seismic source mechanism through an accurate source time function (moment-rate time series), based on the physical characteristics of the impact. We will employ the Spectral Element Method (SEM) implementation of SPECFEM3D Globe for accurate calculation of seismic wave propagation in global 3D heterogeneous Earth models [Komatitsch and Vilotte, 1998, Komatitsch and Tromp, 2002]. The SEM code will generate synthetic seismograms at any location and depth, providing insights into energy focusing and localization.

5.2 Theoretical Background

5.2.1 Impact simulation

In treating our seismic source as an impactor, we will take two pathways. We first consider the impactor as an isotropic explosive source, as has been done in the past [Meschede et al., 2011]. We also take one step further and consider a more realistic source, estimated by using an impact simulation. A brief summary of these two sources is found in the next two

subsections. From the two considerations of sources, we will arrive at a moment tensor and source-time function description of the approximate isotropic explosion source (Section 5.2.1) and the source based on impact physics (Section 5.2.1).

Approximate Source: Scalar seismic moment of an explosion and point source approximation source time function

We first consider the seismic source by constructing a source-time function (STF) and seismic moment tensor as an isotropic explosion. The seismic moment tensor describes the geometry and magnitude of a seismic source. It is often combined with a STF to define the source signal in seismic wave propagation modeling, which corresponds to the evolution of the moment rate as a function of time. It provides information on how the energy is liberated throughout the entire duration of the source radiation. The STF, alongside the location and depth of the source, are enough to characterize the propagation of seismic waves emanating from the source [Vallée et al., 2011]. Since the amplitude of the synthetic wave model is proportional to the seismic moment, synthetic seismograms generated for a given source-time function can be readily rescaled given the seismic moment.

The seismic moment tensor, $\mathbf{M}$, comprises three force dipoles (the diagonal components) and six force couples (the off-diagonal components). For a point source (a common approximation for explosions and impacts), the force couples can be neglected, and $\mathbf{M}$ simplifies to a diagonal tensor. For an isotropic point source, the diagonal elements of the tensor are equal, $M_{ii} = M_{11}$.

It is possible to represent an impact as an explosive source [Meschede et al., 2011] and gain insights into its temporal behavior. This STF is computed based on the total seismic moment. In this case, we will use a Ricker wavelet that appropriately describes the temporal behavior of the explosive source. The functional form of the Ricker wavelet, $\mathcal{M}_R$, is given by:

$$\mathcal{M}_R(f_{\text{exp}}, t_{\text{exp}}, t) = [1 - 2\pi f_{\text{exp}}^2 (t - t_{\text{exp}})^2] \times \exp [-\pi^2 f_{\text{exp}}^2 (t - t_{\text{exp}})^2] \quad (5.1)$$

where f_{exp} and t_{exp} are the dominant frequency and the central time of the explosion, respectively. To scale it with the seismic moment associated with the explosion, we must normalize the Ricker wavelet, $\mathcal{M}_R$. Then we multiply the normalized STF by the maximum seismic moment, M_0 . The value of M_0 will be derived from the output of the impact simulation so that these two approaches may be compared appropriately. The final expression for the scaled Ricker wavelength, $\overline{\mathcal{M}}_R$ becomes

$$\overline{\mathcal{M}}_R(M_0, f_{\text{exp}}, t_{\text{exp}}, t) = \frac{2 M_0}{\sqrt{3\sigma\pi^{\frac{1}{4}}}} \left[1 - \left(\frac{t - t_{\text{exp}}}{\sigma} \right)^2 \right] \times \exp \left[\frac{(t - t_{\text{exp}})^2}{2\sigma} \right], \quad (5.2)$$

where $\sigma = (2\pi f_{\text{exp}})^{-1}$.

Our STF is an isotropic explosion for which the moment tensor is diagonal, with each diagonal component being equal and thus

$$M_{11} = M_{22} = M_{33} = \left(\frac{2}{3}\right)^{1/2} M_0 \quad (5.3)$$

A representation of this simple STF is provided in Figure 5.2b).

Realistic Source: Estimating the seismic source from impact physics

To compare the approximate Ricker wavelet STF with a realistic impactor, we derive our more realistic source by considering output based on impact simulations. Impact simulations play a crucial role in understanding the dynamic response of materials to high-energy events, such as meteorite impacts. Hydrocode simulation software provide a powerful framework for investigating impact processes. Here, we briefly outline the key equations of the impact calculations, but for further details, see Wünnemann et al. [2006].

The equation of state for the target material, denoted by subscript “t”, can be expressed as

$$P_t = P_t(\rho_t, e_t) \quad (5.4)$$

where P_t represents the pressure, ρ_t denotes the density of the target, and e_t the associated internal energy of the target. The equation of state for the projectile material, denoted by subscript “p” is

$$P_p = P_p(\rho_p, e_p) \quad (5.5)$$

where P_p represents the pressure, ρ_p denotes the density of the projectile. The conservation equations for mass, momentum, and energy for the impacted material are given by the Euler equations, which respectively are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (5.6)$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + P \mathbf{I}) = 0, \quad (5.7)$$

$$\frac{\partial e}{\partial t} + \nabla \cdot [(e + P) \mathbf{v}] = 0. \quad (5.8)$$

Here $\mathbf{v}$ is the velocity vector and $\mathbf{I}$ is the identity matrix.

In this work, we use the iSALE-2D shock physics code [Wünnemann et al., 2006], which is based on the SALE hydrocode solution algorithm [Amsden et al., 1980]. The iSALE software employs a combination of smooth particle hydrodynamics (SPH), a Lagrangian method that

discretizes the material into individual particles and approximates the continuum equations using these particles, and finite difference methods to numerically solve the governing equations described above. By using a state-of-the-art strain-based porosity model, an accurate representation of the compaction and fragmentation behavior of materials during impact events is obtained. Because of this, and its efficiency in handling large material deformations and fragmentation, iSALE has become a widely used code for impact modeling. In Section 5.2.3, we discuss the application of iSALE for our purpose.

5.2.2 Coupling of the impact modeling with the wave propagation simulation

In order to accurately take into account the different source time functions, we make use of the representation theorem to decouple the source effects from the wave propagation itself [Aki and Richards, 2002]. The representation theorem states that the response at a receiver location $\mathbf{x}_r$ due to a seismic source located at $\mathbf{x}_s$ can be represented as the convolution of Green's functions with the moment rate time series, $M(\mathbf{x}, t)$, where $M(t)\delta(\mathbf{x} - \mathbf{x}_s)$. Mathematically, it can be expressed as

$$U_j(\mathbf{x}_r; t) = \sum_i \int_{-\infty}^{\infty} \int_V G_{ji}(\mathbf{x}_s, \mathbf{x}_r; t) \cdot M(\mathbf{x}, t - t') \delta(\mathbf{x} - \mathbf{x}_s) d\mathbf{x}^3 dt', \quad (5.9)$$

where $U_j(\mathbf{x}_r; t)$ is the j^{th} component (North, East, Up) of the ground motion time-series recorded at $\mathbf{x}_r$. $G_{ji}(\mathbf{x}_s, \mathbf{x}_r; t)$ is the Green's function that characterizes the response at the receiver $\mathbf{x}_r$ for a unit force deployed on the j^{th} component recorded on the i^{th} component due to a point-source $\mathbf{x}_s$. We consider the impact a point source and so express $M(\mathbf{x}, t')$ as $M(t)\delta(\mathbf{x} - \mathbf{x}_s)$. The convolution may then be succinctly stated as

$$U_j(\mathbf{x}_r; t) = \sum_i G_{ji}(\mathbf{x}_s, \mathbf{x}_r, t) * M(t) \quad (5.10)$$

where the asterisk denotes the space-time convolution operator. The summation over i represents the sum over all the components of the force at which we compute the Green's tensor.

We compute the Green's tensor for each unit direction of the force, recorded on each component at the location of the receiver. In a SEM computation, it is possible to place as many receivers as possible with no extra computational cost. The unit force is applied at the location of the point source, with a smoothed impulse in order to avoid potential numerical instabilities, and no other external forces are considered. We use the robustly benchmarked SPECFEM3D Globe in order to accurately compute the Green's functions, which has both the computational efficiency and versatility to tackle the different 3D Earth models and the propagation tests we wish to explore.

5.2.3 Setting the stage for the case of Chicxulub and the Deccan Traps

In the methodological description above, our discussion remained general for any consideration of wave propagation triggered by an impact. We summarize here the specific settings we consider to address the question of the K-Pg mass extinction.

STF from Chicxulub Impactor

Table 5.1: Chicxulub impact modelling parameters

Target setup	5000×5000 km
Target materials	Calcite - thickness: 3 km; $\rho = 2598 \text{ kg} \cdot \text{m}^{-3}$
	Granite - thickness: 30 km; $\rho = 2628 \text{ kg} \cdot \text{m}^{-3}$
	Dunite - thickness: 325 km; $\rho = 3314 \text{ kg} \cdot \text{m}^{-3}$
Impactor radius	7.2 km
Impactor velocity	$12 \text{ km} \cdot \text{s}^{-1}$
Impactor density	$2628 \text{ kg} \cdot \text{m}^{-3}$
Impact momentum	$4.98 \times 10^{19} \text{ kg} \cdot \text{m} \cdot \text{s}^{-1}$
Kinetic energy	$2.99 \times 10^{23} \text{ J}$

We consider the target domain in a 2D Cartesian domain, with calcite, granitic, and dunite layers. This is thought to be representative of the impact site at Chicxulub [Collins et al., 2008]. Table 5.1 summarizes the dimensions and densities of these layers. For the impactor, we consider a projectile with a radius of 7.2 km, with a uniform composition with a density akin to that of granite. The momentum and kinetic energy of the impact are $4.98 \times 10^{19} \text{ kg m s}^{-1}$ and $2.99 \times 10^{23} \text{ J}$, respectively. Once more, these values are summarized in Table 5.1. These parameters are fed into the iSALE software and the moment rate, as a function of time, i.e., the STF is the output. The moment rate is computed following Wójcicka et al. [2020], further improved by Rajšić et al. [2021], such that:

$$M_z(t) = c_P p_z = c_P \sum_i^n \rho^i \bar{v}_z^i(t) V^i \quad (5.11)$$

where c_P is the P-wave velocity, p_z is the vertical momentum transferred to the target, v_z^i and V^i are the vertical velocity and the volume in the i -th cell, respectively.

The impact modeling has been conducted in collaboration with Brandon Johnson's research group located at Purdue University, and more specifically with the lead authors of Rajšić et al. [2021].

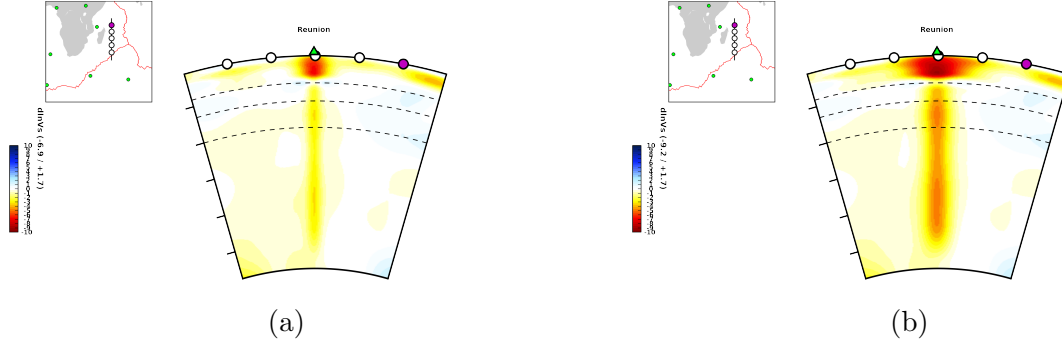


Figure 5.1: Cross-section views of the velocity anomalies (V_s) composing the two types of plumes we superimposed on SEMUCB. Both of them are plotted centered on the modern-day La Réunion plume. The velocity perturbation scale is the same in both figures. The distance between each white dot is $\approx 5^\circ$. On the left panel, we show the added anomaly (denoted WP in Table 5.2) on the SEMUCB background. On the right panel, we show the added strong anomaly (denoted SP in Table 5.2) on the SEMUCB background.

Earth Models for Wave Propagation

Table 5.2: Summary of the characteristics of the plume anomalies superimposed on the two background models of our choice.

Model	Weaker plume (WP)	Stronger plume (SP)
Head max. V_s reduction	6%	10%
Head radius	250 km	500 km
Tail max. V_s reduction	3%	5%
Tail radius	150 km	300 km

While the models we consider have global heterogeneity, we wish to draw particular attention to the plume head that is thought to have fed the volcanism that produced the Deccan Traps. Because of their extreme excess temperatures, the plume head will exhibit low seismic wave speed [Karato, 1993]. Our aim is to focus on the dynamics of the wave propagation within this plume head and evaluate whether the dynamics within this region of heterogeneity might produce phenomena that could lead to states in which the dynamic stresses could trigger an eruption.

In this case, we consider multiple Earth models. Two cases of background models are used: a simple 1D model comprising of a 1D crust and a 3D model, SEMUCB French and Romanowicz [2014]. These two models are considered background models since we do not add the presence of a plume. Against these background models, we test other models, build

on the background 3D model SEMUCB, in which a plume structure is superimposed in the vicinity of present-day La Reunion. We use that location for the anomaly in our model as the Deccan traps resulted from the interaction of a rising plume-head and the lithosphere [e.g. Courtillot et al., 1986], estimating, to a first order, that it remained stationary in the same place for the last 65 million years. This plume-like anomaly comprises a plume head of approximately 350 km depth that reaches the surface and a comparatively thinner plume tail extending all the way to the core-mantle boundary. Since the study primarily focuses on surface wave propagation across the plume head, the significance of the lower mantle velocity structure is less important. We then impose incrementally larger values for the amplitude of the perturbation of the seismic wave velocity within the plume structure. Following Chantel et al. [2016], we first impose a 6% V_s reduction in the plume head, corresponding to $\approx 1\%$ partial melt, for a plume radius of 350 km. This plume model will be labeled “WP” for weaker plume. A plume of stronger seismic anomaly, “SP”, is characterized by 2% partial melt (10% V_s reduction) and a 500 km radius. WP and SP models are incorporated into both the non-plume background models. The added plume anomaly is smoothed with a wide Gaussian filter both laterally and vertically in order to avoid sharp jumps in the meshing for the wave propagation solver. A summary of the different models in which we computed Green’s tensors is provided in Table 5.2.

The 1D model allows us to gain valuable insights into the fundamental principles governing wave propagation and understand the basic behavior of seismic waves in a simplified setting. Once the plume is imposed on the 1D model, we are able to consider the effect of the plume in isolation. The consideration of the 3D model allows us to explore the effect of more realistic patterns of wave propagation.

5.3 Results

5.3.1 Impact simulation: preliminary results for the case of Chicxulub

In Figure 5.2a) we show the resulting moment rate as a function of time as computed by iSALE. The total seismic moment (the integral of the moment rate) is $8.46 \times 10^{24} \text{N} \cdot \text{m}$, which corresponds to a moment magnitude of $M_w = 10.55$. This value is in accordance with the previous studies [e.g. Meschede et al., 2011], although on the higher end of the typical magnitude range, that is $9 < M_w < 11$. The maximum rate of dissipated energy appears shortly after the impact, at around 9 seconds. However, unlike the isotropic Ricker STF shown 5.2b), the energy is asymmetrically distributed and dissipated over a very long timescale. This is illustrated by Figure 5.3, where we integrate both STFs over time, in order to reconstruct the total moment transferred during the impact, dissipated via the seismic waves, as a function of time. With the isotropic source, we quickly reach the final value of M_0 , after about 60s. After that, no more energy is added to the system. With the

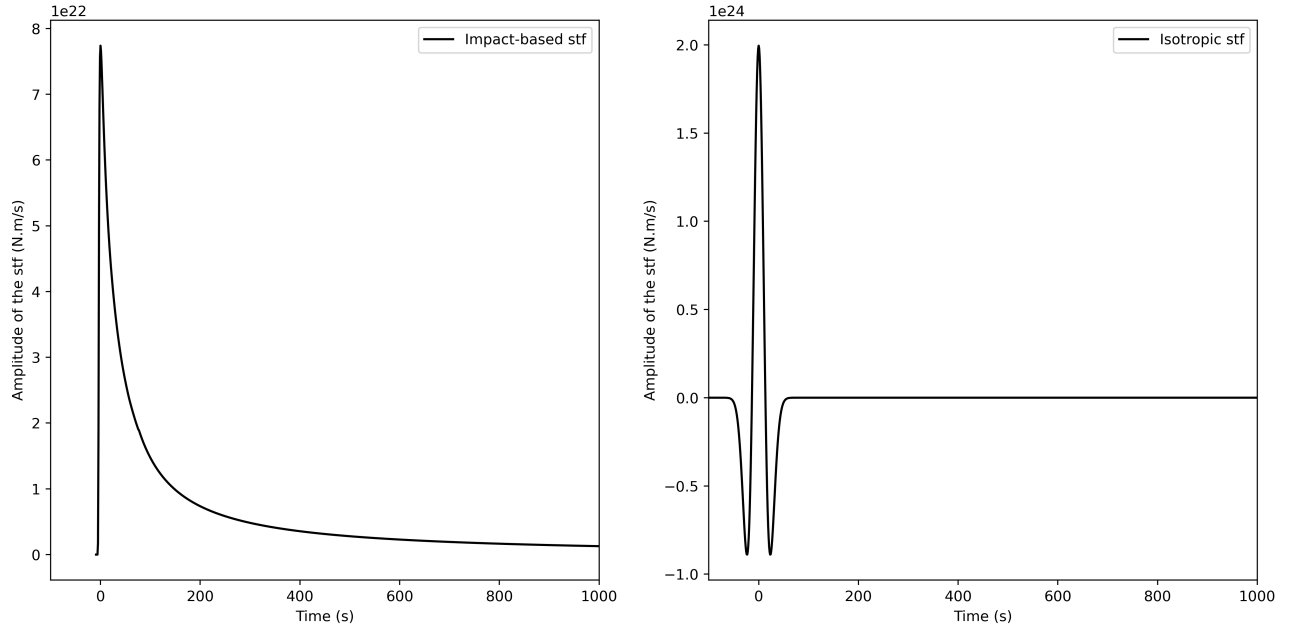


Figure 5.2: Seismic moment rate of the impact as a function of time. For both STF, The total moment computed for this simulation is $8.46 \cdot 10^{24} \text{ N} \cdot \text{m}$. On the left panel, the impact-based, realistic STF as computed by iSALE, with the parameters summarized in Table 5.1. Although the time series stops here at 1000 seconds, the source radiates for 8000 seconds (see Figure 5.3 which represents the integrated moment over time until it reaches its final value. On the right panel, the "point-source" STF, as computed for an isotropic explosive source. It is represented here with a Ricker wave eq. 5.2, with a characteristic frequency of 60 seconds, chosen after Meschede et al. [2011] to correspond to a seismic efficiency of 10^{-4} , which is typical in the literature. Because the Ricker wavelet is anticausal, we choose to differ the center time by t_0 chosen here at 100 seconds. This ensures that all the energy of the impact is taken into account for the later stage of the study.

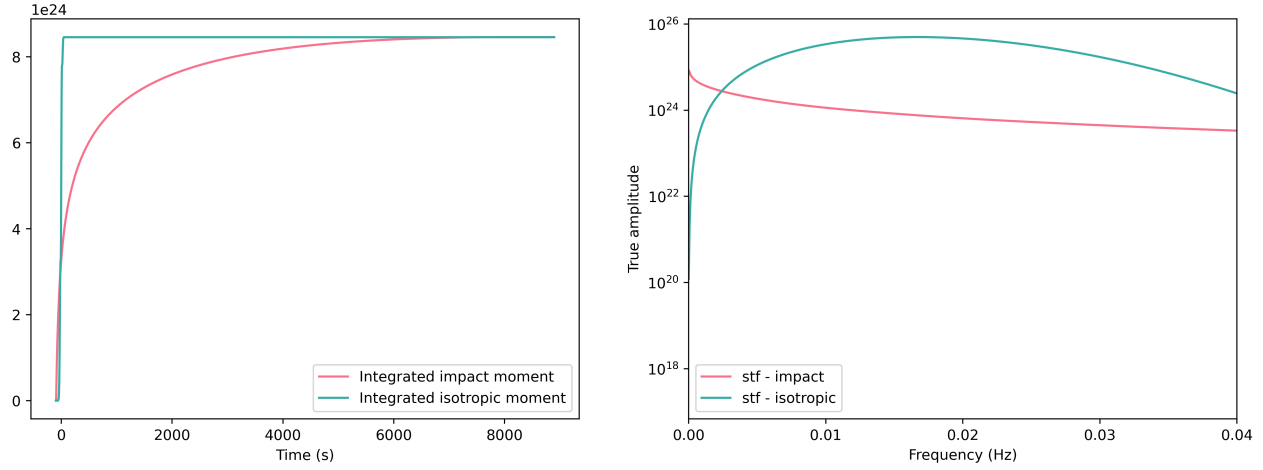


Figure 5.3: Left panel: Integrated equivalent seismic moments as a function of time, for both the isotropic STF and the impact-based STF. The impact-based STF delivers its energy over the course of a much longer time frame, unlike the isotropic STF which delivers its entire energy over a much shorter period of time. Right panel: Spectra of the two different source time function. The impact-based STF dominates the low frequency, but the isotropic STF has the highest amplitudes in the higher frequencies of the considered bandpass.

impact-derived STF on the other hand, although the initial slope is stronger (the first 20 seconds), it keeps liberating its energy in the system for a far much longer time to finally reach M_0 after 6000 seconds. This is partly due to the impact physics, which take into account the energy of the crater formation, and the secondary impacts from the ejecta, constantly adding more vertical momentum to the system, which translates into more wave seismic onsets. Therefore, although the application of the force is reduced to a single point in the wave propagation computation, this method to compute the STF partially lifts the "point-source" approximation, as the crater formation and its area are taken into account in the STF itself.

5.3.2 Computation of synthetic seismograms in different models

Across the SEM wave propagation model domain, we define a dense array of receivers centered around the plume head. These are shown in Figure 5.4, with our 3D background model and SP (Table 5.2). In order to capture the dynamics of the wave propagation in the plume head, our array is actually spread across a three-dimensional domain within the Earth's interior. As well as the array on the surface, shown in Figure 5.4, continue this arrangement by additional "buried" receivers every 50 km, from the surface to 400 km. This allows us to track the deformation induced by the passing waves at every single receiver within the plume head.

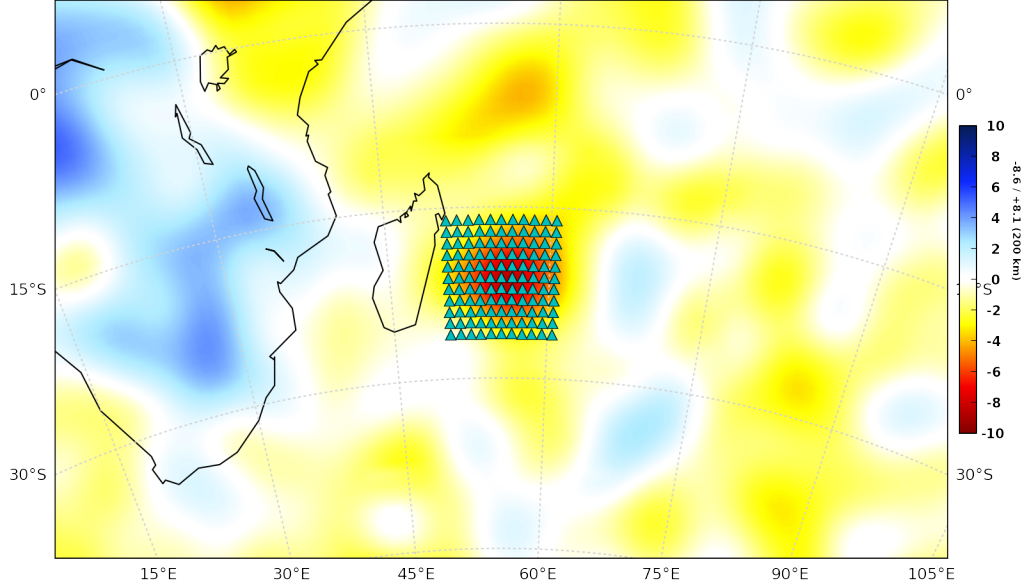


Figure 5.4: A map view of the wave propagation experiment. Each turquoise triangle represents a receiver, for which we compute the displacement at each time step. We have this array of receivers at multiple depths, in order to monitor the strain and the wave propagation inside the plume head. Those depths are 0 (surface), 50km, 100 km, 150 km, 200 km, 250 km, 300 km, 350km, and 400 km, which is the bottom of our plume head. In the background we show the velocity perturbations (for V_S), which consists of SEMUCB + SP (see Table 5.2 for reference).

The resulting seismograms, recorded beyond the center of the anomaly, to take this one into account in the propagation, for the three types of plume (NP, WP, SP), are presented Figure 5.5. We also show for comparison, the seismograms which were obtained in the pure 1D model. The different STF lead to drastically different amplitudes, up to two orders of magnitude higher for the isotropic STF. Because the moment is liberated in a shorter burst (see Figure 5.3), the resulting waveforms show a much higher amplitude than the impact STF. It is hence likely that studies using an isotropic source time function highly overestimate the peak-to-peak displacement and the resulting dynamic strain. In the case of a realistic impact, the energy is released in a much longer time scale, which makes the overall amplitudes lower than those expected in typical earthquakes for such magnitudes. This is particularly visible on the spectral domain (see Figure 5.6), where the seismograms convolved with the isotropic STF show one to two order of magnitudes more energy, especially at the

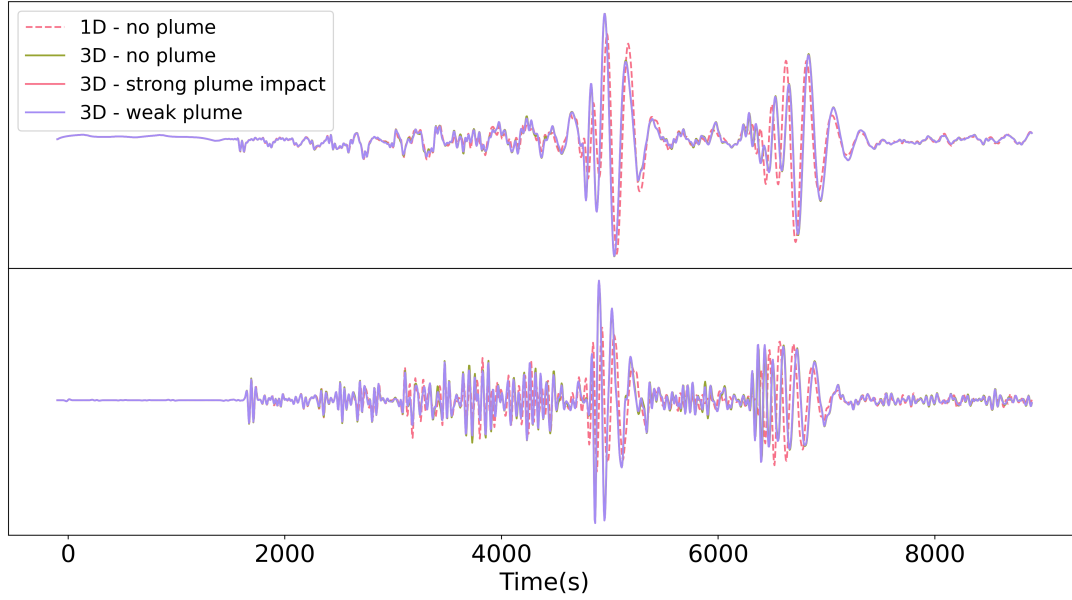


Figure 5.5: Displacement seismograms as a function of time at the center of the plume head and at a depth of 150km. All traces are recorded on the Z component, and filtered using a cosine taper with cutoffs at 24 seconds and 400 seconds, with corner frequencies at 28 seconds and 250 seconds. On the upper panel, we show the convolution with the impact-based STF. The lower panel shows the waveform obtained after the convolution of the Green's functions with the isotropic explosive STF. The minimum period resolved by SPECFEM3D Globe in this simulation is 22 seconds. The distance between the source and receiver is $\approx 147^\circ$. In both panels, the dashed blacked line is the seismogram computed in the background SEMUCB model, with no synthetic plume superimposed on it (NP). The red solid line corresponds to the seismogram computed in the background SEMUCB model + the weak plume anomaly (WP). The solid green line is invisible here as it is covered by the solid red line. It corresponds to the seismogram computed in the background SEMUCB model, with the strong plume superimposed on it (SP). The time 0 corresponds to the impact time.

highest frequencies.

The second point is that there is no visible amplification of the wave amplitude within the plume head due to the different plume models we tried in this study. A figure showing the difference between the seismograms propagated within all our tested models, and zoomed around the time window of the surface wave arrival at around 4500 seconds is presented in Figure 5.7. These traces were recorded on a receiver buried at 150km depth, and located such that the wavefield has to go through the plume head before being recorded. It confirms that the main difference happens between the 1D model and all the other 3D models, with the

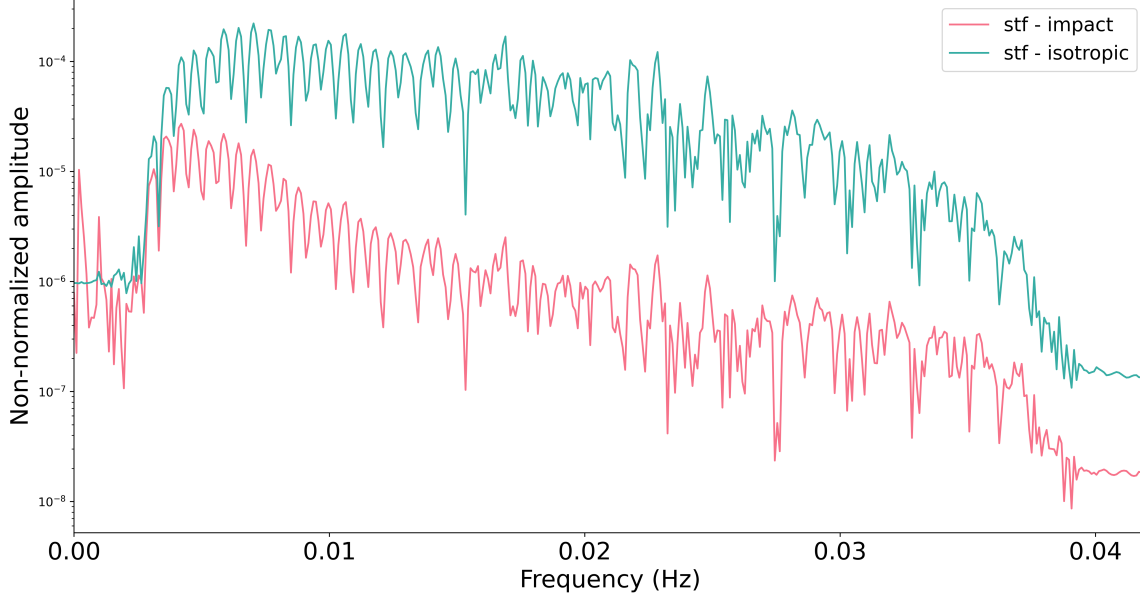


Figure 5.6: We present the spectra of the WP case, shown in Figure 5.5. In green is shown the spectra for the isotropic STF, and in red is shown the spectrum for the impact-based realistic STF. The amplitudes are non-normalized in order to reflect the difference in energy throughout the bandpass considered in our simulation setup. Consistently, the impact-based seismogram is lower in amplitude than the isotropic stf seismogram by one or two orders of magnitude throughout the whole frequency band.

scattering of the background propagation having the most impact. The impact of the plume head represents a few percent difference between the NP and the WP model. Although non-negligible, we do not expect those differences to create a massive difference in the strain field within the magma chamber. On the other hand, the difference between the SP and WP are barely visible on this scale, which confirms the tendency described by Chantel et al. [2016]. Using an unrealistically large low-velocity amplitude changes the results marginally, making it difficult to build up amplification solely based on the elastic parameters. However, this conclusion might be different when taking into account 3D attenuation media and could vary with the shape of the slow-velocity anomalies, and more work is to be done on both hypotheses to draw a more definite conclusion. Finally, even if the overall amplitude between the impact-based STF and the isotropic STF differs by one or two orders of magnitude, that trend remains consistent with both STFs.

In Figure 5.8, we show the evolution of the waveforms with respect to the depth of the receiver. With this figure, it becomes clear that the amplitude generally decreases as a function of depth. In fact, at 400km depth, the recorded amplitude is less than half of the

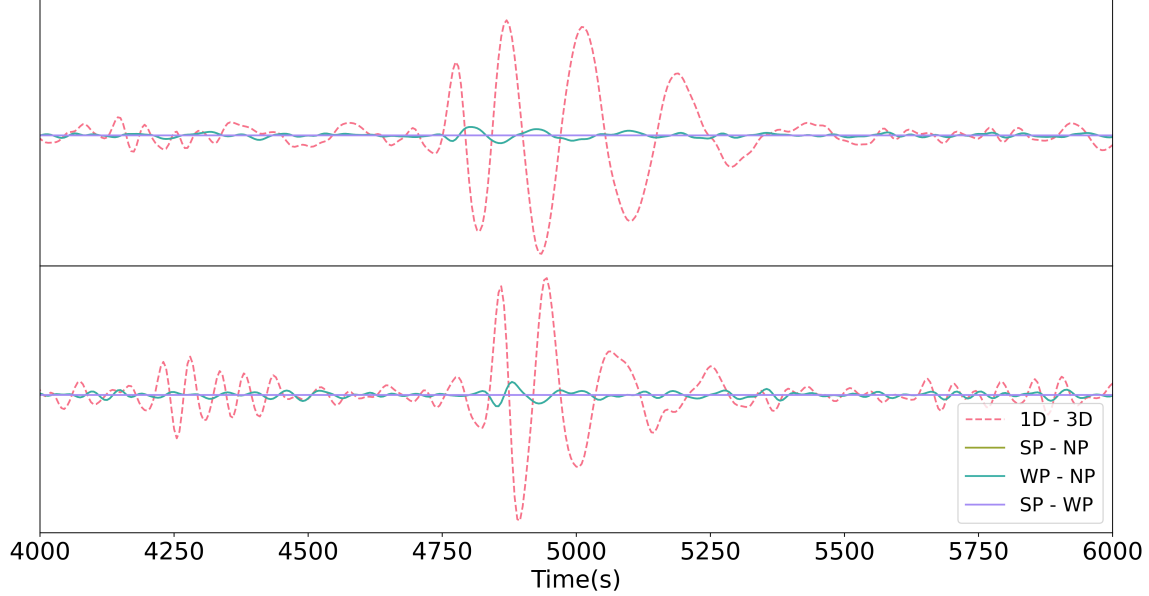


Figure 5.7: Difference of the traces shown Figure 5.5. This time, the traces are shown between 4000 and 6000 seconds, to focus on the main Surface Wave arrivals. All traces are presented on the Z component. The scale of the figure is the same as Figure 5.5. The upper panel shows the case where we have convolved with the impact STF, whereas the lower panel shows the traces obtained for the convolution with the isotropic STF. We observe the biggest differences between the 1D background model, and the 3D background model. However, there is a noticeable difference (10%) between the NP case and the WP. The difference between the WP and SP is one order of magnitude less, and barely visible on this scale.

one recorded at the surface. We can hence rule out a mechanism of focusing at the center of the magma body which would be a potential trigger for potential eruptions.

5.4 Conclusions and Further Work

In addressing the question of whether distant seismic sources and their propagating waves can induce sufficient dynamic stresses to trigger volcanic activity in the case of the K-Pg Mass Extinction, we have, by necessity, taken an interdisciplinary approach. This approach involved: (1) the realistic simulation of a projectile impacting the target set to appropriate values for the Chicxulub impact event, the dynamics of which were calculated by the state-of-the-art iSALE code Wünnemann et al. [2006]. (2) The extraction of the equivalent seismic

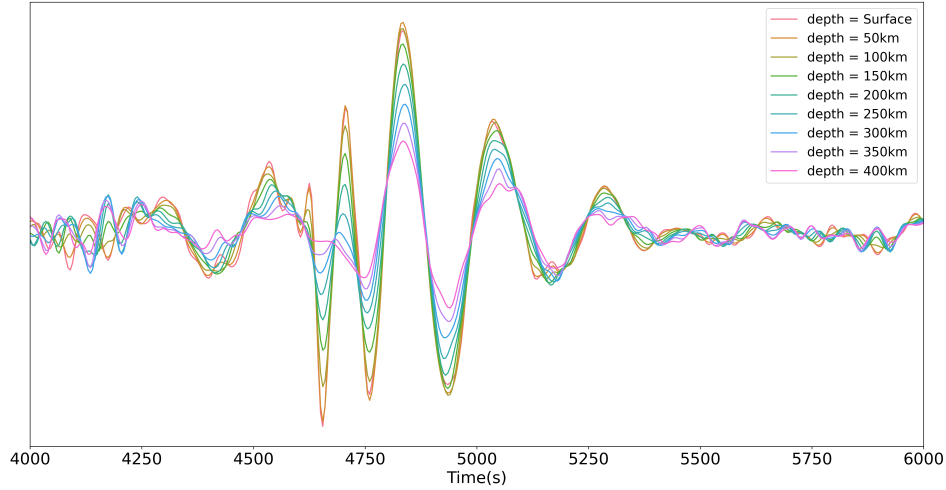


Figure 5.8: Displacement seismograms as a function of time at the center of the plume head and at different depths. Each seismogram is recorded every 50km depth to monitor the evolution of the maximum amplitudes as a function of depth. The time series are shown between 4000 and 6000 seconds, as this is where the Surface Wave train, with the most amplitude is observed. We note a linear trend between the depth of recording and the amplitude, with a noticeable decrease of amplitude as the seismogram is recorded deeper.

moment and source time functions from the impact simulation output. (3) The determination of the Green's Functions for the impulse force for various Earth model settings using the Spectral Element Method wave propagation software SPECFEM Komatitsch and Vilotte [1998]. Finally, (4) the sources and Green's functions were convolved to produce synthetic seismograms which we have presented. We focused on whether the presence of a plume head might change the associated wave propagation physics sufficiently to potentially produce greater dynamic strains.

We find that the effects on wave focusing within the plume are insufficient to distinguish the different cases. The resulting seismograms are not too dissimilar when comparing our background models (without the plume structure). However, we highlighted the importance of using a realistic, impact-based STF in order to not overestimate the peak ground/velocity displacement in the wavefield that results from the impact. Indeed the isotropic STF is too simplistic and fails to transcript the way the energy is liberated in the event of an impact.

However, our conclusions are not sufficient to truly address the question. First, we have considered only two plume configurations. A more exhaustive and systematic consideration of different plume geometries, velocity and Q anomalies should be considered. In fact, one could consider Earth models that honor the difference between present-day and ≈ 65 Ma

mantle heterogeneity. As such, we could also turn to tests in which present-day temperature anomalies within the mantle have been back-advected in time [e.g., Ghelichkhan and Bunge, 2018]. In addition, from the seismograms, dynamic strains may be more accurately estimated. These strains may then be used, as input, to magma chamber models which can fully address whether such induced dynamic strains can trigger volcanism. Such work is underway as we continue to explore this question.

Finally, while we have focused this study on the case of the Chicxulub impactor and the eruption of the Deccan Traps, and a potential link to causality – the workflow and methodology are fully extendable to the broad class of volcanism triggered by distant seismic sources.

Chapter 6

Conclusion

The work presented in this dissertation seeds new lines of investigation in several aspects towards understanding Earth processes. In Chapter 2 we improved the method known as Box Tomography so that it may be applied for realistic Earth geometries. With this advancement, it will be possible to greatly refine seismic models within select regions of Earth’s interior. This flexibility offers a means to honor the reachable range of resolutions within any given dataset and the variation of data coverage within any mantle region. As a complement, with mixed resolution models, or in the event of patching several models into one, in Chapter 3, we introduced a new a tool that allows the merging of mixed resolution models self consistently. This tool will enable analysis of any multi-scale surficial or volumetric spherical field in a manner that does not introduce artefacts. These patching practices are widely used within many subfields of Earth science, and so we anticipate that this tool will be a useful contribution that facilitates research across a broad range of problems. In Chapter 4, we broadened the length and timescale of focus to deep mantle buoyancy, investigating an oscillation in the length-of-day that occurs roughly $\sim$ six years. We concluded that if the oscillation is driven by a mantle-inner core gravitational coupling, then the period of oscillation may prove to be a useful constraint to test competing hypotheses on our ideas of deep mantle buoyancy. In future work, we will consider other competing theories for the six-year oscillation in order to understand the relative contributions and further test whether the oscillation can still be a useful constraint mantle structure. Finally, we tested the hypothesis of whether seismic waves, generated by the Chicxulub impact could trigger volcanism at the Deccan Traps, by simulating wave propagation in a realistic Earth model. We found, in our suite of tests, that the amplification of waves as they focus within the Deccan Trap region is insufficient. However, before ruling this out as a cause, further work aims to explore the sensitivity of the amplification to the magnitude of the seismic anomalies beneath Deccan during that time period (these anomalies have non-negligible uncertainty). As yet, the trigger of the Deccan Trap volcanism remains elusive.

Moving from the short timescale and short wavelength, to the long timescale and long wavelength, and how to consider problems that combine mixed wavelengths, the theme across all these chapters has been to introduce techniques in which we can enhance and

further explore our knowledge on mantle heterogeneity and the associated processes that arise from this heterogeneity.

Appendix A

Supplementary material for chapter 1

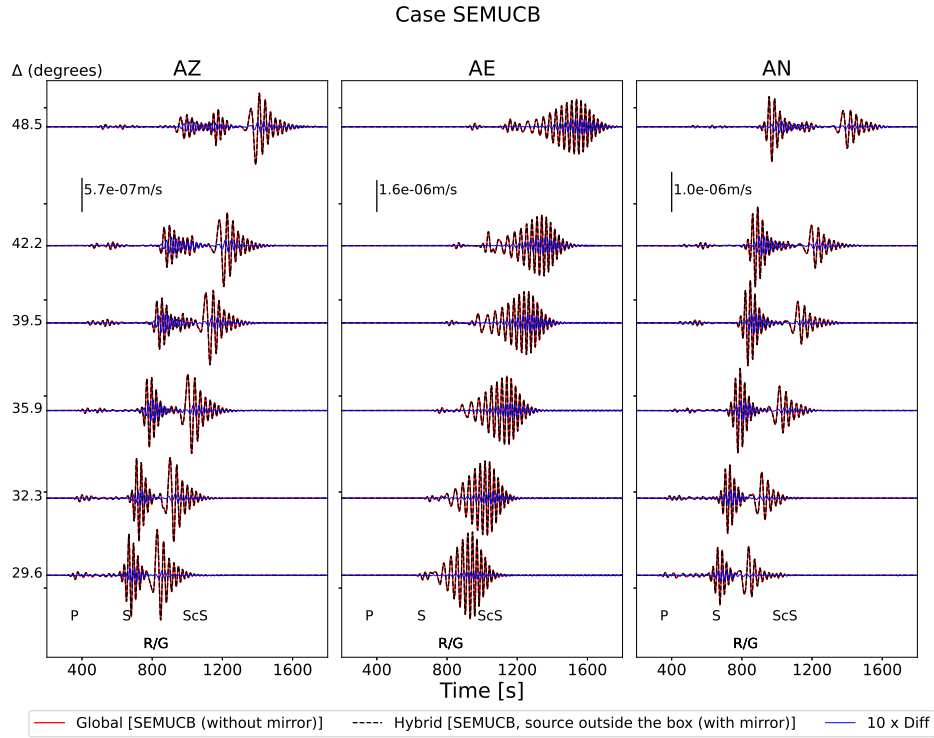


Figure A.1: Benchmark results in the SEMUCB-WM1 model French and Romanowicz [2014], without 3D crust, ocean or anelastic attenuation, for the line A shown in Fig. 4. The reference SPEC-FEM3D_globe solution (red), is compared to the hybrid seismogram obtained with the "box tomography" methodology described in this paper (black dashed line). The difference between the two time-series (blue) is enlarged by a factor of 10. The wavefield is presented in velocity (m/s). Left panel: Vertical component, arranged with distance from the epicenter. Center panel: East component. Right panel: North component.

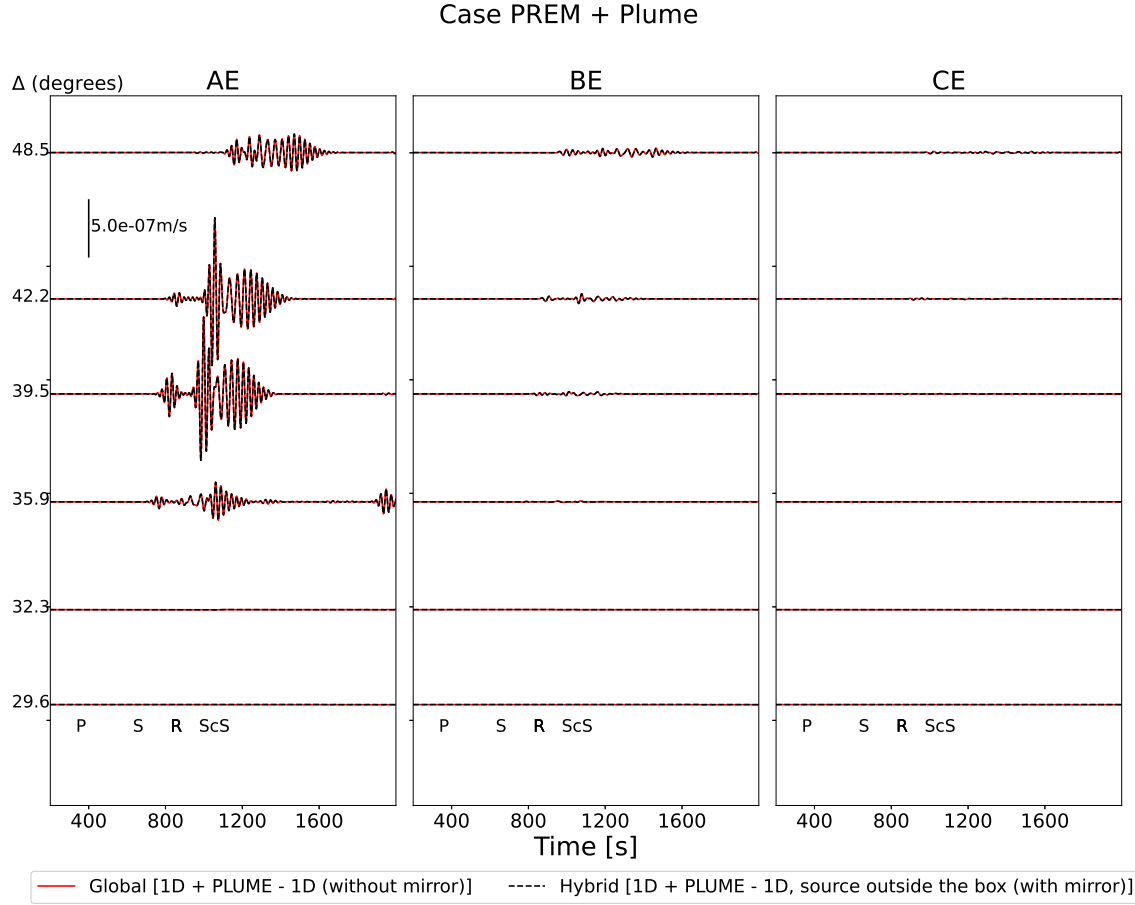


Figure A.2: Benchmark results in the 1D-PREM background model with a plume-like 3D anomaly in the target region for all stations. The results are shown on the same scale, visible at the top left corner of the left panel. Plotted here are the differences between the computations with and without the 3D plume anomaly. The reference SPEC-FEM3D_globe solution (red) shows a good agreement with the hybrid seismogram (dashed black line) obtained with the methodology described in this paper. Left panel: East component of the velocity wavefield, for line A. Center panel: East component of the velocity wavefield, for line B. Right panel: East component of the velocity wavefield, for line C.

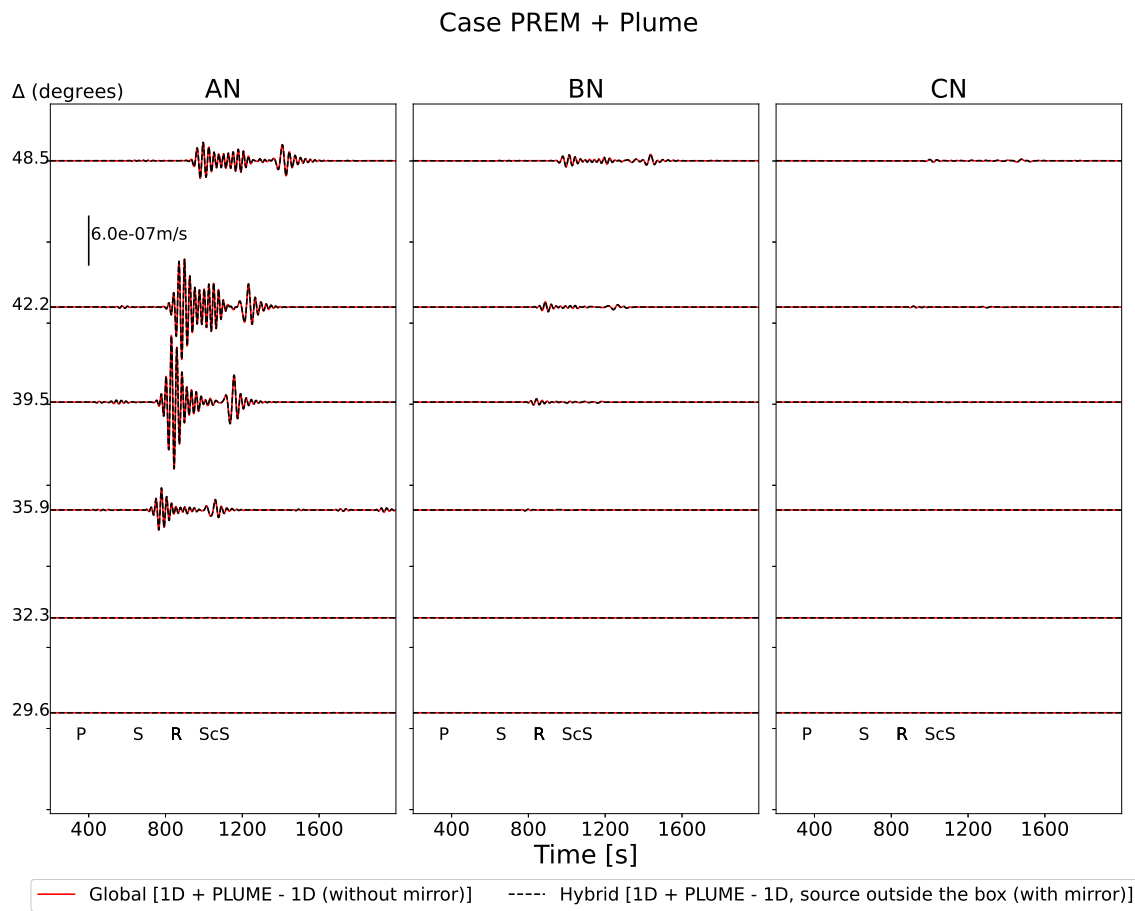


Figure A.3: Same as Fig. A.2, but for the N component in the PREM background model for the entire array, with a 3D plume added in the target region.

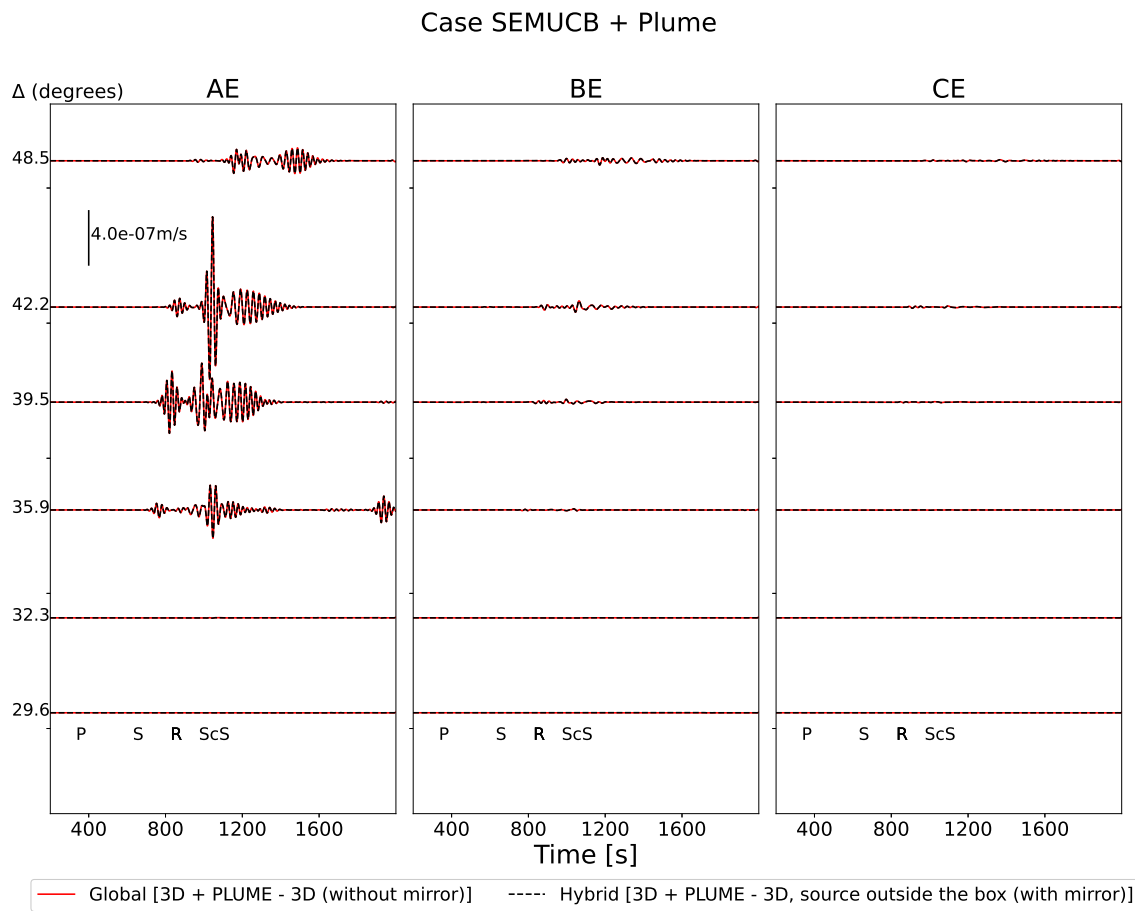


Figure A.4: Same as Fig. A.2, but for the E component in the SEMUCB_WM1 background model, with a 3D plume added in the target region, for the entire array.

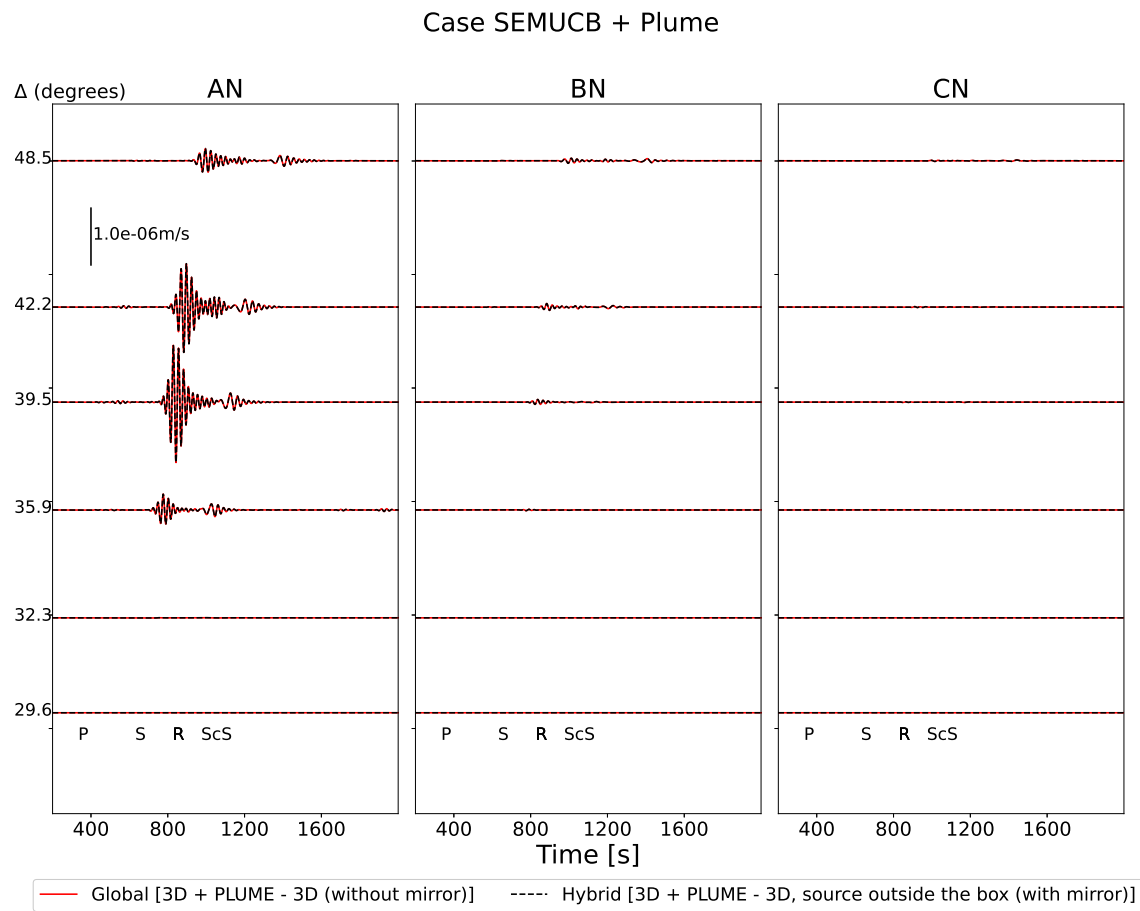


Figure A.5: Figure S5: Same as Fig. A.2, but for the N component in the SEMUCB_WM1 background model, with a 3D plume added in the target region, for the entire array.

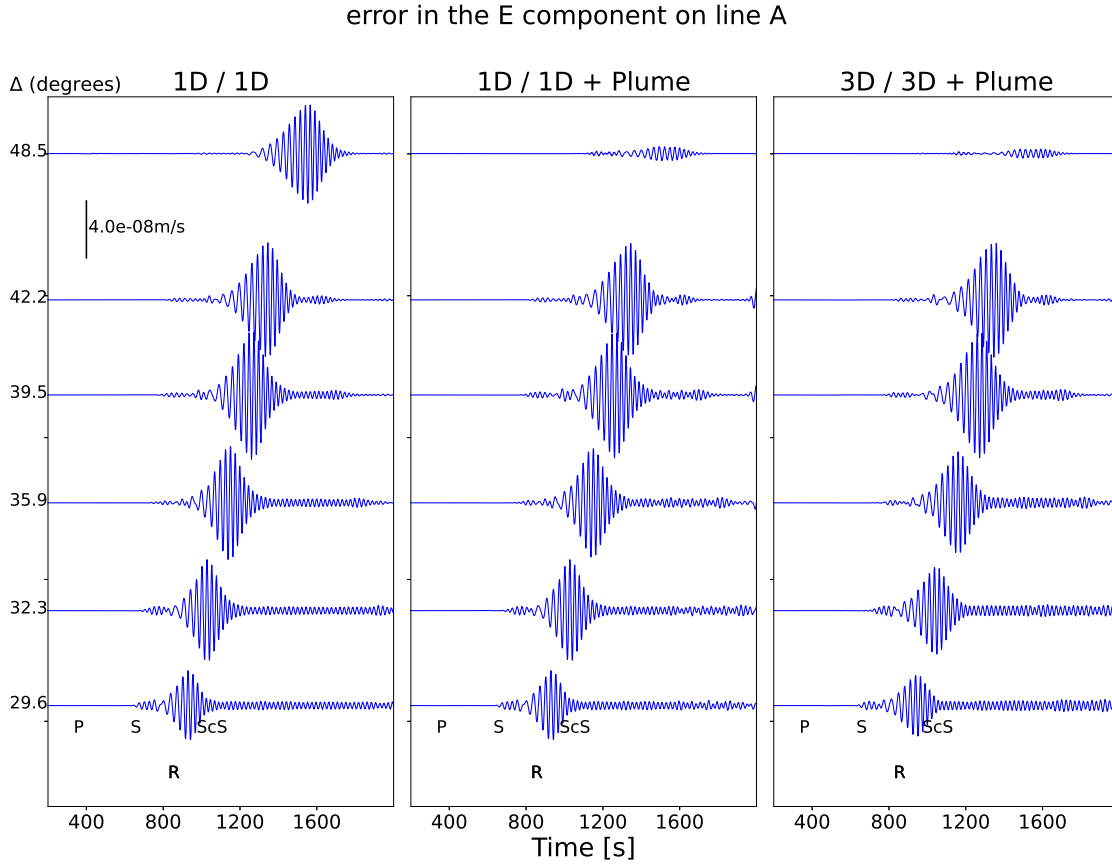


Figure A.6: Differences of the E component between the reference and hybrid seismograms, computed for all three benchmarks for all stations in line A (passing through the synthetic plume) and presented in velocity (m/s). Note the amplitude scale, which is 40 times smaller than in Fig. A.1. The amplitude of the error obtained is consistently below 2.5%, for all the stations. Left panel: Errors for the 1D case. Center panel: Errors for the case with 1D PREM in the background, and a 3D low-velocity plume-like anomaly in the target region. Right panel: Errors for the case where the background model is 3D SEMUCB_WM1, with a low-velocity plume-like anomaly located in the target region.

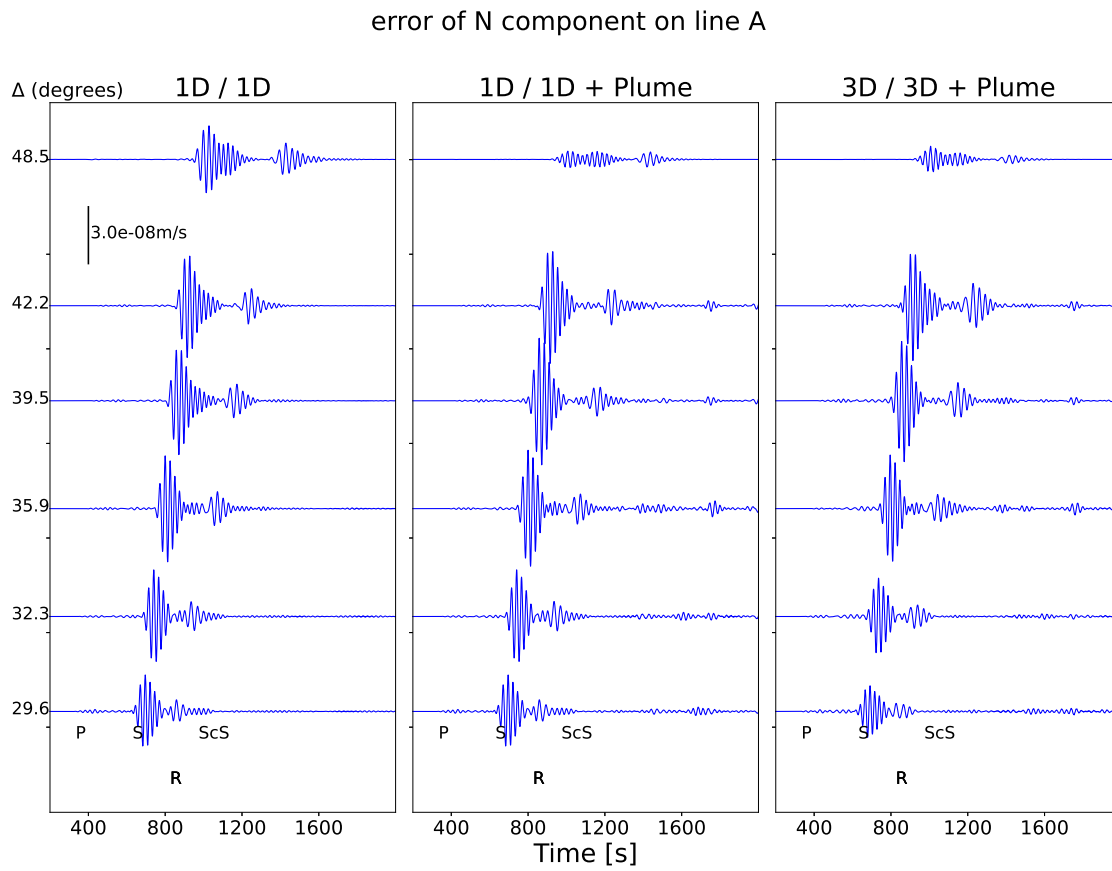


Figure A.7: Same as Fig. A.6, but for the N component.

Appendix B

Real-Time data compression using B-splines

In the classical data resampling approach for compressing real-time signals, the data are first filtered and then decimated e.g. as in Lanczos resampling. Here we adopt a slightly different strategy which is a two-step optimal curve fitting method. The first step is similar to the classical approach as the data are filtered and then decimated in real-time. In the second step, some post-processing is applied to the filtered/decimated recordings to obtain optimal representations of the time series (in the least square sense).

Our objective is to compress a seismogram $d(t)$ output by a numerical solver and represented using its discrete values $d_i = d(t_i = i\Delta_t)$ ($i = 0, N_t$) stored in vector $\mathbf{d}$. We wish to obtain an approximation

$$d^B(t) \approx d(t) \quad (\text{B.1})$$

that is represented by a smaller number of coefficients $N_B \ll N_t$ stored in vector $\mathbf{d}^B$. To do so, we represent $d^B(t)$ as a B-spline curve i.e. as the linear combination

$$d^B(t) = \sum_{i=1}^{N_B} \beta_i B_i^p(t) \quad (\text{B.2})$$

where $B_i^p(x)$ are the N_B basis functions with polynomial order p and can be computed using the Cox de Boor recursion formula:

$$B_i^0(x) = \begin{cases} 1 & \text{if } k_i < x < k_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.3})$$

$$B_i^p(x) = \frac{x - k_i}{k_{i+p} - k_i} B_i^{p-1}(x) + \frac{k_{i+p+1} - x}{k_{i+p+1} - k_{i+1}} B_{i+1}^{p-1}(x). \quad (\text{B.4})$$

We choose the knot vector as $\mathbf{k} = \{k_i = (i - p - 1)\Delta_t^B\}$, where $\Delta_t^B = N_c \Delta_t$ and the integer $N_c \approx N_t/N_B$ is the compression ratio. The basis functions $B_i^p(x)$ are represented in

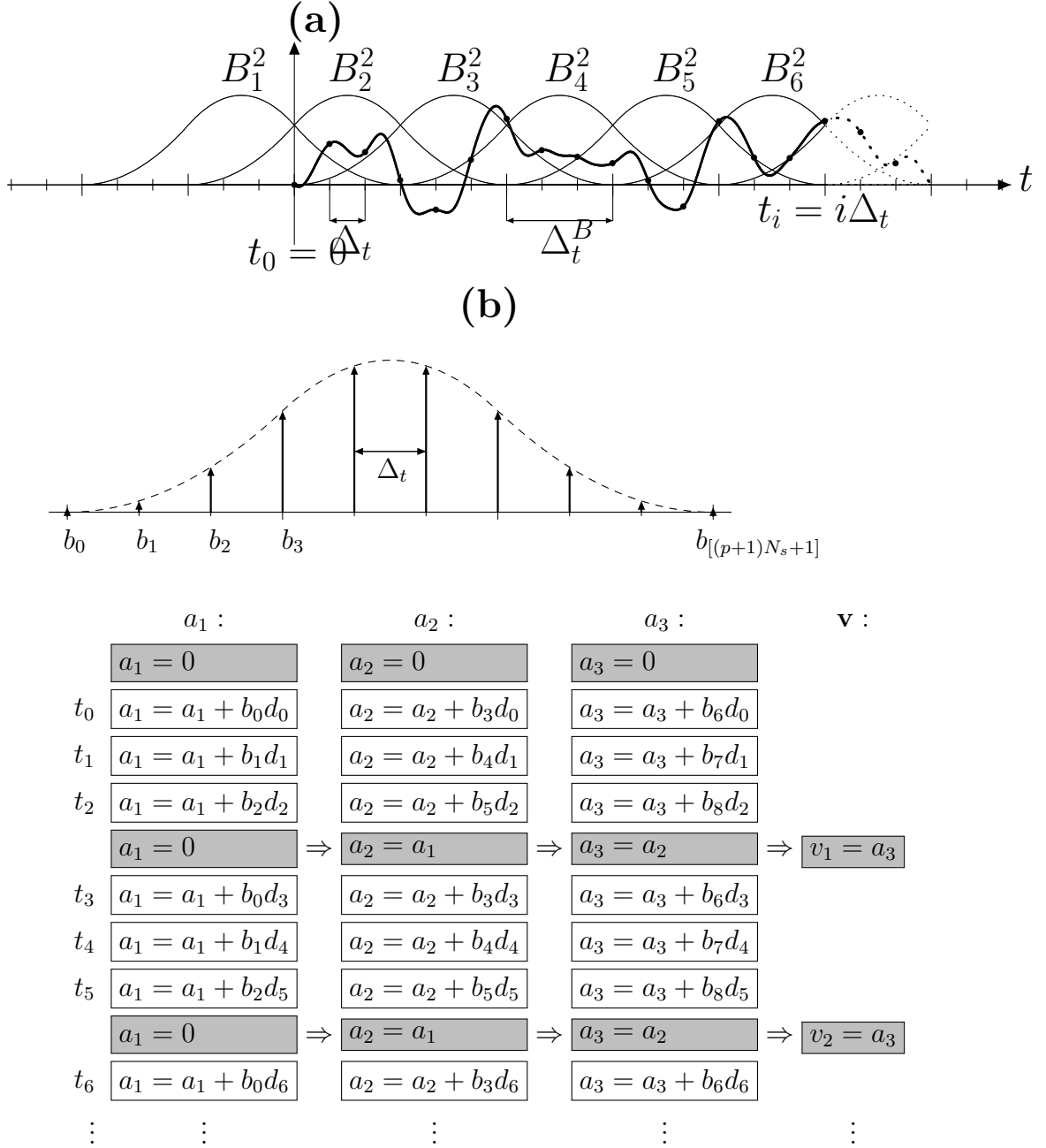


Figure B.1: Continued on the following page

Figure B.1: **(a)** The solid line shows the discrete signal $d(t)$ to be compressed represented by its values $d(t_i)$ at times $t_i = i\Delta_t$. The bell-shaped curves are the first few B-spline basis functions B_i^p constructed using the knot vector $\mathbf{k} = k_i = (i - p - 1)\Delta_t^B$ where $\Delta_t^B = N_c\Delta_t$, $N_c = 3$ and $p = 2$. **(b)** The coefficient $b_i = B_0^p(t_i)$ correspond to the discrete values of the reference basis function evaluated at times $t_i = -(p + 1) * \Delta_t^B + i * \delta_t$. They are employed to update the memory variable in Fig B.1(c). **(c)** Graphic representation of the time marching algorithm employed for evaluating the components of the vector $\mathbf{v} = \mathbf{B}^T \mathbf{d}$ in eq. (B.6). The vector $\mathbf{v}$ is constructed using the memory variables a_i ($i = 1, N_c$). At each time step Δ_t of the simulation, the memory variable incremented accordingly to the assignation inside the boxes. Whenever the discrete t_i time reaches the value $t_i = kN_c - 1$ ($k = 1, 2, 3, \dots$) the memory variable a_{N_c} that is equal to the *kest* value v_i of vector $\mathbf{v}$ is written to disk. At the end of the simulation the element elements in vector $\mathbf{v}$ are filled with the memory variables in consecutive order.

Fig. B.1(a). They are compactly supported inside the intervals $[k_i, k_{i+p+1}]$ and are equal to zero elsewhere. The number of basis functions N_B needed to represent $d^B(t)$ corresponds to the index of the last basis function that has non-zero values inside the interval $[0, N_t\Delta_t]$. By writing eq. (B.1) for all discrete times t_i ($i = 0, N_t$) and using the substitution in eq. (B.2), we obtain the linear system:

$$\mathbf{B} \mathbf{d}^B = \mathbf{d} \quad (\text{B.5})$$

where the matrix $\mathbf{B}$ has dimensions (N_t, N_B) and its *iest* row contains the values of the basis function $B_i^p(x)$ evaluated at times t_i ($i = 0, N_t$). Because $N_B \ll N_t$ the linear system in eq. (B.5) is over-determined, however, a least square solution $\mathbf{d}^B$ can be obtained by solving

$$\mathbf{A} \mathbf{d}^B = \mathbf{B}^T \mathbf{d} = \mathbf{v} \quad (\text{B.6})$$

where $\mathbf{A} = [\mathbf{B}^T \mathbf{B}]$ is a symmetric banded matrix that can be efficiently factorized and stored once and for all using the Cholesky factorization $\mathbf{A} = \mathbf{L} \mathbf{L}^T$. Our compression algorithm thus consists of two steps:

1. In real-time, during the simulation, the product $\mathbf{v}_j = \mathbf{B}^T \mathbf{d}_j$ is evaluated for all seismograms j of interest and stored to disk using the procedure detailed in Fig. B.1. This corresponds to low-pass filtering followed by decimation.
2. As a post-processing step, the linear system $\mathbf{A} \mathbf{d}_j^B = \mathbf{L} \mathbf{L}^T \mathbf{d}_j^B = \mathbf{v}_j$ is solved for all seismograms using forward and backward substitution.

Once the vectors $\mathbf{v}_j$ are known, the compressed seismograms may be evaluated (uncompressed) at an arbitrary time using eq. (B.2).

Appendix C

Convolution of time series in the B-spline domain

Say we want to obtain the discrete convolution product for one point of the mirror:

$$c(t_j) = (G \star f)(t_j) = \sum_{i=-\infty}^{\infty} G(t_i) f(t_j - t_i) \quad t_j = j \Delta_t^c \quad (\text{C.1})$$

between two time-series $G(t)$ and $f(t)$ from their compressed representation $\mathbf{G}^{B_1}$ and $\mathbf{f}^{B_2}$ in bases B_1 and B_2 , respectively. Notice that the sampling rates $\Delta_t^{B_1}$ and $\Delta_t^{B_2}$ of the B-spline basis functions in bases B_1 and B_2 aren't necessarily the same. A simple strategy is to first evaluate $G(t)$ and $f(t)$ (i.e. uncompress $\mathbf{G}^{B_1}$ and $\mathbf{f}^{B_2}$ using eq. (B.2)) at times $t_j = \Delta_t^c$ and then compute $c(t)$ using the discrete convolution product in eq. (C.1). A better strategy is to directly compute the B-spline representation $\mathbf{c}^B$ of the convolution product $c(t)$. By defining the discrete signal:

$$\bar{G}^B(t) = \sum_{i=1}^{N_B} \beta_i \delta(t - (i-1)\Delta_t^B), \quad (\text{C.2})$$

we rewrite eq. (B.2) as the continuous convolution product

$$G^B(t) = \bar{G}^{B_1}(t) \star B_1(t). \quad (\text{C.3})$$

It follows that:

$$c(t) = (G \star f)(t) = \bar{G}^{B_1}(t) \star B_1(t) \star \bar{f}^{B_2}(t) \star B_2(t). \quad (\text{C.4})$$

$$= [\bar{G}^{B_1}(t) \star B_1(t) \star \bar{f}^{B_2}(t)] \star B_2(t). \quad (\text{C.5})$$

$$= [\bar{f}^{B_2}(t) \star B_2(t) \star \bar{G}^{B_1}(t)] \star B_1(t) \quad (\text{C.6})$$

which suggests that the B-spline representation $\mathbf{c}^B$ of the convolution product $c(t)$ can be computed using two approaches: (1) by first evaluating the B-spline curve G^{B_1} at times

$t_i = i\Delta_t^{B_2}$ and then convolving the result vector with vector $\mathbf{f}^{B_2}$ using a discrete convolution to obtain $\mathbf{c}^{B_2}$ represented in basis B_2 , or (2) by first evaluating the B-spline curve f^{B_2} at times $t_i = i\Delta_t^{B_1}$ and then convolving the result vector with vector $\mathbf{G}_1^{B_1}$ using a discrete convolution to obtain $\mathbf{c}^{B_1}$ represented in basis B_1 . Knowing the compressed representation $\mathbf{c}^B$, we can then evaluate $c(t)$ at arbitrary time. Notice that, when $B_1 = B_2$ one may directly convolve vector $\mathbf{G}^B$ with vector $\mathbf{f}^B$ and one obtains the representation $\mathbf{c}^{B^{2p}}$ in basis $B^{2p} = B \star B$.

For performance and stability purposes, each convolution product will be performed in the Fourier domain, using the convolution theorem. The convolution becomes:

$$c(t) = \mathcal{F}^{-1} [\mathcal{F}(G) \times \mathcal{F}(f)] \quad (\text{C.7})$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ represent respectively the Fourier transform and the inverse Fourier transform operation.

Appendix D

Reinterpolate geo-referenced datasets

Let S be a sphere with radius R , and let (θ, ϕ) be spherical coordinates on S . Let $f(\theta, \phi)$ be a function defined on S .

We want to find a function $g(\theta, \phi)$ that interpolates f at a set of N data points (θ_i, ϕ_i) , where $i = 1, 2, \dots, N$.

We construct g as a linear combination of spherical spline basis functions:

$$g(\theta, \phi) = \sum_{i=0}^N c_i B_i(\theta, \phi) \quad (\text{D.1})$$

where $B_i(\theta, \phi)$ are the spline basis functions, and c_i are the coefficients that we want to determine.

To determine the coefficients c_i , we minimize the following expression:

$$E = \sum_{i=0}^N [f(\theta_i, \phi_i) - g(\theta_i, \phi_i)]^2 \quad (\text{D.2})$$

which can be solved as a simple linear system $\mathbf{B} \mathbf{c} = \mathbf{f}$; where $B_{i,j} = B_j(\theta_i, \phi_i)$ ($B_j(\theta_i, \phi_i)$ being the value of the j th spline basis function evaluated at the data point (θ_i, ϕ_i)), $\mathbf{f}_i = f(\theta_i, \phi_i)$ is the column vector containing the values of our function at known latitudes and longitudes, and $\mathbf{c}$ is the column vector containing the coefficients c_i .

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