Numerical seismology across the scale
From experimental acoustic to the core-mantle boundary

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NUMERICAL SEISMOLOGY ACROSS THE SCALE: FROM EXPERIMENTAL ACOUSTIC TO THE CORE-MANTLE BOUNDARY

A thesis submitted to attain the degree of
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Abstract

Numerical techniques are useful in a variety of problems in Seismology and Earth Sciences. Here we present two applications one at large scale and one at small scales that fully benefits from them.

The core-mantle boundary (CMB) is one of the most important global interfaces of the Earth, separating the solid silicate mantle from the fluid iron core. Its topography has not been characterized well yet, although it could provide precious insights about dynamics and thermal profile of the surrounding regions. Complex structures above and below are keys to understand past and future evolution of our planet. In this project, we aim to characterize the sensitivity of seismic waves due to CMB topography in terms of forward and inverse seismic modeling. Our study fully embeds the most recent developments of numerical seismology such as spectral element based waveform inversion and time-frequency seismogram analysis. In chapters 1 and 2 we use the adjoint method to compute sensitivity kernels combined with an efficient spectral-element code to integrate the wave-equation on the full Earth. Using large scale spectral element simulations, we analyse the effects on seismograms due to topography and/or 3-D mantle. In chapter 2 we use and study boundary sensitivity kernels to compute maps of the CMB first using synthetic data for a benchmark and later with real data. Following a similar theoretical, at the end of chapter 2, we introduce a volumetric inversion algorithm based on mantle sensitivity kernels that can be used for mantle tomography, and coupled to the CMB boundary inversions to set up a joint inversion mantle and CMB topography. In a second project, we show how large spectral-element simulations help disentangling the role of source, scattering and reverberations, using the ambient-noise technique to extract the Green's function on a laboratory experiment scale. This technique, which is revolutionary because it does not require earthquakes to infer Earth properties, is expected to be the source of data for global tomographic studies, like the one presented in the first two chapters. Making use of a thin aluminium plate where flexural waves propagates, we focus on the extraction of the coda which contains scattered waves and multiple secondary arrivals. In the study we also consider the influence of the source distribution and the diffusivity of the wave-field.
Sommario

I metodi numerici costituiscono un importante sussidio in molti problemi di sismologia e più in generale, nelle scienze della terra. In questo lavoro ne presentiamo due esempi su scale molto diverse. Il primo rappresenta un problema a scala globale, mentre il secondo è su scala di laboratorio.

Il confine nucleo-mantello (CMB) è una delle più importanti interfacce che caratterizzano la struttura interna della terra. Essa separa il mantello, composto prevalentemente da silicati dal nucleo esterno, composto da ferro liquido ad alta temperatura. La topografia di questa interfaccia non è ancora stata mappata in dettaglio ed i pochi studi effettuati evidenziano sostanziali differenze. Una più approfondita conoscenza della sua topografia potrebbe permetterci di capire la dinamica, la composizione e la temperatura delle regioni che la circondano. Queste complesse strutture al di sopra e al di sotto, sono le chiavi per comprendere l’evoluzione del nostro pianeta. In questo progetto miriamo a caratterizzare la sensitività delle onde sismiche alla topografia del CMB sia dal punto di vista del così detto “problema diretto” che in un’ottica tomografica ovvero, il “problema inverso”. Il nostro studio è supportato interamente dalle più recenti tecniche di calcolo agli elementi spettrali per il problema inverso e di analisi dei sismogrammi nel dominio del tempo o della frequenza. Nel primo e secondo capitolo utilizziamo “l’adjoint method” per calcolare i così detti “sensitivity kernels” utilizzando un efficiente codice agli elementi spettrali per integrare l’equazione d’onda. Attraverso delle simulazioni ottenute su potenti centri di calcolo analizziamo gli effetti sui sismogrammi dovuti alla presenza di topografia e strutture 3-D nel mantello. Nel secondo capitolo utilizziamo e studiamo “kernels” sensibili alla topografia, per ottenere delle mappe del CMB, invertendo prima dei dati sintetici come benchmark e in seguito dati reali. Utilizzando una teoria e degli algoritmi simili a quelli usati per kernels per la topografia, alla fine del secondo capitolo, introduciamo i kernels sensibili alle eterogeneità del mantello utili per ottenere immagini tomografiche del mantello e per essere accoppiati a quelli per la topografia in una così detta “joint-inversion”. In un secondo progetto, che occupa per intero il terzo e ultimo capitolo, utilizziamo le tecniche della sismologia computazionale, (elementi spettrali in particolare) per capire come la funzione di Green viene estratta in un esperimento di acustica in laboratorio basato sull’ambient-noise interferometry. Questa tecnica, rivoluzionaria in quanto non richiede terremoti per ricavare le proprietà del mezzo al contrario della sismologia tradizionale, sembra essere la più promettente fonte di dati per la tomografia globale (ad esempio nell’argomento trattato nei primi due capitoli) negli anni a venire. Utilizzando come mezzo di propagazione una piastra di alluminio sottile e limitata in cui vengono generate “onde flessurali”, studiamo l’estrazione della coda della funzione di Green che contiene lo scattering e gli arrivi successivi al primo. La ricostruzione dello scattering è rimasta finora incompleta in esperimenti numerici e di laboratorio, questo lavoro ne completa la trattazione.
Chapter 1: Seismic waveform sensitivity for global boundary topography  We investigate the implications of lateral variations in the topography of global seismic discontinuities, in the framework of high-resolution forward modelling and seismic imaging. We run 3-D wave-propagation simulations accurate at periods of 10 s and longer, with Earth models including core-mantle boundary (CMB) topography anomalies of \( \sim 1000 \text{ km} \) spatial wavelength and up to 10 km height. We obtain very different waveform signatures for \( P_c P \) (reflected) and \( P_{\text{diff}} \) (diffracted) phases, supporting the theoretical expectation that the latter are sensitive primarily to large scale structure while the former only to small scale, where large and small are relative to the frequency. \( P_c P \) at 10 s seems to be well suited to map such a small scale perturbation while \( P_{\text{diff}} \) at the same frequency carries faint signatures that do not allow any tomographic reconstruction. Only at higher frequency the signature becomes stronger. We present a new algorithm to compute sensitivity kernels relating seismic travel times (measured by cross-correlation of observed and theoretical seismograms) to the topography of seismic discontinuities at any depth in the Earth using full 3-D wave propagation. Calculation of accurate finite-frequency sensitivity kernels is notoriously expensive, but we reduce computational costs drastically by limiting ourselves to spherically symmetric reference models, and exploiting the axial symmetry of the resulting propagating wave-field that collapses to a 2-D numerical domain. We compute and analyse a suite of kernels for upper and lower mantle discontinuities that can be used for finite frequency waveform inversion. The \( P_c P \) and \( P_{\text{diff}} \) sensitivity footprints are in good agreement with the result obtained cross-correlating perturbed and unperturbed seismogram, validating our approach against full 3-D modelling to invert for such structures.

Authors: Andrea Colombi (ETH Zuerich), Tarje Nissen-Meyer (ETH Zuerich), Lapo Boschi (UPMC Paris), Domenico Giardini (ETH Zuerich). Published in Geophysical Journal International

Chapter 2: Efficient waveform inversion for CMB topography  The core mantle boundary and its surrounding regions are partially known and its topography is directly linked to the dynamics of both mantle and outer core. Recent studies produced topography models with mutual agreement up to degree 2. We recently implemented an inversion strategy based on 1st order Born approximation capable of full-waveform inversion down to 10s period with relatively low computational cost. Here, after introducing the inversion scheme, we validate and benchmark its performance using synthetic waveform calculated in theoretical Earth models that include different topography patterns with varying lateral wave-length from 800 to 2500 km and magnitude (\( \sim 10 \text{ km peak-to-peak} \)). The database contains mainly \( P_{\text{diff}}, PKP, P_c P \) and \( ScS \) phases. Our tests show that \( PKP \) branches,
PcP and ScS perform generally good and in a similar fashion, while scarce are the results for $P_{\text{diff}}$.

We investigate also how 3D mantle correction influences the output models finding that, despite the disturbance introduced, the models recovered do not seem biased provided that the 3D model is correct. Using manually picked ISC data and cross-correlated travel-time we propose new topography models derived both from $P$- and $S$-waves, which share some of the features found in previous studies in areas where the coverage is sufficient. By modelling travel-times residual starting from sensitivity kernels, we show how the simultaneous usage of volumetric and boundary kernels may reduce the bias coming from mantle structures.

Authors: Andrea Colombi (ETH Zuerich), Tarje Nissen-Meyer (ETH Zuerich), Lapo Boschi (UPMC Paris), Domenico Giardini (ETH Zuerich), Published in Geophysical Journal International with the title: "Seismic waveform inversion for core-mantle boundary topography"

Chapter 3: Complete Green’s function of a complex medium measured by interferometry: reverberated flexural waves on a thin aluminium plate  

Simulating the propagation of flexural waves on a thin plate, and conducting laboratory experiments on a similar plate, we attempt to identify the relative contribution of reverberation and source distribution to the diffusivity of the ambient wave field and hence to the success of seismic interferometry. The way the plate is excited is critical to the “diffuseness” of the generated wave-field. An air-jet source produces a very diffuse field that lead to the Green’s function after stacking only few cross-correlations regardless to the length of the cross-correlation window. To extract the Green’s function from the cross-correlation of time-space point sources many more realizations are necessary and a sufficiently long time window must be used to smooth out the effects of coherent first arrivals. Because of the design of the plate, the Green’s function extracted contains besides the direct arrival, reverberation from the plate boundaries and, depending on the frequency, scattering. We show that a spatially uniform distribution of point sources over the target area enhances the quality of the reconstruction removing more efficiently spurious arrivals compared to other source distributions.

Authors: Andrea Colombi (ETH Zuerich), Lapo Boschi (UPMC Paris), Philippe Roux (UJF Grenoble), Michel Campillo (UJF Grenoble). Published in the Journal of the Acoustic Society of America with the title: "Green’s function retrieval through cross-correlations in a two-dimensional complex reverberating medium"
General Introduction

Of the three chapters collected in this manuscript, two concern deep mantle seismology while the third concerns a laboratory experiment on seismic interferometry. Although both make use of procedures that belong to the broadly defined “computational seismology” domain, they are certainly two different subjects. The bridge connecting the two is that seismic interferometry may possibly provide improved data for deep mantle in the future. The first two chapters treat the study of the core-mantle boundary (CMB) which develops on the most recent technique of seismic tomography. In the next sections, we first introduce the Earth structure focusing on the deep mantle region (1). Because the study is carried on using tomography, a technique that requires the formulation and the solution of an “inverse problem” (3), it is essential to introduce the “mathematical modelling” as methodology to reproduce and to study physical systems (2). The inverse problem is then practically solved using an optimization algorithm after defining a cost function, that in our case is defined through the “adjoint method” (5). To exploit the full potential of this method the numerical solution of the wave equation is required. We accomplish that using a spectral element method (4). In the last section we introduce seismic interferometry, loosely known as ambient noise tomography by seismologists, which serves as introduction to the final chapter.

2.1 Exploring the core-mantle boundary with modern seismic tomography

Earth seismology aims to better understand structure and composition of the interior of our planet using information from seismic waves propagation at scales ranging from sediments to the inner core. The extraction of Earth section, a tomogram, illustrating the behaviour of some relevant properties is the eventual goal of seismic tomography.

2.1.1 Earth structure and CMB

The Earth at a global scale is approximated by a spherical sphere. Life exists only on top of the crust shaped by plate tectonics, which is responsible of: faulting formation, earthquakes, mountain belts, volcanism, and at a lower extent, the creation of reservoirs. The crust has roots extending between ~ 5 km and ~ 70 km below the free surface, and it is generally characterized by a rigid behaviour. Although relatively close to our living world, this region is only poorly explored and mapped because very complex and heterogeneous. Unbeatable technical obstacles limits our capacity to drill wells
and seismology is one of the few discipline able to image the complex structure that it features. The mantle is located beneath the crust, and with its $\sim 2900$ km depth occupies the bulk of the Earth. Prevalently composed by silicates that because of the pressure and temperature conditions behave as a visco-plastic solid, it is well know in geodynamics for hosting a vigorous convection mostly responsible for driving plate tectonics and cause of the most energetic phenomena visible on the crust (e.g., mid ocean ridges, hot spots, subduction). An intriguing synergy between seismic studies, geodynamical models, gravitation field measurements and mineral physics gave to us during the past years a good knowledge of this region such that it remains to tackle only the small scale structures [e.g., Ita and Stixrude, 1992; Jackson et al., 1993; Ritsema et al., 2010; Soldati et al., 2012]. Beneath the mantle the core occupies the remaining volume. Made prevalently of Iron it is mainly responsible for the Earth mass. Its external layer, the outer core, is behaving as a fluid so that shear waves do not propagate. A vigorous convection, not yet completely mapped, generates the Earth magnetic field, crucial for the existence of life on the planet. The study of the magnetic properties of the Earth, is the primary source of information for the core structure and dynamics. Seismic waves are only partially capable of sampling this region, strong attenuation and biases from overlying structures allow inference on the large scale properties limiting the capability of mapping finer structure. Those regions are separated by boundary layers across which physical and chemical properties change abruptly. The rigid crust is separated from the mantle by the Moho discontinuity (named after its discoverer Mohorovicic). The viscous mantle is separated from the fluid outer core by the core-mantle boundary (CMB) also known as Gutenberg discontinuity. The outer core/inner core interface finally completes the set of the main Earth’s discontinuity layer. Since the pioneering works of Oldham [1906], Gutenberg [1914], and Lehmann [1936], mapping the depth and laterally varying topography of seismic discontinuities has been integral to progress in understanding our planet’s structure and dynamics. Later research has focused on upper-mantle discontinuities, which are sampled by a relatively large quantity of high-quality seismic data. The 220 km, 410 km, 520 km and 660 km discontinuities have been studied in detail since the 1960s and are partly features of the Preliminary Reference Earth Model PREM (Dziewonski and Anderson 1981) still very used nowadays. The “660” in particular characterizes the bottom end of the transition zone, i.e. the boundary separating upper and lower mantle subject to important mineral phase transitions [Ita and Stixrude, 1992]. However a sudden drop of compressional wave-speed from $\sim 13$ km/s to $\sim 7$ km/s and the impossibility of transmitting shear waves, make of the CMB the strongest and most important discontinuity on Earth, yet not completely mapped. This abrupt change must either coincide, be the cause or the consequence of a very dynamic and complex surrounding environment, both from the mantle and the core side. The lowermost part of the Earth’s mantle (Fig. 2.1) just above the core mantle boundary (CMB), known as D”, has been under investigation for several years and it is thought to be crucial for the understanding of many geophysical phenomena connecting global seismology, geodynamics, geomagnetism, mineral physics and geochemistry. The outer core is a liquid layer composed prevalently of Iron and Nickel convecting turbulently. Owing to its boundary layer nature between viscous mantle and fluid iron outer core the CMB-D” is central to the properties of both regions. On the mantle side it may affect the convective regime, triggering uprising plumes, governing the destiny of the sub-ducting plates, and last but not least, ruling the chemical and mineralogical stratification. On the side of the outer core, it can add some constraints on the amount of heat flux and temperature (around 4000° C) which influences the magnetic field generated by the geodynamo. From the seismological perspective, the D” complexity is translated into strong velocity anomalies and anisotropy. Large low velocity provinces, ultra low velocity zones (ULVZ), fast anomalies and phase precursors which indicate the presence of
a moderate topography are observed [Lay and Garnero, 2004; van der Helst et al., 1998]. The effects that the presence of moderate topography at the CMB produces on seismogram trace are similar or sometimes equal to those of velocity anomaly and therefore it may be difficult to separate these effects. For instance the signal produced by ULVZ although very small compared to other large scale structure can be indistinguishable from that of topography producing a bias on either maps. Thus a neat interpretation of $D^\prime$ structures would require the knowledge of the actual shape of the CMB. A similar reasoning may be true if we are to study of the inner-core boundary. There, a moderate ellipticity is known to exist studying seismogram perturbations of magnitude comparable to those of CMB topography [Woodhouse et al., 1986]. Furthermore, geodynamo modelling have proven that even a small CMB topography can have strong influence on the magnetic field and thus it could be ruled out from other effects. The same is true for measurements coming from Earth rotation variations. The torque between mantle and outer core strongly depends on the CMB topography. Seismic tomography is one of the few tools capable of resolving this region. In the latest years this technique has been amended with a solid background theory to compute the actual sensitivity of each seismic phase [Tromp et al., 2005]. Such computation has to be undertaken with spectral element method or finite difference which are notoriously expensive. However the computing resources at the Swiss computing center (CSCS) and at ETH Zurich allowed us to carry on this study at global scale without any compromises.

2.1.2 Numerical modelling in science

Numerical or mathematical modelling of physical phenomena has an increasingly important role in science. The continuous growth of modern computer and new scientific and technological challenges fuel the constant development of new and more sophisticated models. Mathematical and numerical modelling do not exclude the need of analogical or empirical experiments but often they represent an efficient and economic alternative. In other cases, they establish the only approach because the studied phenomenon is not reproducible (earthquakes, meteorology) or at a too large scale (evolution of the universe) or at a nano-scale (atomic iterations). The numerical model has also the advantageous features of being repeatable and reproducible for varying parameters hence simulating multiple sce-
narios. Output data from simulation may be used for a wide range of purposes e.g., benchmark and improvement of theoretical models, explore unknown regions of our planet, improve design of object increase the awareness of the society over a certain phenomena, analysing unlikely scenario and its countermeasures. The data coming from direct observation are used in the same way. In the majority of the cases, numerical simulation means computing the evolution of the relevant quantities over time and space. For instance in elastic wave propagation we will keep track of the stress-strain when the material undergoes excitation by an external force. A model is initially formulated in physical and mathematical terms both based on the direct observation of the phenomena. Often the mathematical formulation of the problem is too complex to lead to a solution in a closed form. We therefore extract an approximated formulation in a discrete form leading to a reduced number of equations associated to a reduced number of unknowns. Those equations are typically solved with appropriated algorithm and the aid of a computer. Each of these phases introduces an error that displaces the approximated solution from the real one. Hence the final solution must be interpreted considering uncertainties, and model calibrated to reduce to a minimum the distance to the real phenomena reproduced. Typically the step between discretization and resolution requires the translation of the problem to a programming language (C, Fortran, Matlab) that can be executed iteratively from a computer. The seismic inverse problem fits particularly to this description, as we will see in the next paragraph and throughout the chapters.

2.1.3 Inverse problem for spherically symmetric Earth models

Non-linear inverse problems are a class of mathematical problems which often features very high complexity and they have rarely proven the existence and uniqueness of the solution by mathematical analysis. The seismic inverse problem next introduced is a perfect example for this class of problems.

We define a numerical technique (the solver, in our case based on spectra element methods, SEM) that discretize and solve the elastodynamics system for any seismic event reading in input a set of model parameters represented by a vector $\mathbf{m}$. This is called the direct problem written as $\mathbf{u} = \mathcal{L}(\mathbf{m})$ where $\mathcal{L}$ is the operator mapping model parameters space into data space. The vector $\mathbf{m}$ may contain: reference Earth model, source parameters, boundary conditions, or any further variable characterizing the solution of the direct problem. The inverse operator $\mathcal{L}^{-1}$ can be considered linear only when strong assumption on the mean properties are taken. For the remaining

Figure 2.2: Deep mantle velocity anomaly and CMB topography map obtained by seismic and geodynamical constraints by Soldati et al. [2012]
case it is highly non-linear [Tarantola, 2005]. The typical approach to circumvent non-linearity consists in a linearisation of the problem around a point of the model parameter space by mean of Taylor series assuming small perturbation. Assumption considered true in global seismology, where the average model parameters $m_{ref}$ of the media under investigation are known and only a refined representation is sought (i.e. we assume that our current Earth model represents well composition and structures. Hence the relative model perturbations to the starting or reference model reads as: $\delta m = m_{ref} - m$. Seismic stations distributed over the earth surface provide us with the data $u$ containing information about Earth’s interior. Data come as waveforms, seismogram records: displacement but also velocity or acceleration. Synthetic waveforms are calculated solving $u_{ref} = L(m_{ref})$. After the definition of a misfit measurement, a relationship that best quantifies the residual difference, $\delta u = u - L(m_{ref}) = u - u_{ref}$ the inverse tomographic problem can be restated, without loss of generalities, in terms of data residuals with respect to model perturbations. Measuring the distance between observation and synthetic via the $L_2$ norms leads to the most used definition of misfit function $X(m) = \frac{1}{2}(u - u_{ref})^T(u - u_{ref})$. Tarantola [2005] discusses all the pros and cons of such a choice. Expanding in Taylor series the cost function around $m$ and truncating at first order we obtain the linearised relationship between model variations and residuals is:

$$\delta u = G\delta m \quad \text{with} \quad G = \frac{\partial X(m)}{\partial m}$$

(2.1)

Here $G$ is known as the 1st order derivative operator (sometime Frechet derivative) with respect to model parameters and $G \cdot \delta u$ the gradient. In Colombi et al. [2012] we deal with the calculation of $G$ for the boundary topography perturbation $\delta d$ causing a travel-time difference $\delta t$ while in section 4.3 $G$ is defined as a matrix, because discretized on the inversion grid and calculated for many $\delta \mathbf{u}$, or travel-time residual $\Delta t$ where we used $\Delta$ because more appropriate for a finite measure. If no further simplifications are introduced the explicit calculation of $G$ will lead to a $O(n^2)$ with respect to $n$ the number of model parameter, i.e. the degrees of freedom of the inversion grid. This factor needs to be multiplied by the cost of each run of the solver. Fortunately the tools provided by the adjoint method allow the computation of the gradient of the misfit function that drastically reduce the computational cost, leading to an almost linear dependency with respect to the number of records included in the dataset. The accuracy extent can be potentially pushed ahead truncating Taylor series at second order. This would allow to solve the non linear problem with a higher order inversion scheme: the Newton method [Quarteroni et al., 2007].

$$m_{n+1} = m_n - [H(m_n)]^{-1}G(m_n)$$

(2.2)

Newton method updates iteratively the model parameter vector until appropriate convergence is reached (minimum distance between data and synthetics) using the Hessian $H$ as preconditioner. In practice the method is not yet applicable because the computation of the Hessian, the second derivatives matrix, is prohibitive.

### 2.1.4 The spectral element method (SEM) in elastodynamics

The SEM has been introduced into seismology in the 90’ and has since become one of the prime techniques for accurate simulations of earthquake waves. Current implementations accommodate elastodynamics including gravity, earth ellipticity and rotation, with anisotropic, (an-)elastic, acous-
tic, poroelastic media containing sharp multi-scale property contrasts and surface topography. The physics of wave propagation is well understood such that the main challenge lies in tackling complex media properties. The success story of the SEM is closely linked to its favourable balance of numerical accuracy, flexibility in accommodating complex structures, and efficiency for large-scale, parallel applications: Retaining spectral convergence due to its polynomial representation of basis functions within finite elements, the version we shall use is based on tensor products and a diagonal mass matrix such that fully explicit time schemes are used and result in extremely efficient parallel behavior. The numerical cost of the scheme is determined by the number of propagated wavelengths in 3-D, which depends upon the total record length, the earthquake source period, and is ultimately constrained by the numerical time step. The source frequency determines the meshing process, in that each element must be smaller than a local wavelength. In order to double the resolution of the simulation at fixed propagation distance, one pays a factor of approximately 16 in terms of CPU time: Two in every spatial direction and approximately half the global time step. The performance of these algorithms is measured in terms of the shortest seismic period that can be modeled. In this work we use two different software implemented with spectral elements which serve at different scopes. The first, used to set up the inverse problem, is very efficient because it relies on 1-D earth model. The second, used for forward modelling can handle full 3-D Earth model but is has very high computational complexity.

1. [Nissen-Meyer et al., 2007b, 2008] have developed a separate, stand-alone spectral-element method that circumvents this issue by assuming spherically symmetric reference models, thereby collapsing the computational domain to 2-D (Fig. 2.3a). Indeed, such spherically symmetric models explain up to 90% of the data and are commonly used as a reference starting point for inversions. For the same reason it is feasible to calculate sensitivity kernel based on an axial symmetric model and use them to perform a 3D inversion. This has the advantage that full waveforms at all frequencies can be used for large datasets. The software is open source and available under GNU license terms.
2. The implementation SPECFEM3D GLOBE [Komatitsch and Tromp, 2002a,b] won the Gordon-Bell prize in 2003. This SEM is a dedicated open-source code specifically designed and optimized for global Earth structure, and is available under GNU license terms through the Computational Infrastructure for Geodynamics (www.geodynamics.org). The SPECFEM3D GLOBE mesh honors all major and minor radial discontinuities as assumed by 1-D reference models. The mesh design is embedded in the software and the grid is structured upon hexahedral elements. The domain decomposition is intrinsic and perfectly load-balanced. No other code in the community is able to replicate such a range of realistic physics, and as such SPECFEM3D GLOBE has enjoyed growing popularity in global seismology. The sphere is meshed using hexahedra elements upon an analytical mapping (cubed sphere, Fig. 2.3b) from the six sides of a unit cube to six blocks on the surface of the Earth. In each element there are $5 \times 5 \times 5$ integration points.

2.1.5 Finite frequency sensitivity and adjoint method

With the increasing power of modern computers, traditional ray theory based tomography [Boschi and Dziewonski, 1999; Valenzuela and Wysession, 1998] is progressively abandoned in favour of more accurate but complex full waveform tomography [Fichtner et al., 2009; Hung et al., 2000; Tromp et al., 2005]. Ray theory is based on the explicit solution of the wave equation assuming the wave travelling at infinite frequency. In this framework a given seismic phase is thought to travel along a ray of infinitesimal width and therefore sensing only the path traversed by the ray. The same principle is used in other tomographic technique but in seismology is known to be a rough approximation of true propagation.

The recent findings applying 1st order Born perturbation theory [Dahlen et al., 2000] and adjoint method [Tarantola and Valette, 1982; Tromp et al., 2005] have shown that the sensitivity zone is much larger than the ray path (Fig. 2.4) and it is inversely proportional to the wavelength. With this new approach, each degree of freedom of the inversion mesh contributes to the total residuals according to the actual sensitivity calculated via the adjoint technique. The adjoint technique requires to calculate a forward and a backward propagating wave-field for every source receiver pair available in the inversion database which are then convolved to give the sensitivity kernels or partial derivatives to the data with respect to the model [Liu and Tromp, 2008]. Forward and backward field are calculated via the spectral element discretization described before. In travel-time tomography the total sensitivity is found by summing over each source receiver pair contribution weighted by a factor proportional to the travel time anomaly. The travel time anomaly is simply the cross-correlated difference in arrival time between real data and modelled data. Embedded in the adjoint framework there are also a wide set of tools for signal processing. With this approach it is also possible to utilize more complex seismic phases (diffracted, head waves, evanescent waves) that were not accounted for in ray theory. Owing to the larger information set that can be feed into the method, we are getting closer to the full waveform tomography advocated first by [Tarantola and Valette, 1982] but never really realized because of computational and data acquisition bounds.

2.2 Seismic interferometry and ambient noise

Classic seismic imaging and monitoring techniques rely on the occurrence of earthquakes or explosive events to extract data illuminating the target area. Earthquakes, which are by definition clustered in few regions, do not provide uniform coverage in time and space and the determination of the
rupture mechanism is a non-trivial task. By means of passive interferometric seismology, i.e. the “ambient noise” technique, these problems are finally circumvented because each seismic station represents potentially a source. By the expression “ambient noise”, seismologists refer to the set of procedures by virtue of which a Green function can be determined empirically based on the signal recorded by two nearby seismic instruments over a long time. This approach was foreseen in the early work of Aki [1957] in small-scale seismology and Lobkis and Weaver [2001] in acoustics, and later applied successfully to helioseismology [Duvall et al., 1993] and Earth seismology [e.g., Shapiro and Campillo, 2004]. Ambient-noise imaging exploits ambient, low-energy signal that seems to be generated continuously by the coupling between oceans and solid Earth and then scattered by Earth heterogeneities. The diffusivity of the ambient wave field, caused by the nature of the source(s) and/or by scattering, is a necessary condition for the successful application of seismic interferometry.

Many studies have already applied passive seismology at the regional scale to image crustal structure (Fig. 2.5), and at smaller scale in the context of hydrocarbon industry and monitoring (i.e. time-depending tomography of volcanoes and seismically active areas). M. Campillo and co-workers have recently analyzed ambient noise records that include the coda generated by earthquakes to show that the full spectra of body waves can be extracted using this technique Poli et al. [2012]. This result was obtained earlier in laboratory acoustics Larose et al. [2006] and it paves the way for many interesting applications in mantle and deep mantle tomography. In spite of much work and significant progress in seismic interferometry over the last decade it remains hard to estimate how good the Green’s function is reconstructed when using real data. Laboratory experiments are a powerful tool to benchmark the theory: as opposed to “field” seismic data, the medium of propagation and source mechanisms used in the laboratory are known and can be controlled. Laboratory experiments are complementary to numerical simulations, as they allow to study the physics of wave propagation in complex media without discretization and the associated approximations.

For the receiver-receiver cross-correlation to coincide with the Green’s function between the two receivers, several assumptions have to be satisfied. The diffusive nature of the wave field, and the
uniform distribution of the noise-sources are, among others, the most important although difficultly met in nature. This technique seems nevertheless to work far beyond the expectations even when initial assumptions are seemingly not met. Answers to the following questions would help clarifying this somewhat unexpected results: How close is ambient noise to being exactly diffuse; what features of the Earth (coupling between oceans and solid Earth, scattering by crustal heterogeneities and so on) contribute to its randomness and complexity? These issues are related to the asymmetry between causal and anti-causal part, to the physical meaning of quantitative measures of phase amplitude of the cross-correlation, and to the issue of reconstructing not only the main phase, but also the coda of the receiver-receiver green function. Addressing them will eventually allow to make reliable measurements of anisotropy and the attenuation (the only seismological observable that can be directly associated with temperature heterogeneity below the earth’s surface) and to reconstruct small scatterers.

Seismic ambient noise has not yet been simulated numerically in the same detail as earthquake-generated wave propagation. This could be explained by the difficulty of implementing or representing diffuse sources, of integrating the effects of scattering and the long simulation time required to reach a diffuse regime [Basini et al., 2013; Peter et al., 2011]. Thanks to the powerful clusters at the Swiss computing center we have exploited a spectral element code to benchmark ambient noise reconstruction using point sources. Simulating the propagation of flexural waves on a thin plate, and conducting laboratory experiments on a similar plate, we attempt to identify the relative contribution of scattering, reverberation and source distribution to the diffusivity of the ambient wave field and hence to the success of seismic interferometry.
Abstract  We investigate the implications of lateral variations in the topography of global seismic discontinuities, in the framework of high-resolution forward modelling and seismic imaging. We run 3-D wave-propagation simulations accurate at periods of 10 s and longer, with Earth models including core-mantle boundary (CMB) topography anomalies of ~1000 km spatial wavelength and up to 10 km height. We obtain very different waveform signatures for PcP (reflected) and P_{diff} (diffracted) phases, supporting the theoretical expectation that the latter are sensitive primarily to large scale structure while the former only to small scale, where large and small are relative to the frequency. PcP at 10 s seems to be well suited to map such a small scale perturbation while P_{diff} at the same frequency carries faint signatures that do not allow any tomographic reconstruction. Only at higher frequency the signature becomes stronger. We present a new algorithm to compute sensitivity kernels relating seismic travel times (measured by cross-correlation of observed and theoretical seismograms) to the topography of seismic discontinuities at any depth in the Earth using full 3-D wave propagation. Calculation of accurate finite-frequency sensitivity kernels is notoriously expensive, but we reduce computational costs drastically by limiting ourselves to spherically symmetric reference models, and exploiting the axial symmetry of the resulting propagating wave-field that collapses to a 2-D numerical domain. We compute and analyse a suite of kernels for upper and lower mantle discontinuities that can be used for finite frequency waveform inversion. The PcP and P_{diff} sensitivity footprints are in good agreement with the result obtained cross-correlating perturbed and unperturbed seismogram, validating our approach against full 3-D modelling to invert for such structures.

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3.1 Introduction

Since the pioneering works of Oldham [1906], Gutenberg [1914], Lehmann [1936], among others, mapping the depth and laterally varying topography of seismic discontinuities has been integral to progress in understanding our planet’s structure and dynamics. Later research has focused on upper-mantle discontinuities, which are sampled by a relatively large quantity of high-quality seismic data. The 220 km, 410 km, 520 km and 660 km discontinuities have been studied in detail since the 1960s and are partly features of PREM (Dziewonski and Anderson 1981). The “660” in particular
characterizes the bottom end of the transition zone, i.e. the boundary separating upper and lower mantle subject to important mineral phase transitions [Ita and Stixrude, 1992].

More recent studies attempted to map the actual topography of the discontinuities mainly using SS and PP precursor differential travel-time, see Deuss [2009] for a review. Discontinuity topography is coupled with mantle structure via convective flow [Flanagan and Shearer, 1999; Gu et al., 1998], so that the tomography maps can serve as constraints for geodynamics models, including the geometry of subducing slabs and presumed mantle plumes. Seismic studies of discontinuity topography have thus far been based on the ray-theory (infinite frequency) approximation; only Lawrence and Shearer [2008] made use of finite-frequency travel-time kernels as provided by Dahlen [2005]. Waveform inversions have not yet been attempted at the global scale.

The strongest discontinuity in the Earth’s interior is the core-mantle boundary (CMB), separating the solid mantle from the fluid outer core. Its topography is very likely related both to the thermal/compositional/viscosity structure (and associated convection) of the mantle [Forte et al., 1995; Soldati et al., 2012], and to the properties of the outer core, where vigorous convection is believed to generate the Earth’s magnetic dynamo [Jackson et al., 1993]. A number of authors, starting with Morelli and Dziewonski [1987], mapped CMB topography based on compressional-wave travel times, while others [e.g., Ishii and Tromp, 2001; Koelemeijer et al., 2012] inverted observations of eigenfrequency splitting, focusing on normal modes sensitive to the CMB. Most ray-theory authors find a similar degree-2 pattern with peak-to-peak topography of a few km (see Fig. 3.1 for an example), but shorter-wavelength structure is more difficult to constrain. Several studies [e.g., Boschi and Dziewonski, 1999; Soldati et al., 2003; Vasco et al., 1999] point to a discrepancy in CMB structure as mapped by core-refracted (various branches of the PKP phase) versus core-reflected seismic waves, which casts some doubt on the validity of CMB maps derived from those data. Soldati et al. [2012] show that the discrepancy can be reduced if one requires the inverse-problem solution for CMB topography to be coupled with seismic structure in the mantle according to the theory of Forte et al. [1995].

With this study we present a wave-based formulation of the seismic inverse problem associated with discontinuity topography, whose future applications to global seismic databases should help to enhance the resolution of our CMB maps. As noted, e.g., by Dahlen [2004] and [Montelli et al., 2004], ray and finite-frequency inversions may give similar results when applied to P or PcP data, but stronger differences are to be expected if the more complex, core-refracted (PKP) or diffracted \( (P_{dif}, S_{dif}) \) waves are taken into account. Our formulation is based on 1st order Born perturbation theory [Nissen-Meyer et al., 2007a] coupled with the adjoint method [Geller and Hara, 1993; Peter et al., 2007; Tarantola, 2005; Tromp et al., 2005]. Boundary sensitivity kernels presented here can naturally be applied in a joint volumetric-discontinuity inversion.

Although algorithms for joint, waveform-inversion of both volumetric and discontinuity heterogeneity are still under development, independent finite-frequency inversions for volumetric or discontinuity structures have been attempted. Much attention was devoted to volumetric inversions [Fichtner et al., 2009; Montelli et al., 2004; Tape et al., 2009], while finite-frequency discontinuity topography has been the subject of very few [Dahlen, 2005; Lawrence and Shearer, 2008; Takeuchi, 2005] studies. Discontinuity imaging is, in fact, more difficult than volumetric tomography: while the latter aims at constraining structures that presumably extend for hundreds of km in all directions, the topography of known mantle discontinuities never exceeds a few km radially and thus requires very specific source-receiver layout.

A methodology for joint volumetric-discontinuity finite-frequency inversions of seismic data is proposed by Mora [1989] in the context of exploration seismology. The treatment that we shall de-
3.2 The forward problem: Effects of boundary perturbation on seismograms

3.2.1 Global wave propagation: notation and analytic background

In our convention, vectors are denoted as boldface lower-case letters (\(u, v, \ldots\)) and tensors as uppercase letters (\(T, E, \ldots\)). Vectors and tensors are real valued functions \(\mathbb{R}^3\). For further reference about vector conventions and operations used in this article, refer to [Dahlen and Tromp, 1998].

The physical quantities have the usual meaning of linear elasticity problems formulated from a Lagrangian perspective. We define three-component vectors \(u(\mathbf{x}, t)\) as the displacement at point \(\mathbf{x}\) at time \(t\), measured in \([m]\). The first and second derivative with respect to \(t\) are respectively
velocity: \( \mathbf{u}(x, t), \partial_t \mathbf{u}(x, t) \) measured in \([m/s]\) and acceleration \( \ddot{\mathbf{u}}(x, t) \) or \( \partial_t^2 \mathbf{u}(x, t) \) measured in \([m/s^2]\). Whenever possible, we render the dependence of various physical quantities on \( x \) and \( t \) implicit.

The adimensional strain tensor is defined as the symmetric part of the displacement gradient, \( \mathbf{E} = \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \). Hooke’s relationship then gives the stress tensor: \( \mathbf{T} = \mathbf{C} : \mathbf{E} \) measured in \([Pa]\) upon the definition of \( \mathbf{C} \), the 4\(^{\text{th}}\)-order tensor containing at most 21 independent elastic constants. The practical case studies are limited here to isotropy, but our formulation remains valid for general anisotropic media.

At the global scale, the phenomenon of seismic wave propagation is explained well by linear elasticity theory. The effects of Earth’s rotation and gravitation and of the oceans are all negligible at the frequency band \((40 – 100 \text{ mHz})\) and geographic scale length \((20^\circ – 180^\circ)\) that will be considered here [Dahlen and Tromp, 1998; Komatitsch and Tromp, 2002b], while those of the Earth’s ellipticity can be accounted for by simply applying a linear correction on the data as shown by Dziewonski and Gilbert [1976].

Under these assumptions and after defining an Earth model \( \mathbf{m} \), wave propagation in the whole volume of the Earth \( \Omega \) is described by the system:

\[
\begin{align*}
\partial_t^2 \mathbf{u}(x, t) + \nabla \cdot \mathbf{T}(x, t, \mathbf{m}) &= \mathbf{f}(x, t) \quad &\text{in } \Omega \quad (3.1a) \\
\mathbf{T}(x, t, \mathbf{m}) &= \mathbf{C}(\mathbf{m}) : \mathbf{E}(x, t) \quad &\text{in } \Omega \quad (3.1b) \\
\hat{n} \cdot \mathbf{T} &= 0 \quad &\text{on } \partial \Omega \quad (3.1c) \\
\text{Interface Condition on } \Sigma \quad (3.1d) \\
\mathbf{u}(x, 0) &= 0 \quad \partial_t \mathbf{u}(x, t) = 0 \quad (3.1e)
\end{align*}
\]

where \( \hat{n} \) is the normal vector and \( \partial \Omega \) the surface of the Earth. Eq. (3.1a) expresses conservation of momentum, with the forcing term \( \mathbf{f}(x, t) = \mathbf{M} \dot{\mathbf{m}}(t) \) a function of the focal mechanism (through the moment tensor \( \mathbf{M} \)) and of the source-time function \( \dot{m}(t) \) of the earthquake. Eq. (3.1b) is known as the constitutive relationship which is defined by the selected Earth’s reference model and in seismology is often taken to coincide with Hooke’s law. The boundary conditions (3.1c) require the outer surface of the Earth to be free of tractions. Interface condition (3.1d) links regions with different physics or discontinuous properties. The solution of a differential equation like (3.1) requires the initial conditions (3.1e). In our case, the Earth is considered to be at rest at \( t = 0 \), prior to occurrence of an indigenous seismic event represented by the forcing term \( \mathbf{f}(x, t) \).

When Eq. (3.1) is used to model the propagation of realistic seismic waves in the Earth, it is crucial to choose the source-time function \( \dot{m}(t) \) appropriately. We assume \( \dot{m}(t) \) to be Gaussian; this is common practice in seismology, signal processing and image processing, and be written as: \( m(t) = \exp \left( -\gamma (t + T_0 - \tau)^2 \right) \) where \( T_0 \) is the dominant period, \( \tau \) the shift from \( t = 0 \) and \( \gamma \) the shape factor.

Improving the level of detail and elaborating models which are consistent with geological, geodynamic and geomagnetic constraints is the main goal of seismic tomography. While most authors currently agree on the long-wavelength (\( \gg 1000 \text{ km} \)) pattern of mantle structure (e.g., Becker and Boschi 2002), no agreement has been achieved on the nature of relatively small-scale tomographic features interpreted as, e.g., mantle plumes or subducting slabs. Spherically symmetric models such as PREM [Dziewonski and Anderson, 1981] explain up to 90% of travel-time observations. This is justified by the fact that very strong lateral variations are expected only in a small portion of the total volume of the Earth: the highly heterogeneous crust, and the area surrounding the CMB, while
the remaining volume is characterized by heterogeneity of small amplitude (\( \sim 1\% \) for P and \( \sim 2\% \) S velocity).

### 3.2.2 Boundary conditions

Regardless of the reference model considered, all global tomographic models share some similarities. Spherically symmetric reference models are defined as the union of spherical-shells domain \( \Omega = \Omega_1 \cup \Omega_2 \cup \ldots \), interfaces \( \Sigma \) linking different domains, and free surface \( \partial \Omega \) that bounds the outer domain where external forces are applied. Domains are all solid except for the outer core. Oceans are directly modelled at local scale, while for global studies they can be treated as external forces [Komatitsch and Tromp, 2002b]. Continuity between domains is guaranteed by the transmission condition defined at various interfaces. Depending on the nature of the two domains only certain quantities may be transmitted.

The jump of a quantity \( [u]^+ \) across an interface is obtained taking the difference of the value starting from the outer (+) to the inner (−) boundary. The transmission conditions at interface (3.1d) then read

\[
[u]^+ = 0 \quad \text{and} \quad [T]^+ = 0 \quad \text{on} \quad \Sigma_{SS}, \\
[u \cdot \hat{n}]^+ = 0 \quad \text{and} \quad [T \cdot \hat{n}]^+ = 0 \quad \text{on} \quad \Sigma_{SF},
\]

where \( \Sigma_{SS} \) and \( \Sigma_{SF} \) denote the union of all solid-solid, and all solid-fluid interfaces, respectively. Eq. (3.2b) is also valid for time-derivatives of enclosed quantities. Material properties vary smoothly within each layer. In the case of PREM they are analytically defined as 1D polynomial functions [Dziewonski and Anderson, 1981].

The solid-solid condition is naturally embedded inside the elastodynamic system. When equations are solved via finite element methods, these conditions are fundamental part of the discretization procedure (hence the jump of the quantities across the interface is entirely due to the discontinuity in the material property).

Solid-fluid boundaries, on the other hand, involve a change in the physics of wave propagation, as no shear waves can exist in a fluid medium. The elastodynamic system becomes a scalar problem formulated in terms of a potential function. The two systems are coupled together, for instance as in Nissen-Meyer et al. [2008].

### 3.2.3 Computational cost of global-scale wave propagation modelling

Although high-resolution 3-D models of the entire Earth’s mantle [e.g., Bijwaard et al., 1998; Della Mora et al., 2011; Li et al., 2008; Montelli et al., 2006; Obayashi et al., 2009; Ritsema et al., 2010; Simmons et al., 2010] are available, their direct application is bounded by computational resources, particularly if notoriously expensive waveform inversion were to be conducted. Fig. (3.2) shows that computation time for a global 3-D simulation (SPECFEM3D GLOBE of Komatitsch and Tromp [2002a]) is roughly inversely proportional to the cube of the shortest resolved period \( T_0 \). The axi-symmetric spectral element code by Nissen-Meyer et al. [2008], hereafter named AXISEM, models exact 3-D wave propagation in a spherically symmetric Earth by solving the equations of motion numerically on a 2-D disc; the size of the mesh, and, consequently, the computational costs are massively reduced, with runtime inversely proportional to the square of \( T_0 \).
3.2.4 Ground-truth synthetic database via 3-D modelling

The adjoint technique is at the core of finite-frequency full waveform tomography for computational reasons, relies on 1st order perturbation theory, i.e. a linearization that might or might not be valid depending on how far the starting model is from the true one. Its accuracy and applicability depend on data type and frequency, their error statistics, the chosen misfit function, the sparsity of data coverage, the wavelength of the anomaly we wish to resolve, the signal-to-noise ratio and inversion parameterization. Before addressing the inverse problem, forward simulations of core-sensitive seismic phases are useful to evaluate the effects of the mentioned parameters. We construct a synthetic database based on numerical integration of the equation of motion via SPECFEM3D GLOBE [Komatitsch and Tromp, 2002a]. Unlike AXISEM, SPECFEM3D GLOBE accommodates 3-D velocity and/or topography heterogeneity; comparing the results of SPECFEM3D GLOBE with those of 1st order perturbation theory allows us to quantify the accuracy of the latter for different wavelength-to-topography length-scales and seismic phases and determine settings which optimally highlight topography.

Our experimental setup is illustrated in Fig. (3.3). To isolate the effects of CMB topography, we assume a spherically symmetric Earth model (PREM). For the sake of simplicity, we neglect the effects of surface topography, crustal heterogeneity, ellipticity and gravitation (relevant at $T_0 \geq 100$ s). We simulate explosive events located around a single region of anomalous, smooth CMB topography. Seismograms calculated with SPECFEM3D GLOBE are valid down to 10 s period.
After the simulation, we can filter the modelled traces to isolate any desired frequency band, with no need to repeat the same simulation for different frequencies.

We utilize different source-station distributions depending on the phase that we wish to analyse. Fig. 3.4a shows a dense, relatively low-aperture receiver network designed for the small-aperture phase $P_cP$: a $60^\circ \times 60^\circ$ area around the center of the anomalous CMB area is covered by receivers every $1^\circ$. The $P_{diff}$ phase is naturally characterized by a broader range of possible epicentral distances, and is accordingly analyzed on the wider-aperture array ($120^\circ \times 120^\circ$ with $2^\circ$ spacing) of Fig. 3.4b. We also experiment with different patterns of CMB topography: closely-spaced depression and uplift (Fig. 3.5b), defined by the colatitude-derivative of a Gaussian function, or a broad (Gaussian) uplifted region (Fig. 3.5a). A section of seismograms due to an event at the bottom-left for the rightmost column of receivers depicted in the event-receiver layout in Fig. 3.4a is portrayed in Fig. 3.6.

As anticipated by Fig. 3.2, these tests are computationally very expensive. To simulate a 25 min-long seismic record accurate down to 10 s period, we need 200 Gbyte of system memory distributed over 486 processors for a wall clock time of about 3 hours. The construction of a (complete) database spanning several combinations of simulation parameters required $\sim 5 \times 10^5$ CPU hours.

### 3.2.5 Probing the database for body-wave-CMB interaction

We measure the residual time $\delta t = t_{prem} - t_{topo}$ of a given phase as the cross correlated time difference between perturbed $t_{topo}$ and unperturbed seismogram $t_{prem}$. The cross-correlation window is centered at the expected arrival time, calculated with TauP (http://www.seis.sc.edu/software/TauP/), and its width is proportional to the frequency content of the seismogram. Seismograms are filtered with a Gaussian function with half-width/period corresponding to the target frequency. We investigate 4 different frequency bands with periods: 30, 20, 15, 10 s, filtering seismograms before cross-correlation. We iteratively tune the cross-correlation window’s width in order to optimize its bounds with respect to the anomaly.

We notice first of all, and show in Fig. 3.7, that, as predicted by finite-frequency theory, the effect of a CMB topography anomaly on a seismic measurement can be significant even if the associated ray path does not sample the anomaly directly.

#### $PcP$ synthetics

We show in Fig. 3.8 a set of cross-correlation-based $PcP$ travel-time anomalies for different source-anomaly-receiver geometries and different CMB topography patterns. The plots define the pattern of residuals as a function of receiver location, with a CMB uplift resulting in earlier $PcP$ arrivals, and a CMB depression in delayed arrivals. The misfit also depends upon the relative position of the source with respect to the topography anomaly, and phases that bottom (in a ray-theoretical sense) between $20^\circ$ and $30^\circ$ away from the source are more strongly affected by CMB topography.

To summarize the cumulative effect of CMB heterogeneity on the entire synthetic database, we introduce the misfit functions

$$L_1 = \sum_{i=1}^{N} |\delta t_i| \quad \text{and} \quad L_\infty = \max_N |\delta t_i|,$$

with $N$ the total number of source-receiver pairs. The $L_\infty$ norm reflects the maximum residual time present in the database, while the $L_1$ norm gives an idea of what portion of seismograms (i.e. source-
Figure 3.3: (Top) A section of the Earth showing one of our synthetic CMB topography models: in this case, topography is Gaussian with a maximum height of 11 km and a lateral extension of \( \sim 800 \) km. The anomalous CMB area is visible as a dark circle at the center of the plot. A cross section of the global mesh taken at the CMB shows the stretching (10 times exaggerated) of mesh elements to accommodate topography. A 100 km-deep explosive event was located at 30° S and 10° E. (Bottom) reference (CMB with constant radius) (blue line) and perturbed (red line) seismograms predicted at a station aligned with source and CMB anomaly, 23° away from the source. The largest misfit corresponds to the \( P_cP \) arrival time. The perturbed seismogram is obtained after amplifying topography to 70 km, to emphasize its effects.
Figure 3.4: (a) The layout of receivers (red crosses), events (green stars) and topography-anomaly (yellow triangle) for low-aperture phases like $P_{cP}$, $ScS$, $PcS$. (b) Same as (a), but for long-epicentral-distance phases like $P_{diff}$, $PKP$.

Figure 3.5: Patterns of synthetic topography models used in this study; the lateral extent of both maps is ~800 km.
Figure 3.6: Vertical component section of 61 stations for one of the source-receiver configurations of Fig. 3.4. Main phase arrival times are also marked. The $y$–axis shows epicentral distance, and $x$–axis time in seconds. Colours depend on the magnitude of the displacement in [m].

Figure 3.7: Ray paths for 3 different stations are plotted along with the measured misfit. The effects of topography on SPECfEM3D GLOBE synthetics are not only evident for rays bottoming at the center of the anomaly, but also for those grazing its sides, for which ray theory predicts no travel-time anomaly.
Figure 3.8: PREM vs PREM + topo residual PnP travel-times plotted at each receiver’s location. Two different (left vs. right panels) source locations, marked by a red star in the top panels, are simulated. The top four residual maps refer to the topography model of Fig. 3.5a. Seismograms are filtered around the dominant period (10 or 20 s) specified to the right of each row. The bottom four panels refer to the topography model of Fig. 3.5b with analogous source position.
receiver couples) are affected by the anomaly. \( L_\infty \) and \( L_1 \) misfits for two different realizations of the \( PcP \) synthetic database are shown in Fig. 3.9. We also compute the ray-theoretical residual

\[
\delta t_{ray} = -2 \frac{\delta d}{r} \sqrt{\left( \frac{r}{v(r)} \right)^2 - p^2}
\]  

(3.4)

[e.g., Morelli and Dziewonski, 1987] (where \( r \) is the unperturbed CMB radius, \( \delta d \) its perturbation at the bounce point, \( v(r) \) the P-wave speed and \( p \) the ray parameter), and show the corresponding \( L_\infty \) norm in Fig. 3.9. For the \( L_1 \) norm, ray-theoretical values are not shown as they are out of scale.

The \( L_\infty \) norm in Fig. 3.9 indicates a maximum residual of \( \sim 1 \) s, lower than the 1.5 s residual predicted by eq. (3.4). Errors on these values associated with our automated cross-correlation procedure can vary roughly between 0.1 and 0.2 s. The discrepancy between ray-theory predictions and numerical results grows with increasing period, as is to be expected given that ray theory is strictly valid only at the infinite-frequency limit. Synthetics do not converge to the ray-theoretical value because they are calculated for a perfect vertical reflection that is not visible from synthetics. Hence the actual upper bound is positioned slightly below.

It is also clear from Fig. 3.9 that the potential to resolve topography (as well as volumetric) heterogeneity depends strongly on the frequency of the analysed signal: filtering the synthetics around 30 s would essentially obliterate the CMB-topography signature and we should utilize data at \( \sim 10 \) s or lower to be able to detect these signatures i.e. keeping the lateral length-scale to wave-length ratio \( \geq 5 \). Decreasing the lateral extension of anomalous topography does not affect strongly the \( L_\infty \) misfit as the height does, indicating that seismic waves are more sensitive to the amplitude of topography rather than its shape. The \( L_1 \) misfit shows a lower value as expected with a reduced extension of the topography.

A similar experiment can be conducted upon the CMB topography of Fig. 3.5b, with positive and negative peaks at \( \pm 6 \) km. The resulting residual travel-time maps are shown in Fig. 3.8. The abrupt change in the sign of the residual again reflects the high sensitivity to the anomaly height.

Because of their reflected origin, \( PcP \) signals are very sensitive to the height of the topography rather than its lateral extent. If on one hand we can get useful data from reflected phases, on the other hand we also need to be particularly careful about their spatial coverage, since they might be very strongly affected by topography heterogeneities of very small scale.

\( P_{diff} \) synthetics

Fig. 3.10 shows that even at the relatively short period of 10 s, the assumed CMB anomaly (Fig. 3.5a) has a very faint effect on travel-times of \( P_{diff} \). Residuals remain small even if the lateral extent of the topography anomaly is doubled. At longer periods (not shown here for brevity) the signal is lost completely. These observations are confirmed by direct inspection of individual seismograms.

3.3 The inverse problem for topography

Full waveform inversion can make complete usage of the residuals computed in the previous section, but expensive computation of the Fréchet derivatives of data with respect to model parameters have to be carried out (fortunately the adjoint methodology comes into help, making this computation feasible).
Figure 3.9: The $L_\infty$ (top) and $L_1$ (bottom) cumulative misfits between PREM synthetics and two sets of anomalous-CMB $PcP$ synthetics, as a function of the dominant period of filtered signal, generated after imposing a Gaussian-shaped topography anomaly with a maximum height of 11 km (continuous) and 6 km (dashed), and a lateral extent of (red) 800 km, and (blue) 500 km. The green lines in the top panel show the frequency-independent prediction of ray theory, for the ray-path bouncing at the highest topographic peak ($L_\infty$ misfit).
Figure 3.10: Residual \( P_{\text{diff}} \) travel times plotted at each receiver’s location, similar to Fig. (3.8). Two different (left vs. right panels) source locations, marked by a red star in the top panels, are simulated. Residuals generated by two Gaussian CMB topography models: (top) 800 km in lateral extent and 11 km in maximum height, and (bottom) 1600 km lateral extent, same height.
3.3.1 Seismic sensitivity kernel foundations

A seismic anomaly $\delta u$ is linked to model perturbations $\delta v$ and $\delta d$, respectively volumetric and boundary, through sensitivity kernels $\tilde{K}_v$ and $\tilde{K}_d$:

$$\delta u(t) = \int_{\Omega} \delta v \tilde{K}_v(x,t) \, dx + \int_{\Sigma} \delta d \tilde{K}_d(x,t) \, dx. \quad (3.5)$$

Here we just focus on the boundary contribution.

Boundary sensitivity kernels in the 1st order Born approximation were first obtained analytically by Dahlen [2005], following the scheme first developed for volumetric kernels by Dahlen et al. [2000] and Hung et al. [2000]. The numerical implementation of terms $\tilde{K}_v$ and $\tilde{K}_d$ in Eq. (3.5) is computationally prohibitive for full 3-D wave propagation at high resolution. Computational cost is reduced particularly if, as mentioned above, a 1-D reference model is used leading to the integration of the equations of motion on a 2-D disc, as in Nissen-Meyer et al. [2007b, 2008]. We follow these studies, and complement the corresponding software with an additional module, which provides seismic sensitivity to boundary topography for any of the interfaces included in the selected reference model such as upper mantle discontinuities and both core boundaries.

3.3.2 Waveform sensitivity to boundary perturbations

The calculation of boundary sensitivity requires the decomposition of a vector in normal and tangential component: $u = u \hat{n} + u^\Sigma$. The surface gradient and divergence [Dahlen and Tromp, 1998] are accordingly defined:

$$\text{surface gradient of } u : \quad \nabla^\Sigma u = \nabla u - \hat{n}(\hat{n} \cdot \nabla u), \quad (3.6)$$
$$\text{surface divergence of } u : \quad \nabla^\Sigma \cdot u = tr(\nabla^\Sigma u). \quad (3.7)$$

Where $tr()$ is the tensor-trace operator. For notational brevity we denote with $*$ the convolution between two time-dependent quantities (written in the time domain).

$$g(t) * f(t) = \int_0^t g(t) f(t - \tau) \, d\tau. \quad (3.8)$$

The convolution between vector (tensor) quantities is a scalar, and involves (double) contraction, i.e.

$$g(t) * h(t) = \int_0^t g(t) : h(t - \tau) \, d\tau \quad \text{vectors} \quad (3.9)$$
$$G(t) * H(t) = \int_0^t G(t) : H(t - \tau) \, d\tau \quad \text{tensors} \quad (3.10)$$

The model parameter vector $m$ is defined as the input of the forward problem, and the unknown of the inverse problem. $m$ can in principle include all the elastic parameters of the medium of propagation including shear and compressional velocity, their anisotropy, density, as well as source mechanism and location. In the framework of 1st-order perturbation theory, it is more convenient to consider its variation $\delta m$. For brevity we assume that we solve an inverse problem for boundary perturbation alone: $\delta m = [\delta d]$. The boundary perturbation $\delta d$ must be small enough for the 1st order perturbation theory to be a valid approximation. Our formulation is valid for any discontinuity defined by the reference model.
The boundary sensitivity kernel has a more complicated form than the volumetric type [Nissen-Meyer et al., 2007a]. The expression calculated for the frequency domain by Dahlen [2005] may be computed for the time domain and, making use of (3.10) to avoid clutter, we can write:

\[
\tilde{K}_d(x, t) = \left[ \rho \partial_t \tilde{u} + \partial_x \tilde{u} + \bar{T} \ast \tilde{E} - \tilde{t} \ast \nabla_n \tilde{u} - \tilde{t} \ast \nabla_n \tilde{u} \right]_{\text{general interface}}
\]

\[
- \tilde{n} \cdot \tilde{t} \ast \nabla^F \tilde{u} - \tilde{n} \cdot \tilde{t} \ast \nabla^F \tilde{u} - \tilde{u} \ast \nabla^E (\tilde{n} \cdot \tilde{t}) - \tilde{u} \ast \nabla^E (\tilde{n} \cdot \tilde{t}) \right],
\]

where \( \tilde{K}_d(x, t) \) is the time-dependent sensitivity of the waveform with respect to the boundary topography and \( t \) the traction acting on the interface. The solid-fluid term arises from interface conditions (3.2b). We denote with a right-pointing arrow as in \( \tilde{u} \), the ”forward field”, i.e. the regular propagating field from instant \( t = 0 \) to \( t = T \) emanating from the earthquake location \( x_s \), while the backward field, denoted by a left-pointing arrow, is a time-reversed field going from negative time \( t = -T \) to \( t = 0 \), emanating from the receiver position \( x_r \). Derived quantities such as \( \tilde{E} = \frac{1}{2} [\nabla \tilde{u} + (\nabla \tilde{u})^T] \) and \( \bar{T} = C : \bar{E} \) are calculated in the same way in both forward and backward fields.

In the adjoint framework the definition of misfit modifies the expression for \( \tilde{f} \) and hence the form of the backward field [Fichtner et al., 2009; Peter et al., 2007; Tromp et al., 2005].

The forward field \( \tilde{u} \) is now defined as the solution of equation (3.1) for a moment tensor source centred at \( x_s \),

\[
\tilde{f}(x, t) = M \tilde{m}(t) \delta(x - x_s),
\]

where \( M \tilde{m}(t) \) has been defined in section 3.2.1. The backward field is instead the time reversed solution to (3.1) for an impulsive forcing term

\[
\tilde{f}(x, t) = \tilde{x}_r \delta(x - x_r) \delta(T - t),
\]

i.e. the Green’s function associated with (3.1) and the receiver locations, \( x_r \). The vector \( \tilde{x}_r \) points in the same direction of the seismogram component used to measure \( \delta u \). For instance, if only vertical components are used to compute \( \tilde{K}_d \), then \( \tilde{f} \) is a vertical single force and the backward field the numerical solution to the heterogeneous extension of Lamb’s problem [Lamb, 1904]. Note that only one simulation is necessary for all distances and configurations.

### 3.3.3 Travel-time sensitivity to boundary perturbations

The most general expression relating a seismic travel-time anomaly observation to discontinuity topography in the first-order approximation is implicitly found from eq. (3.5) after dropping the volumetric term,

\[
\delta t = \int_\Sigma \delta \tilde{d}(x) K_d(x) d\Sigma^2,
\]

where the sensitivity kernel \( K_d(x) \) is naturally not the same as that of eq. (3.5). Notice that (3.11) is independent from the measured misfit. Only after having defined an appropriate misfit measure (here \( L_2 \) travel-time residual \( \delta t \) norm), the static kernel in (3.15) and the instantaneous sensitivity in (3.11) can be linked together.
Static travel-time kernel and waveform sensitivity are coupled through

\[ K_d(x) = \frac{1}{N_r} \int_0^T w_r(t)v(x_r, t)\tilde{K}_d(x, t) \, dt, \]  

(3.16)

where the boxcar function \( w_r(t) \) equals 1 inside the window where the sought phase arrives and \( v(x_r, t) \) is the velocity seismogram due to (3.13) recorded at station \( r \). This is derived in equivalence to the cross-correlation travel-time perturbation as a function of \( \delta u \) in Dahlen et al. [2000]. A scaling factor

\[ N_r = \int_0^T \omega_r(t)v^2(x_r, t) \, dt, \]  

(3.17)

is introduced, to rescale the kernel so it does not depend on the source magnitude.

Finally, if the misfit function is computed with the \( L_2 \) norm, the optimization problem associated with travel-time tomography is defined as follows for the combination of all travel-time observations:

\[
\text{find } m \text{ such that } \min \frac{1}{2} |t(m) - t_{\text{obs}}|^2,
\]

(3.18)

where \( t(m) \) is solution of equation (3.1). This expression allows equation (3.15), once the problem is discretized on an inversion grid, to be solved in least square sense as \( \delta t_i = G_{ij}\delta d_j \), where the matrix \( G_{ij} \) contains the discrete sensitivity kernels through the integral (3.15).

### 3.3.4 Sensitivity kernel computational outline

Nissen-Meyer and Fournier [submitted] describe the work-flow to compute volumetric sensitivity kernels using the AXISEM software. Here we extend their procedure to allow the computation of discontinuity kernels \( K_d(x) \), introducing further numerical optimization described in appendix B. By collapsing the equation of motion onto a 2-D grid, AXISEM reduces the storage-space requirement, so that it becomes possible to save the propagating wave-field in time at any resolution scale. An analogous process for similar resolution would not be feasible if a full 3-D solver was used.

The moment tensor calculation for Eq. (3.1) in AXISEM is subdivided into 4 different simulations for as many independent moment tensor components \( M_m \). Separate contributions, owing to the linearity of eq. (3.1), can be simply summed to recover the full moment-tensor wave-field [Nissen-Meyer et al., 2007b]. The same property applies to kernels:

\[ u = \sum_m M_m u_m \rightarrow K = \sum_m K_m \]  

(3.19)

(valid for both boundary and volumetric kernels).

Spatial and temporal wave-field derivatives are computed on-the-fly in (3.11). We also examined the \( C_0 \) feature of the wave-field at the CMB regarding the normal component of the traction \( t \cdot \hat{n} \). Second-order space derivatives across the solid-fluid boundary are accurate for all settings that we deem relevant, and only display slight inaccuracies after long simulation times.

In general P-waves are always fine, S-waves travelling very long might be affected. The displacement gradient in the axi-symmetric domain is defined in Appendix (A.8). Its knowledge, together with that of the surface gradient and divergence (3.6), completely define the discontinuity kernel according to expression (3.11).
Figure 3.11: The kernel mesh (we removed a slice for clarity reasons) is constructed starting from the interface layer of the spectral element mesh (the gridded semi-disc). Here, for instance, the CMB layer is depicted. The spacing between $\Delta \phi$ is chosen to respect minimum point spacing. Magenta semi-circumferences represents the interface on the AXISEM mesh.

From the semi-disc-shaped domain (Fig. 3.11) we store, as a 1D array, the values along the desired interface (a semi-circumference) in time. The simplest approach is to generate the spherical-kernel mesh, straight out of the spectral-element mesh. This latter procedure has the advantage of preserving the $\hat{s}$, $\hat{z}$ components of AXISEM mesh points, acting only on the $\hat{\phi}$ component. Thus, no interpolation for any field variable is needed. One disadvantage is the point-clustering at the poles. Our procedure as well as the reference frame involved are illustrated in Fig. 3.11 and can be outlined as follows:

- The cylindrical coordinates of the point lying on the discontinuity (highlighted in magenta Fig. 3.11) are copied from the AXISEM mesh of Fig. 3.11. By construction they will all have $\hat{\phi}$ component equal to zero.

- We select an appropriate $\Delta \phi$ and, moving in counter-clockwise direction, we loop over $\phi$ from 0 to $2\pi$. The value of $\Delta \phi$ is such that the spatial resolution along the colatitude direction is equal to the longitudinal one at the equator (dedicated box in Fig. 3.11).

- The grid-point coordinates are converted from cylindrical coordinates $(\hat{s}, \hat{\phi}, \hat{z})$ to Cartesian $(\hat{x}, \hat{y}, \hat{z})$ using equation (A.6).

For convenience we define the kernel mesh with the $z$-axis pointing north, the same convention used in AXISEM. Both forward and backward field are north pole oriented when saved from AXISEM while they must be rotated when computing the kernel to their actual source or receiver positions. This rotation of the grid-point coordinates to the actual source location $(\phi_s, \theta_s)$ or receiver location $(\phi_r, \theta_r)$ boils down to coordinates and quantities to be remapped and will be described later. In our procedure, each grid-point is associated with 3 different coordinate values: one for the kernel mesh, one for the forward field and one for backward. If we define the position of the new coordinate system
as \( \mathbf{x}' \) (either for source or receiver) we may write: \( \mathbf{x}' = \mathbf{Rx} \), where \( \mathbf{R} \) is defined for a given source or receiver position, \((\phi_s, \theta_s)\) and \((\phi_r, \theta_r)\) in Eq. (A.6).

The cylindrical frame is defined starting from the Cartesian frame through Eq. (A.7), such that a rotation of this latter produces the same rotation on the first. The coordinate basis vectors \( \hat{s}, \hat{z} \) correspond to the Cartesian \( \hat{x}, \hat{z} \) for \( \phi = 0 \) and \( y = 0 \), respectively. To each grid-points corresponds a unique point onto the 2-D semi-disc as Fig. A.1 in appendix A shows. Vice-versa, to each 2-D mesh point correspond multiple kernel mesh-points along each azimuth.

The projection of the 3-D Cartesian point onto the 2-D semi-disc is achieved through (A.7). Hence we run a linear search over the kernel mesh points to obtain the permutation array mapping the north-pole oriented reference frame to the new desired position. The permutation always maps from the kernel mesh (3-D) to the AXISEM boundary mesh (2-D). The points from the 3-D mesh are projected onto the 2-D semi-disc. For each kernel grid-point \( (i) \) we measure the Euclidean distance from the 2-D points and a linear search to find the closer \( (j) \). The permutation array \( P \) for grid-points \( i \) is: \( P(i) = j \).

The azimuthal pre-factors applied to the 2-D wave-field serve to reconstruct the 3-D field and are computed using \( \phi \) values. Fig. A.2 depicts \( \phi \) values for a given source-receiver pair \((\phi_s, \theta_s)\) and \((\phi_r, \theta_r)\). Eq. A.1 in appendix A shows how pre-factors are applied to vector and tensor quantities depending on the moment tensor term currently computed. When the 3-D wave-field has been calculated we can convert the field values to Cartesian coordinates. Again, the procedure uses the corresponding \( \phi \) value for forward and backward fields. This is achieved applying a change of basis matrix \( \mathbf{B}(\phi) \) as described in appendix A. Wave-fields now in Cartesian coordinates are written for two different coordinates systems: one with the z-axis pointing towards the source location and the other pointing towards the receiver.

Before calculating (3.15), we unify forward and backward field reference systems to the north pole oriented reference frame of the kernel mesh applying the same rotation matrix \( \mathbf{R} \) used to calculate rotated coordinates.

\[
\begin{align*}
\text{vectors: } \mathbf{u}_{\text{cart}} &= R^T \mathbf{u}_{\text{cyl}}, \\
\text{tensors: } \mathbf{E}_{\text{cart}} &= R^T \mathbf{E}_{\text{cyl}} R.
\end{align*}
\] (3.20)
The entries $r_{ij}$ of $R$ are defined in appendix A. Note that this rotation maps source/receiver rotated Cartesian frame to the north pole rotated frame while the mesh coordinate’s rotation previously defined mapped north pole oriented to source/receiver rotated. This difference boils down taking the transpose of the rotation matrix $R$. For scalar quantities no rotations are necessary as they are invariant. The result of these procedures are the forward and backward field as if we were to use the any other 3-D code and they are depicted for different time step in Fig. 3.12 Finally the sensitivity kernel due to moment tensor $M_m$ can be computed for any desired seismogram window.

3.4 Boundary sensitivity kernels

The software described in appendix B provides boundary sensitivity kernels according to the procedure described in section 3.3.4. We apply this to compute kernels at dominant periods of 10 and 25 s, using the source time function introduced in section 3.2.1. For the sake of simplicity we limit ourselves to monopole (explosive) sources, and accordingly only consider compressional waves. The sampling rate of modeled seismograms and wave-fields by AXISEM is selected after a number of preliminary experiments. As noted by Fichtner et al. [2009], different sampling rates must be compared to identify the minimum rate threshold, so that time aliasing of the seismic signal and of the sensitivity pattern is prevented. We typically sample the signal 10 times per dominant period, but we verify that this rate may be further reduced to limit the number of time steps needed to calculate the convolution in Eq. (3.11).

The time integration window in Eq. (3.16) is chosen such that the whole signal is enclosed inside, equivalent to section 3.2.5 for the cross-correlation. We tuned specifically the size for every case to avoid the inclusion of other signals that may spoil the kernel-phase signature. A negative (positive) sensitivity value means that a positive topography anomaly will delay (accelerate) the arrival of the phase on the seismogram, and vice-versa, a depression would produce a positive (negative) arrival.

Most of our computations are carried out at the Swiss Center for Scientific Computing (http://www.cscs.ch). The computational cost for this not yet optimized algorithm (i.e., number of processors and wall-clock time) depends on the shortest modelled period, and on the depth range of the modelled discontinuity. It spans from few minutes on 4 processors for the CMB kernels at 25 s to ~1 hour on 24 processors for 10-s upper-mantle-discontinuity sensitivity kernels. Upper-mantle discontinuities are generally more expensive because of the different spatial sampling used to mesh the upper vs. the lower mantle when designing the spectral element grid [Nissen-Meyer et al., 2008].

3.4.1 Transition-zone discontinuities

The seismic phases $P410P$, $P520P$ and $P660P$ (Fig. 3.13) associated with underside reflection of $P$ waves at the ~410, ~520 and ~660 km discontinuities, respectively, have been extensively used to map their topography [e.g., Deuss, 2009; Flanagan and Shearer, 1999; Gu et al., 1998; Gu and Dziewonski, 2002]. We determine the frequency-dependent sensitivity of these phases to discontinuity topography using an explosive event at a depth of 100 km. Because the source is isotropic, kernels are symmetric with respect to the vertical plane defined by source-receiver-center of the Earth. The $P660P$ sensitivity kernel in Fig. 3.14 is characteristically X-shaped [Lawrence and Shearer, 2008]. Using differential travel-times the effects of structure elsewhere (crust and upper mantle for instance) may be removed, focusing the sensitivity only on the boundary. As demonstrated by Dahlen [2005] taking the differential travel-time exactly relates to computing the differential sensitivity kernels.
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Figure 3.13: (top) Cartoon showing the ray trajectories of the $PP$ phase and its precursor discussed in section 3.4.1. (bottom) ray trajectories of the core-reflected, -refracted and -diffracted phases of section 3.4.2.

Figure 3.14: The $KP_{660}P$ kernel for 140º epicentral distance and its associated vertical velocity component for dominant period of 10 s. Black dots mark source (depth 100 km) and receiver locations. Values are all scaled in $10^{-4}$ km s$^{-1}$. The kernel is projected on the "660" surface.
Figure 3.15: The $K_{P660P}$ kernel for 95° epicentral distance on the left and the $K_{PP} - K_{P660P}$ on the right. The dominant period is 10 s. Black dots depict the source (depth 100 km) and receiver location. Values are all scaled in $[10^{-4} \frac{m}{s^2}]$. The kernels are projected on the "660" surface.

$K_{PP} - K_{P660P}$. Because of the small magnitude of the $K_{PP}$ on the boundary, it amounts to $K_{PP} - K_{P660P} \approx -K_{P660P}$ as Fig. 3.15 witnesses. The same results may be obtained using other underside reflection precursors such as $S_{660S}$, $P_{410P}$ or $S_{410S}$. In particular, secondary-wave precursor are well suited for transition zone studies because the impedance contrast for $S$ waves is higher than for $P$ waves with a consequently stronger signature in the seismogram providing better signal-to-noise ratio.

Our AXISEM-based kernels can be compared with those found by Dahlen [2005] and Lawrence and Shearer [2008] using the ray-theory finite frequency approximation, and those found by Liu and Tromp [2008] using the adjoint technique combined with a 3-D spectral-element method. In spite of the difficulty of making direct comparisons when many parameters may differ slightly (source-time function, dominant period, source-receiver locations, etc.) our results are generally consistent with earlier findings (Fig. 3.19).

3.4.2 CMB discontinuity

The $PcP$, $P_{dif}$ and various branches of $PKP$ travel times (Fig. 3.13) have been extensively used to infer properties of lower mantle and core-mantle boundary in many previous studies [Boschi and Dziewonski, 2000; Morelli and Dziewonski, 1987; Soldati et al., 2012; Tanaka, 2010; van der Hilst et al., 1998; Vasco et al., 1999].

We calculate CMB sensitivity using an explosive event at a depth of 650 km. We mainly consider $P$-waves and we record the vertical component of the seismograms. Again, since the source is isotropic, kernels are symmetric with respect to the vertical source-receiver plane. Results in section 3.2.5 show the high sensitivity of $PcP$ phases to the magnitude of the topography in the range between 30° and 70° epicentral distance. The sensitivity kernels displayed in Fig. 3.16 point in the same direction as the synthetic test of section 3.2.5, supporting that the bulk of the sensitivity is clustered in a relatively small area that slowly enlarges as the frequency decreases. We next present (Figs. 3.17 and 3.18) finite-frequency sensitivity kernels associated with $P_{dif}$, for which (unlike, e.g., $PcP$) no asymptotic
Figure 3.16: The $P_{cP}$ boundary sensitivity kernel for 25 s (left) and 10 s dominant periods (right) for an epicentral distance of 60°. It is elongated in the source-receiver direction, the area of non-negligible sensitivity extending up to 2000 km around the predicted bounce point for the 25 s case and roughly 1000 km for the 10 s case. The two dots indicate the location of source (depth 650 km) and receiver. Values are scaled to $10^{-5} \text{s km}^{-3}$.

Figure 3.17: $P_{diff}$ sensitivity kernels associated with different epicentral distances, as specified, at 25 s dominant period. Notice how the sensitivity imprint becomes wider with growing epicentral distance. Values are scaled to $10^{-5} \text{s km}^{-3}$. The depth of the event was 650 km.
Figure 3.18: The $P_{\text{diff}}$ sensitivity kernel for $155^\circ$ epicentral distance (the maximum for $P_{\text{diff}}$ being $157^\circ$), for (left) 25 s and (right) 10 s dominant period. The vertical component of our modelled trace is very weak at 25 s period, but it becomes clearer as the frequency increases. The same is true of this phases sensitivity to CMB topography. Values are scaled to $10^{-5} \frac{s}{\text{km}^3}$. The depth of the event was 650 km.

solution is available. The large width of the area where sensitivity is non-negligible confirms our finding that this phase is sensitive to large-scale variations rather than small-scale (results found also in section 3.2.5) and that positive topography might result in a delayed arrival time depending on its position relative to the source-receiver plane. Fig. 3.17 shows this phase for a suite of epicentral distances spanning its entire existence-range for 25 s dominant period. In spite of the seismic signal being extremely small for $155^\circ$, the $P_{\text{diff}}$ sensitivity kernel can still be computed as Fig. 3.18 shows.

Finally, the sensitivity of the $PKIKP$ phase, and of the $ab$ branch of $PKP$ to CMB topography is illustrated in Fig. 3.20. Sensitivity is limited to the vicinity of the associated ray-path entry and exit points into and from the core. The pattern is similar, but the sign reversed with respect to $PcP$ sensitivity. Positive topography at and close to the entry/exit points causes a delayed arrival. As a final demonstration of the capability of our algorithm we show in Fig. 3.21 the sensitivity kernel for $SKIKS$ for a dominant period of 5 s. Because of the epicentral distance chosen, other $SKS$ branches arrives simultaneously. A $M_{\text{dip}}$ dipole moment-tensor source was used as source and the azimuthal pre-factors (A.1) were applied to the wave-field.

Comparison with other techniques both for $PcP$ and $P_{\text{diff}}$, although only qualitatively possible, may be done looking at the work from Dahlen [2005] and Liu and Tromp [2008]. We also computed with SPECFEM3D GLOBE 3.19 a $P_{\text{diff}}$ kernel for 25 s dominant period (Fig. 3.19). The sensitivity pattern is similar to the one shown in Fig. 3.17. Small differences are attributed to the different algorithm used to solve Eq. (3.1), the implementation of the adjoint source, the numerical time-sampling, the selection of the time window and the meshing strategy.
Figure 3.19: The $P_{\text{diff}}$ sensitivity kernel at 155° calculated using the adjoint method implementation of SPECFEM3D GLOBE. The depth of the event was 650 km. Values are scaled to $10^{-5}$ s km$^{-2}$. This results may be compared with what obtained in figure 3.17.

3.4.3 Drawing connections: travel-time residual reconstructed with sensitivity kernels

One way to validate AXISEM-computed kernels and to show their applicability in tomography consists in reverse (Born) modelling the cross-correlated time residual using the kernels computed in the previous section. The first order relationship (Eq. (3.15)),

$$
\delta t = \int \delta d \, K_d \, dx^2
$$

is calculated evaluating the integral over a finite set of $N$ constant basis functions [e.g., Boschi and Dziewonski, 1999] $i \in \{1, ..., N\}$ that reduces to a scalar product between two vectors:

$$
\delta t = G_i \delta d_i.
$$

Clearly this holds for one specific event-topography-receiver configuration contained in the database causing the travel-time anomaly $\delta t$. Selecting one configuration of the many proposed throughout section 3.2.5, we can compare reverse-modelled $\delta t$ obtained through Eq. 3.21 with previously computed SPECFEM3D-based quantities. We then evaluate the magnitude difference by constructing residual maps. For the sake of correctness, we ignore values $\leq 0.2$ s as they may be strongly influenced by small errors. The travel-time maps are depicted in Fig. 3.22a and 3.22b. Fig. 3.22c shows that AXISEM-based reverse models slightly but systematically overestimates SPECFEM3D synthetics. The reason for this is presumably twofold: on the data acquisition side, the cross-correlation may underestimate such small signals, and the sampling rate (each 0.1 s) of the seismogram may not be sufficient. On the model side, the chain of approximations (including 1st order) used to build the discrete model parameter vector $m_i$, the gradient $G_i$, and the small rounding used to construct the curved surface inside SPECFEM3D may play an important role. The consequences of this discrepancy are a slight underestimation of the magnitude of the topography at inversion time. We however infer that accuracy of AXISEM kernels is sufficient for application to typical (noisy and non-uniformly distributed) real seismic observations.
Figure 3.20: *PKIKP* and *PKPab* for 160° epicentral distance and a dominant period of 10 s. For the *PKIKP* the plot is taken looking at a cross-section throughout the core mantle boundary to ease the visualization of both entry and exit points sensitivity. The black dotted line represents the theoretical ray path. The explosions and triangle marks respectively indicates a epicenter and receiver location. Values are scaled to $10^{-5} \frac{\text{rad}}{\text{km}^2}$. The depth of the event was 650 km.
Figure 3.21: The figure shows the SKIKS kernel for an epicentral distance of 140° for 5s dominant period. The entry point is located on the left-side where the sensitivity is larger. A smaller sensitivity characterize the exit point (on the right-side). The pale signature on the background may be the effect of other SKS branches arriving almost simultaneously for this distance-depth range. Values are scaled to $10^{-4} \frac{s}{km^3}$. The depth of the event was 650 km.

Figure 3.22: The results of the reverse modelling applying Eq. 3.21 in panel (a) and those obtained by cross-correlating SPECFEM3D seismograms (b). While the patterns are practically identical, the magnitude of the $\delta t$ differs as shown in the last plot (c). The continuous line represent perfect matching between the two measures, while asterisks the actual measured residuals. Cross-correlation residuals are divided in discrete band because of the finite sampling of the seismograms while those from reverse modelling are more scattered around. We intentionally left out from plot (c) values lower than 0.2 s as they are not reliable.
3.5 Discussion

This paper addresses the effect of global seismic boundary topography on waveforms as well as sensitivity kernels, i.e. the basis for tomographic imaging within the framework of full-wave theory. In the first part, we computed a large ground-truth database to examine the parameter space spanned by boundary perturbation geometry, epicentral distance, seismic phase, and frequency on seismograms. This is to be seen as a guide for optimal data configurations to illuminate such topography. In particular, $P_cP$ phases are, as expected, useful to detect CMB topography, whereas $P_{diff}$ are less sensitive to such undulations. Our synthetic experiments highlight the importance of reflected phases to map discontinuity topography. The poor sensitivity shown by diffracted waves may represent two pitfalls of this analysis: $T_0 = 10$ s is not sufficient to constrain CMB topography (also for medium-scale structure) and travel-time analysis probably may not represent the ideal misfit measurement. A method based on phase-envelopes as in Bozdag et al. [2011] might amplify the differences. Repeating this analysis with stronger topography will certainly lead to stronger signals but would violate the constraint that the majority of CMB-sensitive observations impose on their magnitude. The database has been computed using full 3-D wave propagation, and as such the prohibitive cost at high resolution (e.g. below periods of 10 s) prevents us from an analysis covering the full spectrum. As tomographic inversions must be conducted at sufficiently high frequency (below 10 s) to detect this topography, we must rely on computationally more efficient methods than full 3-D wave propagation to construct sensitivity kernels.

In the second part, we implemented boundary sensitivity kernels using 1$^{st}$ order perturbation theory following Dahlen [2005], using the axisymmetric spectral-element code AXISEM. This methodology allows to model frequencies as high as required by the database analysis, even in the framework of large-scale tomographic datasets. Those kernels, representing the Fréchet derivatives of perturbations of data with respect to topography, account for finite-frequency effects and can be used in waveform inversion to invert for boundary perturbation. Our kernels share similar properties with kernels calculated in other studies [Dahlen, 2005; Hung et al., 2000; Liu and Tromp, 2008; Peter et al., 2007]. The dependency of the area of non-negligible sensitivity and amplitude upon the period is evident in all cases considered here. Its extension scales with the wavelength and it asymptotically collapses to the ray size at infinite frequency. The values of maximum and minimum sensitivity change correspondingly to accommodate the area change. Varying the epicentral distance produces similar effects. From the perspective of section 3.4, in our future finite-frequency imaging of the CMB, the inclusion of $PKP$ should also be considered as the sensitivity footprint (particularly true for $PKIKP$) is similar to $PcP$. The reverse modelling illustrated in section 3.4.3 confirms the robustness of our approach against more general 3-D wave propagation.

The inclusion of volumetric perturbation combined with topography will be the next step towards waveform inversion accounting for the strong connection between boundary topography and the surrounding volumetric structure. Mantle and crust corrections are known to heavily trade-off with topography in the target area as discussed by Flanagan and Shearer [1999]. Combining the boundary sensitivity algorithm with the work from Nissen-Meyer and Fournier [submitted] will allow a joint volumetric-boundary full-waveform inversion work-flow at global scale, scalable to any resolution. Before reaching this stage, further time has to be devoted to assessing the resolution power of this methodology based on spherical Earth models. This will be achieved by inverting the synthetic seismograms calculated in section 3.2.5 and verifying how well input structures are recovered. A study on waveforms as in section 3.2.5 can be extended to the combined effect of boundary plus
volumetric anomalies: first to assess how the two trade off one another and later to benchmark the joint waveform inversion.

Before implementing the inversion technique, further numerical and computational optimization is needed. In spite of the efficiency of the software by Nissen-Meyer et al. [2007b], computing global sensitivity kernels at periods smaller than 5s is quite expensive. Preliminary application to GPU hardware shows that GPU computing may be a key factor to making this endeavour affordable, besides reverting to frequency-domain convolutions [Nissen-Meyer and Fournier, submitted].
Abstract The topography of the core mantle boundary, directly linked to the dynamics of both mantle and outer core, is only partially known. Recent studies produced topography models with mutual agreement up to degree 2. It is here introduced an inversion strategy based on 1st order Born approximation capable of broadband waveforms inversion with relatively low computational cost. After introducing the inversion scheme, we validate and benchmark its performance using synthetic waveforms calculated in theoretical Earth models that include different topography patterns with varying lateral wave-length from 800 to 2500 km and magnitude (~10km peak-to-peak). The source-receiver geometry focuses on mainly $P_{\text{diff}}$, $PKP$, $PcP$ and $ScS$ phases. The results show that $PKP$ branches, $PcP$ and $ScS$ perform generally good and in a similar fashion, while $P_{\text{diff}}$ yields unsatisfactory results. We investigate also how 3-D mantle correction influences the output models and find that, despite the disturbance introduced, the models recovered do not seem biased provided that the 3-D model is correct. Using cross-correlated travel-time we derive new topography models both from $P$- and $S$-waves. Static corrections used to remove the mantle effect are likely to affect the inversion output. By modelling travel-times residual starting from sensitivity kernels, we show how the simultaneous usage of volumetric and boundary kernels may reduce the bias coming from mantle structures.

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4.1 Introduction

The Gutenberg or core-mantle boundary, (CMB), is the strongest discontinuity in the Earth’s interior, separating the solid mantle from the fluid outer core. Its topography is very likely related both to the thermal/compositional/viscosity structure and associated convection of the mantle [Forte et al., 1995; Soldati et al., 2012], and to the properties of the outer core, where vigorous convection is believed to generate the Earth’s magnetic dynamo [e.g., Jackson et al., 1993]. A number of authors, starting with Morelli and Dziewonski [1987], mapped CMB topography based on compressional-wave travel times, while others [e.g., Ishii and Tromp, 2001; Li et al., 1991] inverted observations of eigenfrequency splitting, focusing on normal modes sensitive to the CMB. Most ray-based models feature a similar degree-2 pattern with peak-to-peak topography of a few km, but shorter-wavelength structure is more difficult to constrain similar to volumetric tomography. Several studies [e.g., Boschi and Dziewonski, 1999; Soldati et al., 2003; Vasco et al., 1999] point to a discrepancy in CMB structure as mapped by
core-refracted (various branches of the PKP phase) versus core-reflected seismic waves, which casts some doubt on the validity of CMB maps derived from those data. Soldati et al. [2012] however show that the discrepancy is at least partially solved if one requires the inverse-problem solution for CMB topography to be coupled with seismic structure in the mantle according to the theory of Forte et al. [1995].

Seismically slower fluid outer core and complex 3-D structures above this region cause of tripli- cation, caustics, scattering and attenuation prevent from obtaining good quality global seismic data i.e., with sufficient signal to noise ratio [Valenzuela and Wysession, 1998]. The few broadband observations available are normally clustered in particular regions as for instance in the studies of Thorne et al. [2007]; Vanacore et al. [2010]. From the installation of dense acquisition grids such as USArray Garnero [2006] we can have access to a large amount of data for global/regional deep mantle stud- ies. Feeding these data into adjoint-like inversion scheme [e.g. Fichtner et al., 2008; Tromp et al., 2005] combined with spectral element (SEM) simulation allows to calculate frequency dependent sensitivity and should eventually improve the results of the inversion [e.g. Fichtner et al., 2009]. For spherically symmetric background models the work from Nissen-Meyer et al. [2008] provides a spectral element code capable of solving the wave equation down to 5-10s period with reasonable computational resources. This allowed us to compute in Colombi et al. [2012] boundary sensitivity kernels for 1-D background models in an efficient way compared to other more expensive technique for 3-D models [e.g., Fichtner et al., 2009; Liu and Tromp, 2008]. So far only Lawrence and Shearer [2008] constrained upper mantle discontinuities following a similar (although hinged on ray-theory) approach. One possible way to discriminate which among the various CMB-sensitive phase are best for constraining topography is through sensitivity study of CMB-phases using synthetic data calculated with large spectral elements simulation through various topographic CMB models as in Colombi et al. [2012]. Core reflections (PcP, ScS) and core diffraction (PKP) provide better images of the CMB topography while diffracted waves perform poorly. With the exception of differential travel-time measurements, like PmKP - PcP from Tanaka [2010] absolute travel-times suffer the disturbing effects of crust and mantle. The appropriate correction of those effects is key to success and and it is a central challenge for such studies. Static corrections calculated upon ray tracing are the most common method, and many database [e.g., Ritsema et al., 2010] are released along with the residuals travel-time correction for crust and mantle structures. The simultaneous joint inversion [e.g., Vasco et al., 1995], although potentially capable of solving this issue, has never been used in CMB studies. Because it requires good data coverage it has been more applied in exploration seismology with Hobro et al. [2003], but without accounting for finite-frequency sensitivity and ray-theory was used instead.

In this article we implement volumetric and boundary sensitivity kernels first introduced in Colombi et al. [2012] in an inversion scheme relying on 1-D background parametrization. In section 4.2 we discuss the implications of CMB boundary topography on wave propagation and we present various synthetic datasets for P and S phases used for testing and benchmarks. Section 4.3 deals with the formulation of the matrix inverse problem for a single class of parameters (topography anomaly) or for the simultaneous joint inversion of volumetric and boundary anomaly. Section 4.4 contains a suite of synthetic inversions for varying topography, dominant period, parametrization and seismic phase. We also address the problem connected to the simultaneous effect of 3-D mantle + topography when using an automated measuring technique for cross-correlation and analyse the effect of source-receiver distribution. In section 4.5 we make use of our algorithm to invert a public available dataset containing various phases and we discuss analogies and similarity with other studies and geodynamic implications. Finally we try, using volumetric sensitivity kernels, to discriminate
between mantle and boundary contribution and we and argue that a joint inversion can resolve this trade off. An appendix clarifying our approach on the solution of the inverse problem completes the work.

4.2 Global synthetic waveform database

4.2.1 Global wave propagation: analytical background

The Earth is a heterogeneous body characterized by strong discontinuities causing significant complexity in the wave-field. At the global scale, the phenomenon of seismic wave propagation is well explained by linear elastodynamics theory. The presence of a fluid outer core is modelled by coupling the acoustic wave-equation with the elastic-wave equation through transmission conditions at the core-mantle boundary [Komatitsch and Tromp, 2002a; Nissen-Meyer et al., 2007b]. Those interface conditions are crucial for the derivation of boundary sensitivity kernels with the approach of Dahlen [2005] using Born theory [Dahlen and Tromp, 1998]. At first order, spherical symmetric background models such as PREM [Dziewonski and Anderson, 1981] containing all major discontinuities and depth dependent mechanical properties are sufficiently accurate for the computation of sensitivity kernels.

The effects of Earth’s rotation and gravitation, and of the oceans, are all negligible at the frequency band (40 – 100 mHz) and geographic scale length (20° – 180°) considered here [Dahlen and Tromp, 1998; Komatitsch and Tromp, 2002b], while those of the Earth’s ellipticity are accounted for by applying a linear correction on the data as shown by Dziewonski and Gilbert [1976]. The seismic event is introduced in the wave equation in the form of a source-time function applied to the moment tensor \( M \), containing information about the radiation pattern of the rupture. To highlight the structural effect of this methodology we only consider explosive events for P-waves or dipole (e.g. dip-slip) in the case of S-waves.

4.2.2 CMB topography

Most published models of CMB topography share the same degree 2 pattern as in Soldati et al. [2012]; Tanaka [2010]. Structures are in the order of few thousands of kilometres, while smaller features are difficult to constrain owing to several reasons: lack of coverage, noise and ray-theory flaws. The sensitivity of seismic waves is scalable as a function of the frequency. Higher frequencies should be more sensitive to smaller topography (in a lateral length-scale sense). We test if a medium-small (~ 800÷1200km) topography at global scale can be constrained successfully with 20s or 10s dominant period that amounts to a length-scale over wave-length (\( \mu \)) ratio of \( \sim 3 \div 10 \). If it is the case, it means that current models could be retrieved with much longer period signal, or vice-versa, that with shorter period data and good coverage, CMB maps can be improved. We use two different anomaly patterns, as in Fig. 4.1.e,f to check whether positive/negative topography introduce some bias with respect to the easiest case where only topography was inserted. The magnitude, chosen respecting what previous studies have shown [see Koelemeijer et al., 2012, for a review of the models], is between 5 and 10 km measured peak to peak. Fig. 4.1.e,f show that topographies inserted in the model, stay within the small perturbation regime.
4.2.3 Selected seismic phases and acquisition grid

Our synthetic database contains several datasets (Tab. 4.1), is an extension of that introduced in Colombi et al. [2012]. The software SPECFEM3D GLOBE [Komatitsch and Tromp, 2002a] was used to calculate perturbed and unperturbed waveform down to a period of 10s. The perturbation consists of an anomaly $\delta r$ (positive or negative) of different magnitudes, shapes, and lateral length-scale superimposed on the native global mesh (Fig. 4.1e-f) at the CMB. The mantle is modelled either with PREM [Dziewonski and Anderson, 1981] or with a full 3-D model [Ritsema et al., 2010].

Travel-time residuals are calculated with cross-correlation applying the procedure described in Colombi et al. [2012]. The output of this operation is simply a travel-time residual $\Delta t$ at the desired dominant period (in this work 10 s or 20 s) calculated for a time window around the predicted arrival of the interesting phase using TauP-2.0 (http://www.seis.sc.edu/software/TauP/). For explosive sources we considered only the vertical components of the seismogram while for those generating S-waves we look at the transverse component (ScS).

The database used in Colombi et al. [2012] contains only $PcP$ and $P_{diff}$ while here, to broadly cover the spectrum of energy partitions at the CMB we calculated also $PKP$ branches and ScS. The ray-paths of the phases are depicted in Fig. 4.1a.

The $PKP$ and $PcP$ branches have been used in several studies to constrain CMB topography [Morelli and Dziewonski, 1987; Soldati et al., 2003, 2012; Sze and Van der Hilst, 2003] or small-scale structure of the lower mantle [Lay and Garnero, 2004; Vanacore et al., 2010] in local or regional studies. Tanaka [2010] considers differential travel-time from $PmKP - PcP$ to eliminate mantle effects. Unfortunately those phases require more than double CPU run-time and therefore will not be considered here. The usage of $P_{diff}$ is not that common [e.g. Valenzuela and Wysession, 1998] because modelling $P_{diff}$ correctly using ray theory is difficult. Recently few global data from ScS phases became available from the work of Ritsema et al. [2010] but it has yet to be inverted for CMB topography. $S$-waves reflection looks to be easily identifiable at longer period (10s) because of the higher reflection coefficient at the CMB than $PcP$ (Ritsema personal communication). These phases have very different propagation path as seen in Fig. 4.1a, to capture them correctly we arranged the layout of source-receivers in different ways upon the corresponding epicentral distance.

Colombi et al. [2012] carried an extensive broadband analysis for multiple frequencies over $PcP$ and $P_{diff}$ data (see for instance Figs. 8 9 and 10 of that article). While for the $ScS$ data the sensitivity is very similar to $PcP$, interesting results have been obtained from $PKP$ branches. Especially for $PKIKP$, the sensitivity kernels look very similar to those of $PcP$ or $ScS$ even if double sided because of different entry and exit point. The residuals for one of the source/receiver configuration are shown in Fig. 4.2b,c. They are measured from the vertical components for $PKIKP$ and $PKPbc$ phases filtered at 10s dominant period. When infinite frequency is used, the magnitude of the residual travel-time is approximately half of that expected for $PcP$ [e.g. Morelli and Dziewonski, 1987] because the sensitivity is partitioned in two sides [Colombi et al., 2012], for an equal anomaly $\delta r$. The reason why only $PKIKP$ carries strong signature in our experiment is two-folds: as Fig. 4.2a shows the $PKPbc$ ray (blue) passes slightly off the topography because the take off angle is not as high as for $PKIKP$ (red) which are sensing closer the anomaly. Second, the sensitivity kernels shows milder sensitivity compared to $PKIKP$ resulting in a smoothed effect. The residuals for 20s (not shown here) lead to similar considerations even if smaller in magnitude because of the frequency dependent sensitivity. It is reasonable to expect a similar behaviour when dealing with $SKS$ phases not considered in the synthetic database for computational reasons but used for actual inversion.
Figure 4.1: (a) The ray-path for the CMB seismic phases considered in our database. (b-d) The source-receiver layout for respectively $P_{cP}$, $P_{diff}$ and $PKP + P_{Cp}$ phases. Red dots show the station while stars represents the events. The spacing between each station is 1° in both directions for $PKP$ and $P_{cP}$ while 2° for $P_{diff}$. (e,f) Two CMB-map views, a bell shaped topography is obtained by projecting a Gaussian distribution, and its first derivative along one major-arc. For each spectral-element simulation, we modify lateral extension and magnitude of the topography.
Figure 4.2: (a) Ray trajectory for the $PKIKP$ and $PKP_{bc}$ leave the epicenter towards the stations, and the map of the CMB shows the topography located at the source. The color map on the receivers indicates the magnitude of the $\Delta t$. (b, c) Residual travel-times for $PKIKP$ and $PKP_{bc}$, measured on the vertical component. The dominant period is 10 s, and the event was located at a depth of 100 km, on top of the topography.

<table>
<thead>
<tr>
<th>phase-topography</th>
<th>model</th>
<th>$10s$</th>
<th>$20s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$PcP \sim 1200km \times 10km$</td>
<td>PREM</td>
<td>3561</td>
<td>2691</td>
</tr>
<tr>
<td>$PcP \sim 800km \times \pm5km$</td>
<td>PREM</td>
<td>3321</td>
<td>2411</td>
</tr>
<tr>
<td>$ScS \sim 1200km \times 10km$</td>
<td>PREM</td>
<td>4385</td>
<td>3657</td>
</tr>
<tr>
<td>$ScS \sim 800km \times \pm5km$</td>
<td>PREM</td>
<td>4185</td>
<td>3375</td>
</tr>
<tr>
<td>$P_{diff} \sim 1200km \times 10km$</td>
<td>PREM</td>
<td>2988</td>
<td>none</td>
</tr>
<tr>
<td>$P_{diff} \sim 2500km \times \pm5km$</td>
<td>PREM</td>
<td>2718</td>
<td>none</td>
</tr>
<tr>
<td>$PKP \sim 1200km \times 10km$</td>
<td>PREM</td>
<td>2532</td>
<td>1825</td>
</tr>
<tr>
<td>$PKP \sim 800km \times \pm5km$</td>
<td>PREM</td>
<td>2347</td>
<td>1762</td>
</tr>
<tr>
<td>$PcP \sim 1200km \times 10km$</td>
<td>S40RTS</td>
<td>9450</td>
<td>7459</td>
</tr>
<tr>
<td>$PcP \sim 800km \times \pm5km$</td>
<td>S40RTS</td>
<td>8610</td>
<td>6753</td>
</tr>
</tbody>
</table>

Table 4.1: Number of observation ($\Delta t$) for each of the inversion upon topography size and dominant period. $PKP$ means $PKIKP + PKP_{bc}$. 
4.2.4 Background models

The knowledge of the mantle structure is a pre-requisite to any CMB topography study. The bulk of the database has been calculated using PREM as background model to highlight topographic effects first. To give a more realistic imprint we also considered for the \( P_{cP} \) data a recent 3-D mantle model. SPECFEM3D GLOBE embeds the recent shear wave model by Ritsema et al. [2010] S40RTS, hence it is easy to simulate the effect of full 3-D mantle and CMB topography altogether (Fig. 4.3). Details on how this model is discretized and how the \( P \)-wave velocity is obtained starting from the \( S \)-wave velocity model can be found in Komatitsch and Tromp [2002b]. Even if S40RTS is an \( S \)-wave based velocity model the important point for us was to insert perturbations in the mantle regardless their actual fit to the reality. The topography patterns are the same as those in Fig. 4.1a-b, paired with the \( P_{cP} \) source-receiver layout. The question whether discontinuity topography can be mapped also in the presence of realistic mantle perturbation can be addressed in a straight-forward way. For each source-topography-receiver configuration we run one simulation with PREM, another with only 3-D mantle and another with 3-D mantle plus topography while the pure effect of topography was calculated in section 4.2.3. If the mantle has little influence on the measurements, the effect of topography remains more or less the same. We measured with cross-correlation the travel-time residual \( \Delta t_{\text{prem}}^{\text{topo}} \) for \( P_{cP} \). We explained in section 4.2.3 how \( \Delta t_{\text{prem}}^{\text{topo}} \) is calculated, we add the subscript PREM as a reminder that a 1-D background model was used. Here we extend this procedure to: \( \Delta t_{\text{S40RTS}}^{\text{notopo}} \), the travel-time residual owing to solely S40RTS with respect to PREM and \( \Delta t_{\text{S40RTS}}^{\text{topo}} \) the joint effect of CMB topography plus mantle travel-time residual with respect to PREM. If the mantle does not affect the measurement of the \( \Delta t_{\text{prem}}^{\text{topo}} \) the following relationship holds:

\[
\Delta t_{\text{prem}}^{\text{topo}} \approx \Delta t_{\text{S40RTS}}^{\text{topo}} - \Delta t_{\text{S40RTS}}^{\text{notopo}}
\]  \hspace{1cm} (4.1)

Fig. 4.4 shows the result of this analysis for the \( P_{cP} \) case. At first sight the effect of 3-D mantle
structure has a great effect on $\Delta t_{\text{topo}}$ but if we consider that the magnitude of $\Delta t_{\text{notopo}}^{S40.rts}$ is up to 10 times larger $\Delta t_{\text{prem}}^{S40.rts}$, the results obtained are overall good (topography produces a maximum residual upon ray-theory of $\sim 0.15s/km$ for PcP phase). $\Delta t_{\text{topo}}$ in Fig. 4.4b is obtained by applying Eq. (4.1). The difference between this latter and the reference $\Delta t_{\text{prem}}^{S40.rts}$ (Fig. 4.4a) is depicted in Fig. 4.4c. The strongest component of the signature is correctly retrieved (white stripe in the middle) while smaller magnitude residuals appear around the darker area. This might be considered part of the error, either due to the automated measuring strategy or non-linearity due to coupled effect of topography and 3-D mantle. In section 4.4 we show that this small error does not compromise the results of the inversions. During the test at different frequencies, we observed an increasing number of outliers (i.e. residuals with infeasible high magnitude) for smaller dominant period. This is probably due to the occurrence of cycle skipping [Virieux and Operto, 2009], an anomalous phase difference between reference and perturbed seismogram that induce cross-correlation to fail. We manually excluded them from the analysis in Fig. 4.4.

### 4.3 Inversion algorithm

We use the approach developed in Colombi et al. [2012] to compute sensitivity kernels for each source-receiver pair used for the inversion. The inverse problem is then solved with a standard sparse matrix inversion. The procedure remains identical for synthetics and actual data inversion.
4.3.1 Boundary sensitivity waveform kernels

The central point of the work by Colombi et al. [2012] is the implementation of an efficient method to compute sensitivity kernels based on 1-D reference models upon the Born approximation, such that the travel-time sensitivity to boundary perturbation is defined by the following integral:

$$\Delta t = \int_S \delta r(x) K_d(x) \, dx,$$

(4.2)

Sensitivity kernels for each source-receiver couple are then expanded on a set of \(i=1, \ldots, N\) basis functions \(\varphi_i\). Choosing a “pixel” parametrization as described by Boschi and Dziewonski [1999], with local basis functions that take unitary values only in the pixel, reduces Eq. (4.2) to a simple scalar product between two vectors (making use of the Einstein summation convention):

$$\Delta t = G_i \delta r_i.$$  

(4.3)

Clearly this holds for one specific event-topography-receiver configuration contained in the database associated to the travel-time anomaly \(\Delta t\). The difference between ray-theory and finite-frequency tomography lies in the construction of \(G_i\) (see Tape et al. [2006] or Peter et al. [2007] for further details about the analogies). The integral appearing in Eq. (4.2) is solved by quadrature with trapezoidal rule [Quarteroni et al., 2007], that after discretization, amounts to a simple element-wise product:

$$G_i = K_i A_i,$$  

(4.4)

where \(A_i\) is the \(i\)-th pixel area. This approximation holds as long as the pixel size is small enough to sufficiently replicate the kernel pattern (see Fig. 4.6). If our database contains \(j=1, \ldots, M\) travel-time observations that we collect in a residual travel-time vector \(\Delta t\), the linearised inverse problem takes the following (matrix) form

$$\Delta t = G \cdot \delta r,$$  

(4.5)

where \(G\) is a \(M \times N\) matrix and each row \(G_i\) corresponds to one discrete sensitivity kernel (4.3). The model update vector \(\delta r\) can be computed easily when \(G\) is not too large using a least square method, that in canonical form for mixed-determined problem takes the following form [Boschi and Dziewonski, 1999]:

$$\Delta r = (G^T \cdot G + \lambda^2 I)^{-1} \cdot G^T \Delta t,$$  

(4.6)

where the regularization term \(\lambda\) helps to stabilize the inversion. The correct value of this term is chosen by exploring the \(L\)-curves (Fig. 4.5d). Depending on the extension of the sensitivity area, the matrix will become relatively sparse which we solve with a conjugated gradient algorithm (Bi-CGSTab, see der Vorst [1992]). We tested our scheme inverting \((G^T \cdot G + \lambda^2 I)\) directly using Gauss elimination, obtaining no significant differences in the output from the iterative solver. To further increase smoothness of the solution, one could also damp the roughness of the solution using an operator \(B\) which applied to \(m\) gives the gradient of the misfit function [Boschi and Dziewonski, 1999] and the final form of (4.6) is:

$$\delta r = (G^T \cdot G + \lambda_1^2 I + \lambda_2^2 B \cdot B^T)^{-1} \cdot G^T \Delta t,$$  

(4.7)

where \(\lambda_2\) is the amount of roughness damping we introduce in the inversion. Regardless of the method used to invert the matrix \(G\) our tomographic inversion is non-iterative, i.e. the procedure ends after the first update of the model is computed. The reason resides in the spectral element code used to compute boundary kernels based on 1-D background models [Nissen-Meyer et al., 2008]. In this work we do not consider a priori information, data correlation matrix or posteriori probability. The
Figure 4.5: Various features of the inversion strategy for $PcP$ dataset. (a) The gradient of the misfit function we want to minimize with the inversion. The gradient, Eq. 4.8, contains information about the magnitude and direction of the model updates. (b) The main diagonal of the incomplete Hessian matrix $G^T \cdot G$, used to explore the data coverage. (c) The sparsity pattern of the $G^T \cdot G$ matrix for $1^\circ$ large pixel. The number of non-zero entries is mainly responsible for the computational complexity of the inversion. (d) The $L$-curve used to trim the damping parameter $\lambda$ used to stabilise the inversion of the system in (4.6)

Fréchet derivative of the misfit function projected on the residual vector, associated to travel-time tomography is calculated as:

$$g = -G^T \Delta t$$

(4.8)

that gives information about the direction and the magnitude of the model updates. The term ($G^T \cdot G$) is known as the incomplete Hessian, an approximation of the full Hessian, cheaper to compute but valid only for linear inverse problems. The values on the diagonal are used as proxy to the data coverage, as the ray plots, or hit-count were used in the case of ray-theory tomography [Tape et al., 2006; Zhou et al., 2005]. The diagonal of the incomplete Hessian in Fig. 4.5b can be compared with hit-count in Fig. 4.13e to appreciate the more uniform coverage provided by finite-frequency. Since the residuals we use for the inversions cover only a small area of the CMB as the diagonal of the Hessian indicates, the addition of the dumping term $\lambda_1$ makes the system solvable (i.e. saying that unconstrained pixels have no variation), despite in most of the synthetic inversions $N \gg M$. 
CHAPTER 4. EFFICIENT WAVEFORM INVERSION FOR CMB TOPOGRAPHY

Figure 4.6: (a) The sensitivity kernel for a PcP phase at 50° epicentral distance for an explosive event with 20s dominant period. (b-d) The same kernels expanded on inversion grids with respectively 2°, 3° and 5° large pixels. The pixel are constructed on equal-area basis on a spherical surface.

<table>
<thead>
<tr>
<th>Grid size</th>
<th>Model parameters</th>
<th>phases suited</th>
</tr>
</thead>
<tbody>
<tr>
<td>2°</td>
<td>10316</td>
<td>ScS, PcP, P_{diff}, PKP, SKS</td>
</tr>
<tr>
<td>3°</td>
<td>4592</td>
<td>ScS, PcP, P_{diff}, PKP, SKS</td>
</tr>
<tr>
<td>5°</td>
<td>1656</td>
<td>P_{diff}</td>
</tr>
</tbody>
</table>

Table 4.2: Depending on the size of the sensitivity area, different pixel size may be suited. In this table we summarize the parametrization best suited for our inversions.

4.3.2 Continuous vs. discrete kernels

The term “continuous” indicates that the mesh on which the kernel is calculated is much finer than the inversion mesh. The transition from continuous to discrete is illustrated in Fig. (4.6) where a sensitivity function $K(x)$ for PcP phase is projected onto the inversion grid made of equal area pixels. The figure highlights a key point of the inversion strategy: if the size of the inversion grid is not sufficiently small the topology of the kernel is lost, as it is shown in Fig. 4.6d. As demonstrated by Panning et al. [2009] using volumetric kernels, the size of the 1st Fresnel zone is directly related to the anomaly length-scale we want to map. This factor along with the data coverage drives the choice of the inversion grid. We investigate the implication of these parameters in section 4.4. For the synthetic inversion we employ various inversion grid parametrizations: 2°, 3°, 5°-sized pixels. Depending on the size of the 1st Fresnel zone, different parametrizations may have different effects on the results. As a general rule we state that 2°, 3° work fairly well for PcP, ScS and PKP and 5° is insufficient. $P_{diff}$ sensitivity, being larger, enable us to use up to 5° large pixel. The number of model parameters given by each parametrization and the phases suited for each pixel size are summarized in Tab. 4.2.

Not only the number of parameters determine the time to solve the system (4.5) but also the size of non negligible sensitivity that dominates the sparsity of $G^T \cdot G$. The number of observations depends on the seismic phase, the topography and on the dominant period used to filter the seismogram. Tab. 4.1 summarizes the number of synthetics inverted in the next section.
4.3.3 Volumetric and boundary sensitivity: the joint approach

A seismic waveform anomaly $\delta u$ is associated to the model perturbations $\delta v$ and $\delta d$ namely, volumetric and boundary, through the corresponding volumetric and boundary sensitivity kernels $K_v$ and $K_d$:

$$\delta u(t) = \int \delta v K_v(x, t) \, dx + \int \delta d K_d(x, t) \, dx^2. \quad (4.9)$$

In this section we focus on the volumetric term and couple its discrete form with the boundary sensitivity previously computed. Assuming an isotropic elastic Earth, fulfilling the approximation introduced in Colombi et al. [2012], we can relate waveform perturbations for volumetric heterogeneities to material properties using: density $\rho$, Young’s modulus $\lambda$ and shear modulus $\mu$. The volumetric sensitivity kernels calculated for the frequency domain by Nissen-Meyer et al. [2007a] may be computed for the time domain and they can be written as follow:

$$K_{\mu}(x, t) = \partial_t \bar{u} \star \partial_t \bar{u}; \quad (4.10a)$$

$$K_{\lambda}(x, t) = tr(\bar{E}) \star tr(\bar{E}); \quad (4.10b)$$

$$K_p(x, t) = \bar{E} \star \bar{E}; \quad (4.10c)$$

All the terms appearing in Eq. (4.10) have been properly described in Colombi et al. [2012], including the notion of backward and forward fields. Following an analogous procedure, we transform waveform kernels $\tilde{K}_{\mu}, \tilde{K}_p$ and $\tilde{K}_\lambda$ to static kernels, to obtains the travel-time sensitivity to volumetric anomaly, in a continuous form:

$$\Delta t = \int_{\Omega} \left[ \delta \rho(x) K_{\rho}(x) + \delta \mu(x) K_{\mu}(x) + \delta \lambda(x) K_{\lambda}(x) \right] \, dx^3; \quad (4.11)$$

Because we compute wave-fields solving the elastic system using the axial-symmetric code from Nissen-Meyer et al. [2007b] we follow the computational outline introduced Colombi et al. [2012] to calculate Eq. 4.11. In this framework, it looks particularly convenient for us to compute the $\lambda$ kernels $K_\lambda$ as it involves only scalar products. $K_\lambda$ expresses directly the sensitivity to $v_p$, the $P$-wave speed, such that we can consider the travel-time sensitivity in the following simplified manner:

$$\Delta t = \int_{\Omega} \delta v_p(x) K_{v_p}(x) \, dx^3. \quad (4.12)$$

Other relationships between $\rho, \mu$ and $v_s$ can be found for instance in Tromp et al. [2005]. Few examples of $K_{v_p}$ are visible in Fig. 4.8. In equivalence with to the boundary sensitivity, by choosing a set of $i = 1, \ldots, N$ base functions $\varphi_i$ and a “voxel”, Eq. (4.12) reduces to a simple scalar product between two vectors:

$$\Delta t = G_i \delta v_i. \quad (4.13)$$

where $\delta v_i$ now is the $P$–velocity perturbation in the voxel $i$, and $G_i = K_i V_i$, is obtained by quadrature [e.g. Quarteroni et al., 2007] on the $i$-th voxel volume $V_i$. If our database contains $j = 1, \ldots, M$ travel-time observations that we collect in a residual travel-time vector $\Delta t$ the linearised inverse problem takes the following (matrix) form

$$\Delta t = G \cdot \delta v. \quad (4.14)$$

where $G$ is a $M \times N$ matrix and each row $G_i$ corresponds to one discrete sensitivity kernel (Eq. (4.13)). Analogous considerations concerning the differences between continuous vs. discrete kernels as explained in section 4.3.2 apply in the volumetric case. The rectangular system in Eq. (4.14)
Figure 4.7: The joint sensitivity matrix. The block in blue represent rows purely sensitive to the mantle and therefore associated to \( P^- \) phase, notice the 0 where the columns associated to CMB are. In yellow we represent the portion of sensitivity associated to the mantle for \( PcP \) and in green those associated to the CMB.

can now be inverted using least square with a procedure analogous to Eq. (4.7) and the appropriate choice of norm and roughness damping. The discrete equivalence of Eq. (4.9) can easily be re-written combining results from section 4.3.1 obtaining the following linear system, the simultaneous joint inversion:

\[
\Delta t = G_{v_p} \cdot \delta v + G_r \cdot \delta r.
\]  

(4.15)

In practice each row of \( G_{v_p+r} \) will have a number of columns which amounts to the number of pixels + number of voxels, i.e., the global number of unknowns. The joint-volume boundary inversion grid is constructed such that voxels at the level of the CMB will match exactly the pixels of the CMB. A dimensional analysis of the quantities in Eqs. (4.9), according to the expression of forward and backward fields, shows that \( K_{v_p} \) is measured in \( s/m^4 \) while \( K_r \) is measured in \( s/m^3 \), thus the quantities in Eq. (4.15) are correctly scaled and lead uniquely to a travel-time anomaly. However the different magnitude of the sensitivity kernels may drive the inversion preferentially in one direction. A number of authors studied this problem and tried to solve it with different approaches. Greenhalgh et al. [2006]; Kennett et al. [1988] use a subspace method that seeks the solution within each parameter space. Hobro et al. [2003] proposed a simpler method that by scaling each class of model parameters, eliminates the discrepancy between different type of sensitivity. We prefer this latter approach because it is more intuitive and it matches with our formulation of joint-sensitivity matrix. The method requires to calculate a normalization factor \( n_c \) for each class of parameter (in our case \( c = 1, 2 \)) using the following relationship:
(a) $P$ kernel at 70° and 40 s

(b) $PcP$ kernel at 70° and 40 s

Figure 4.8: (a) The $P$-wave travel-time kernel at a depth of 600 km, 70° and 40 s (b) The $PcP$-wave travel-time kernel at a depth of 600 km, 70° and 40 s.

$n_c = \sqrt{\sum_{i,j} |K_{c_{ij}}|^2}$

(4.16)

where $[K_{c_{ij}}]$ are the entries corresponding to one type of sensitivity. For the volumetric part it will be the entries in the blue and yellow region while those in green for the boundary entries. The new sensitivity matrix is then obtained by dividing each sensitivity kernel by the appropriate $n_c$. This procedure regularizes the gradient of the misfit function, thereby stabilizing the inversion.

### 4.4 Inversion of synthetic data

Combining the residual waveform data computed via spectral element simulations using SPECFEM3D GLOBE as described in section 4.2.3, and the inversion scheme discussed in section 4.3 using the axisymmetric solver, we test the performance of the inversion algorithm. We also compare it to ray theory inversion and we check the applicability of our method despite the distortions introduced by the presence of 3-D mantle structures. The amount of data used by each inversion, and the number of model parameters for each grid is shown respectively in Tab. 4.1 and Tab. 4.2. An interesting aspect of this approach is the possibility to obtain images for different frequency bands. Residuals are calculated from synthetics at 20 s and 10 s dominant period and sensitivity kernels are computed accordingly. The sizes of the inversion grids are those described in Fig. 4.6. The best damping factor $\lambda_1$ is adjusted using the $L$-curve (Fig. 4.5d) calculated upon the variance reduction introduced in Boschi and Dziewonski [1999]. For the synthetic inversion we did no make use of roughness damping, hence $\lambda_2 = 0$. The choice of $\lambda_1$ did not play an important role because the model variations are small and noise is negligible, nevertheless a $\lambda \neq 0$ is requested to avoid matrix singularities. We will often relate the lateral extension of the anomaly in terms of wave-length $\mu$. The images of the model shown in this section are all calculated for 3°-large pixel inversion grid.
4.4.1 How different phases see the CMB

CMB topography with ScS/PcP

PcP and ScS performed in a similar fashion and for brevity reasons, we show only the results obtained for ScS which are more easily recorded. Fig. 4.10 presents the inversion results for two different anomalies with medium (≈ 11µ for ~10s, ≈ 4µ for 20s) and small length-scale (≈ 6µ for 10 s, ≈ 3µ for 20 s). A vertical cross-section going through the topography peak along a meridian (Fig. 4.10d,i) helps to compare the inversion output with the reference. Models with larger lateral length-scale are sufficiently reconstructed for the 20s case despite the expected amplitude reduction (Fig. 4.10a-d) i.e. the magnitude of the topography/depression is smaller. The second input model has shorter length-scale and the reconstruction is acceptable when 10s kernels are used (Fig. 4.10f-i). The models upon 20s kernels are poor in amplitude and lateral resolution, furthermore the topography peaks are slightly misplaced.

CMB topography with PKP

The PKP branches, used in several study to constrain CMB topography [Morelli and Dziewonski, 1987; Soldati et al., 2003, 2012] or structure of the lower mantle [Lay and Garnero, 2004; Vanacore et al., 2010], are characterized by double sided sensitivity, i.e. on the entry and the exit point. Plots of the sensitivity kernels show a 1st Fresnel zone of size comparable with that of PcP (see Colombi et al. [2012] for sample images). Fig. 4.2a, explains why we used only synthetic events located right on top of the topography. Observations are mainly represented by PKIKP and only few from PKPab/bc, are inverted but they are unlikely to be relevant. Fig. 4.11 presents the results for the inversion using the second input model of the ScS/PcP case. We used a global map instead of regional to check whether mapping on the exit point occurs. Positive and negative anomalies with a smaller lateral wavelength to length-scale ratio are more difficult to retrieve at 20s and artefacts are
Figure 4.10: Synthetic inversion results using $ScS$ phase. (a) The input model inserted in SPECFEM3D GLOBE. (b) The recovered pattern using $3^\circ$ spaced pixel at 20s dominant period; Picture (c) the same but at 10s dominant period. (d) The value of topography taken along the meridian-cross section (where topography is centred) for the different dominant period/pixel size. (e-h) The same as above but for a different input model. The colorbar is in [km].
on the exit point, we used global projection, rather than regional projection. The dominant periods perform. The color map is in [km]. To determine whether something was mapped on the exit point, we used global projection, rather than regional. To check whether something was mapped on the exit point, we used global projection, rather than regional projection.

Figure 4.11: Topography inverted from the 

![Image](image_url)

(a) input \( \sim 800 \text{km} \times \pm 5 \text{km} \\
(b) 3^\circ \times 3^\circ 20 \text{s} \\
(c) 3^\circ \times 3^\circ 10 \text{s} \\
(d) Meridian cross-section

Figure 4.11: Topography inverted from the \( PKP \) branches. (b) Inversion output for 20-s dominant period and different grid parameterization using \( PKIKP \) recorded by the layout in Figure 4.2 for the topography in (a). (c) As for (b), but for a dominant period of 10 s. (d) Cross-section value along the meridian passing through the center of the topography, which shows how different parameterization/dominant periods perform. The color map is in [km]. To determine whether something was mapped on the exit point, we used global projection, rather than regional projection.
introduced while good results are ensured at 10s dominant period with an overall accuracy similar to $ScS/PcP$ (Fig. 4.11b-e). The coverage is good enough such that almost nothing is mapped on the exit side of the $PKIKP$ branch but for a weak signal in Fig. 4.11b. The settings of this test resemble regional studies like Vanacore et al. [2010] for instance, which uses observations from single or just few earthquakes assuming good sensibility of this phase over a quite dense and closely spaced array of receivers.

**CMB topography with $P_{diff}$**

Core diffracted waves $P_{diff}$ do not carry as much information for topography as in the $ScS/PcP$ case. We nearly doubled the lateral length-scale ($\sim 18\mu$ for 10s) of the anomaly to obtain usable imprints out of the cross-correlation. In spite of this, residuals can be measured only for 10s dominant period waveform. Kernels and inversions are therefore restricted to this case. The tomographic maps in Fig. 4.12 show a poor reconstruction. This conclusion could be drawn a priori just by looking at the magnitude of the residual travel-time, less than a tenth in magnitude than what reflected or transmitted phases could provide [Colombi et al., 2012]. The impossibility of reproducing a topography of a significant lateral length-scale and consistent magnitude for higher dominant period prevents us from frequency dependent comparisons. Our claim for this lack of sensitivity is:

1. the non negligible sensitivity surface is significantly larger than that of reflected phases;

2. the wave-front healing effect cancels the effect of the anomaly as documented in Malcolm and Trampert [2010].

We conclude that core diffracted waves are not suited for CMB topographic inversions because they produce not accurate results.

### 4.4.2 Finite frequency vs ray-theory

A rigorous test against ray-theory should consider only infinite frequency kernels, but for sake of completeness and curiosity, we present the model obtained inverting our database with ray-theory. We selected our shortest period dataset (10s) for one of the topography models available and we use the residual travel-time for the ray-theory code developed by Soldati et al. [2012] that solves CMB topography. Their inverse problem has been parametrized in a similar fashion, but the iterative solver was LSQR of Paige and Saunders [1982]. The results shows that ray-theory reconstructs quite well the anomaly provided that the inversion grid ensures sufficient coverage. Looking at the hit-count table in Fig. 4.13e we see that coverage is missing in some areas and the corresponding output map is biased. With finite-frequency this does not happen because the smoothing effect of the kernels produce smoother maps also where ray-coverage is not perfect. This can be deduced by looking at the diagonal of the Hessian in Fig. 4.5b, where the coverage with finite frequency looks more uniform (considering the same dataset).

This suggests that finite-frequency may perform better on smaller pixel grids than ray-theory, or in other words, that finite-frequency with the same parametrization needs less data to constrain the model space similarly.
Figure 4.12: Inversion results using $P_{diff}$ phase. (a) The input model inserted in SPECFEM3D GLOBE. (b) The recovered pattern using $3^\circ$ spaced pixel at 10s dominant period. (c) The value of topography taken along the meridian-cross section (where topography is centered) for the different dominant pixel size. (d,e) The same as before but for a different input model.
Figure 4.13: Ray-theory inversion test. (a) The input model already used in Fig. 4.10 and Fig. 4.11. (b) The ray-theory model. The colorbar is in [km]. (c) Meridian cross-section. (d) The hit-count map associated to each inversion parametrization.
4.4.3 Influence of the source-receiver distribution and density

The source-receiver layout used for the previous test represent an ideal case, rarely found in reality, however our approach quickly allows to verify resolution and coverage capacities of kernels. To do so, we now arrange the source-receiver layout in various ways.

**Acquisition grid coarsening**

We eliminate records from the database to reach $2^\circ, 4^\circ, 6^\circ$ and $8^\circ$ spaced receivers. We repeat this experiment for PcP because the coverage with this phase was good and such were the inversion results. In the interest of conciseness, we do not show results for each model but rather measure the $L_2$ norm difference from the input model:

$$\chi = \sum_N \delta r_{\text{input}} - \delta r^2,$$

where the sum is intended over the inversion parameters $\delta r = \delta r_i$ with $i = 1, \ldots, N$, and the input model discretized over the same grid. We show the result only for the topography in Fig. 4.10f, as it represents the most challenging case. The plot in Fig. 4.14 shows on the $y$-axis the value of $\chi$ normalized over the initial misfit $\chi_0$, therefore differences are interpreted in a relative sense. The smoothing effect of the kernels helps keeping the inversion solution stable, however for more than $4^\circ$ the solution is not satisfactory anymore; magnitude and shape in particular are lost. The number of observations drastically reduces and the stations with dominant $\Delta t$ do not enter in the inversion. The degradation is slightly more pronounced when the grid used has smaller pixel as shown by Fig. 4.14b.

**USArray-like distribution**

By virtue of symmetry we can change our database as it was covering North America and we can select the stations close to their actual USArray position. We do not have the same flexibility for the Earthquake distribution, hence we select a group as shown in Fig. 4.15. The input anomaly is the one in Fig. 4.10a and it represents the most challenging test using 10s data. Although worse than those in Fig. 4.10 the shape and magnitude of the anomalies are quite well reconstructed. Notice that this
was possible only using $\sim 500$ measurements. In practice, a receiver distribution like USArray should be able to reconstruct such features even better because a larger number of Earthquakes covering a broader azimuth and area is available.

### 4.5 Seismic data inversion

We now use our algorithm to invert the cross-correlated travel-times collected by Ritsema et al. [2010]. The regularization scheme is based on norm and roughness damping to stabilize the solution and to smooth out the variations. We base the choice of $\lambda_1$ and $\lambda_2$ on the $L$-curve analysis introduced in Fig. 4.5. The CMB topography maps in Fig. 4.16 are combined with coverage maps showing the regions where there is sufficient data coverage, thus results are more reliable. The coverage is estimated using the diagonal of the approximated Hessian, i.e., $G^T \cdot G$ which gives a proxy to the data coverage [Fichtner and Trampert, 2011; Tape et al., 2006]. We filter the spherical harmonic spectrum of the tomographic maps to eliminate noise at $l > 10$. Tomographic inversions are computed using cross-correlated travel-times calculated by Ritsema et al. [2010]. This database includes $\sim 35000$ SKSac, $\sim 18000$ and PKIKP, $\sim 9000$ ScS phases. The number of this latter observation is too small to be used for a ScS only map and therefore it is not shown. The data have been relocated and corrected for ellipticity. Crustal corrections are based upon CRUST 2.0 [Bassin et al., 2000] and added to the residual travel-time as static corrections. Mantle corrections provided by the author and our corrections implemented using the body waves in the database of Ritsema et al. [2010] give similar results. We used the former to correct for mantle structures, such that the residual travel-times should then be approximately sensitive only to the CMB. The effect of the outer core on the PKIKP and SKS is assumed to be negligible. The sensitivity kernels for $S$-data are computed for a dipole moment tensor at 18s located at varying depths according to 20 km bins. Same period but explosive source is used for the $P$-data. The vertical component of the velocity seismograms was used for the SKS and PKIKP. We first observe that the coverage is sufficient only along the pacific rim. In the illuminated regions we recognize some analogies with other models [e.g. Soldati et al., 2012].
Figure 4.16: CMB topography maps from S40RTS cross-correlated travel-time data on a $3^\circ \times 3^\circ$ grid filtered up to a spherical harmonic degree 10. Contour lines isolate the regions where the data ensure sufficient coverage. (a) Topography map obtained using SKS\textit{ac} data and its relative data coverage. The damping used is: $\lambda_1 = 3$ and $\lambda_2 = 3$. (b) Topography map obtained using PKIKP data and its relative data coverage. The damping used is: $\lambda_1 = 1$ and $\lambda_2 = 4$. Colorbar for topography maps is in [km].
The presumed presence of deep subduction results into a depressed CMB (blue areas), especially in the $PKIKP$ model. The difference between Fig. 4.16a and b indicates that resolution is limited, which could be explained by limited data quality or by the difficulties inherent to the presence of heterogeneity throughout the mantle, as discussed in the next section.

4.5.1 3-D mantle and topography

A classic way to account for the mantle effect on travel-time, is to eliminate its contribution to the total travel-time anomaly as described by Eq. (4.1) (static corrections). These corrections are calculated from an a priori 3-D mantle model which should represent as faithfully as possible the real mantle (see also section 4.2.4). If this is the case, and finite frequency effects are taken into account in both mantle and the CMB, the mantle effect can be ruled out completely as as shown in Fig. 4.17.

For this example we used the synthetics corrected for the S40RTS mantle in Fig. 4.4. To estimate the errors that inaccuracies in the mantle model would thus cause in our CMB maps, we conduct the following test, exaggerating the mantle bias. Synthetics are those associated with model S40RTS, but the mantle correction is now wrongly calculated after dividing S40RTS amplitude by 2 upon Eq. (4.1). The result is shown in Fig. 4.18 where the input model is compared with the biased output model. Artefacts appears because the mantle is mapped into the CMB. The error can be caused not only by a biased mantle model, but in a finite frequency context, from an incorrect calculation of the frequency dependent travel-time misfit by cross-correlation. In other words mantle correction applied to the CMB data must be calculated for the same frequency for Eq. (4.1) to be valid. Probably the only valid approach to tackle the problem of the mantle correction is through a mantle+CMB joint inversion, further discussed in the next section.

4.6 Outlooks for joint volumetric and topography inversion.

We next use the joint sensitivity, introduced in section 4.3.3 to investigate how simultaneous joint inversion could improve the CMB maps obtained previously. A qualitative way to assess if the delay due to the mantle on CMB sensitive phases can be isolated, is by reverse modelling residual travel-times due to both mantle anomalies and CMB topography. Focusing only on $P$ and $PcP$ phases, we compute sensitivity kernels for source receiver pairs that experience similar sensitivity through the mantle in a simplified scenario. We compute $G_{v}$ for the source-receiver layout of Fig. 4.1d. We select source-receiver couples for which the epicentral distance is between 65° ± 80°. For this distance-range the volumetric sensitivity of $P$ and $PcP$ phases is similar in the first ~1000 km depth (as Fig. 4.8 shows) and therefore an anomaly located in this area should be felt in a similar way. This idealized scenario is represented in Fig. 4.19. A fast anomaly, inserted between 100 and 900 km depth and 45° × 45° large, is located directly above a positive CMB topography of the type in Fig. 4.1e, 30 km height and ~6000 km large. The receiver grid and the fast anomaly are centered above the topography peak. In second example we move the fast anomaly in the deep mantle between 1900 and 2700 km.

Using the procedure in sections 4.3.3 and 4.4 we compute $K_{v}$ for $P$ and $[K_{v}, K_{d}]$ for $PcP$ phases that we then project onto the inversion grid. The normalization factor appearing in Eq. 4.16 is not necessary because we use the travel-time residuals and not directly the kernels. The computations are done at 40 s to reduce the computational effort in calculating volumetric kernels. To compensate the reduction of sensitivity that longer period waves have, we increase the size and the extension of
Figure 4.17: CMB inversion with 3-D mantle correction according to Eq. (4.1). (a-b) The input models. (c-d) The tomographic output for 20 s and (e-f) the output model for 10s data. (g) The meridian cross section comparing results with and without the mantle effects.
the topography anomaly according to the results obtained by Colombi et al. [2012] during synthetic and reverse modelling tests. The distance range is sufficiently large for an accurate projection on to a $3^\circ \times 3^\circ$ inversion grid of $P$ kernels. The source-receiver layout chosen ensures sufficient coverage along all the azimuths surrounding the anomaly for a total $\sim 4500$ observation of $P$ and $PcP$ phases.

The choice of using the differential $P$-$PcP$ sensitivity to correct for overlying structures is known in seismic tomography. We claim that although this method is good for crust and upper mantle heterogeneities because the sensitivity is similar (both using ray-theory and finite frequency), it may fail for anomalies located in the lower mantle where sensitivity patterns differ. We now model travel-time residuals $\Delta t$ using Eqs. 4.13 and 4.3 for each source-receiver pair. The net effect of the mantle $\Delta t_P$ captured by the $P$ phase is subtracted from the $\Delta t_{PcP}$ which contains both. The result is a proxy for the residual due to the CMB. Because of the large number of source-receiver pairs sampling anomalies in various ways, it is important to filter results using summary data, like the maximum or minimum value over all the dataset. Both the fast anomaly and the positive topography produce a negative residual, anticipating the arrival time of the phase. This helps avoiding ambiguity in our analysis. Over all the possible source receivers pairs (that are within the distance range) we calculate the maximum value of $\Delta t_{PcP} - \Delta t_P$ and $\Delta t_P$ for the same distance ranges. The distance range and the kernels are calculated using 1-degree bins. In Fig. 4.20(a) we plot the value of $\Delta t_P$ (red line) and $\Delta t_{PcP} - \Delta t_P$ (blue) as a function of the epicentral distance. This latter represents the travel-time residual due to topography. It shows a monotone decrease that agrees with the average travel-time anomaly due to the CMB topography only for each epicentral-distance bin. The travel-time residuals generated from the mantle (red line) feature stronger oscillation due to the irregular sampling of the velocity anomaly. Those oscillations do not seem to propagate in the blue line. On the other hand, Fig. 4.20(b) shows that when the velocity anomaly is located in the lower mantle this method fails, because the sensitivity in that region differs too much. Bearing in mind that the $K_{vp}$ component of $P$ and $PcP$ sensitivity kernels are very similar only in the upper mantle, we can conclude that the monotone trend of the blue line (CMB topography effect) is a good indicator that the mantle contribution can be ruled out from the combined effect of mantle heterogeneities and
CMB topography. Therefore a joint inversion featuring data with good coverage of the whole mantle can successfully capture the volumetric effect. It is however to be verified the validity of such a test and the coverage required in the presence of complex mantle and CMB structures with various length-scale.

### 4.7 Conclusion

Using a comprehensive synthetic database, we tested the theory and the methodology for constraining boundary topography developed in Colombi et al. [2012] and applied it to real global seismic datasets of both compressional and shear waves. With respect to Colombi et al. [2012], our synthetic database is more complete in that it contains waveforms for $PKP$ and $ScS$ arrivals associated with a set of different CMB and mantle models. To account for complex laterally varying mantle models, part of the synthetics database is obtained using a 3-D background model S40RTS by Ritsema et al. [2010] down to a period of 10s. Using this latter we verify that static corrections derived from 3-D model are valid, and provided that the mantle model is correct, the effect of boundary topography is separable from that of the mantle. Exploring into the synthetic data we found that the magnitude of the travel-time anomaly is as small as a tenth of the travel-time anomaly caused by mantle heterogeneities if any of the current CMB topography model would be used. This forces us to conclude that CMB topography is not a sufficiently isolated effect in the waveforms compared to mantle contributions, as expected. The dependence of the residual magnitude calculated with cross-correlation on the dominant period used appears clearly. In the analytical section 4.3 we outline the formulation of the inverse problem in a least square sense using roughness and norm damping starting from the results in Colombi et al. [2012]. The algebraic system is solved with an iterative solver and the result is the
model update. We complete the section providing the expressions for mantle sensitivity kernels and we show how they can be merged with boundary kernels to set up a simultaneous joint inversion for compressional wave-speed and CMB topography. A normalization factor between the two classes of parameters is however necessary.

The results of the synthetic inversions for $PcP$, $ScS$ and $PKP$ phases lead to interesting conclusions, using the correct frequency contents, the input model can be retrieved successfully, both in magnitude and pattern, while those of $P_{diff}$ could not be retrieved in a satisfactory manner. We highlight the importance of choosing the correct parametrization in accordance with the wavelength of the anomaly we want to constrain and consequently the dominant period at which kernels are calculated. These parameters have to be chosen accordingly to the data-coverage, which can be verified using the diagonal of the approximated Hessian as we did in section 4.3 and 4.5. According to our results, at fixed frequency-range, the output from $PcP$, $ScS$ and $PKP$ should be almost the same. Ray-theory does not perform much worse than finite-frequency for our specific setting but some issue with the model coverage emerged when inverting one synthetic dataset. Using an excessively fine parametrization is discouraged as it gives rise to spurious small-scale features as in section 4.4.2. Varying the source-receiver layout to approximate real coverage shows that more than the position of the earthquakes, a dense acquisition grid similar to that installed by USarray is more important. With the dominant period used in this work (10-20 s), the structures appearing in current models should be perfectly reconstructible.

Starting from a 1-D CMB model we separately invert cross-correlated travel-time data for $PKIKP$ and $SKSac$ from Ritsema et al. [2010] obtaining maps characterized by non-uniform coverage. Although part of the resolved structures are consistent with geodynamical models of the deep mantle, the difference between the two maps may indicate lack of data resolution or a biasing effect due to mantle correction. With a synthetic inversion we show how this may limit the capacity to resolve CMB topography. With the aim of setting up in a future study a simultaneous joint inversion, we verify the capacity of mantle sensitivity kernel of capturing the travel-time anomaly due purely to mantle heterogeneities, with respect to the joint effect of topography and mantle. The results from the reverse modelling show that in a simple scenario with just a layer of negative anomaly in the

Figure 4.20: (a) Summary travel-time residuals for mantle only and topography calculated for equal source-receiver only $P$, (red line) and $PcP$ kernels (blue line) as if these latter would feel only the CMB. The anomaly was located in the upper mantle. (b) Same as (a) but for a wave-speed anomaly located in the lower mantle.
upper mantle and a simple CMB topography, the delay times due to the mantle calculated from $P$ kernels are correctly extracted from that of $PcP$ kernels containing both. Conversely if the anomaly is located in the lower mantle the topography signature is less accurately retrieved because the sensitivity tradeoff due to deep-mantle heterogeneities. The results from this test suggest that a joint inversion, featuring mantle and CMB sensitive data and their associated sensitivity kernels, will improve the visibility of the CMB topography. Before doing that we need to collect an adequate dataset of cross-correlated travel-times that ensure, besides a good CMB coverage, also a good sampling of upper and lower mantle.
**Abstract**  Simulating the propagation of flexural waves on a thin plate, and conducting laboratory experiments on a similar plate, it is possible to identify the relative contributions of reverberation and source distribution to the diffusivity of the ambient wave field and hence to the success of seismic interferometry. For a diffuse wave field, ensemble-averaged cross-correlations of continuous recordings made at two different locations on the plate approximate the Green’s function associated with those locations, including reverberations from the boundaries of the plate. Studying the performance of receiver-receiver interferometry at retrieving the Green’s function, exciting the plate in different ways, it is shown that a spatially uniform distribution of point sources is more effective than an azimuthally uniform source distribution at enhancing the fit between cross-correlation and Green’s function. How the plate is excited is critical to the “diffuseness” of the generated wave-field. An air-jet source produces a very diffuse field that leads to retrieval of the Green’s function after stacking only few cross-correlations. To extract the Green’s function from the cross-correlation of time-space point sources many more realizations are needed, and a sufficiently long time window must be used to smooth out the effects of the more energetic first arrivals.

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### 5.1 Introduction

Ensemble-averaging of field cross-correlation over long time window is a powerful tool in seismic, acoustic, helioseismic imaging [Aki, 1957; Duvall et al., 1993; Lobkis and Weaver, 2001; Sabra et al., 2005; Shapiro and Campillo, 2004].

In seismology, this approach has the particularly significant merit of allowing seismic tomography even in the absence of earthquakes or other “deterministic” sources. Regions of the Earth that were previously invisible to tomographers are now illuminated by cross-correlation observations. Since most ambient noise observed on Earth propagates in the form of short-period (~10s) surface waves [Hillers et al., 2012], this is particularly relevant to crust-lithosphere imaging; yet, recent work shows
that the same techniques can be applied to broad-band signal sampling the entire mantle down to the core Nishida [2013]; Poli et al. [2012].

The cross-correlation of the signal recorded at two stations consists of a so-called “causal” contribution, which contains energy traveling from a reference station to another, and an “anti-causal” one, traveling from the second station towards the reference one. If noise sources are uniformly distributed or just sampling the stationary-phase region [Curtis et al., 2012; Roux et al., 2005; Snieder, 2004], the causal and anti-causal parts of the cross-correlation are symmetric with respect to zero time [Fan and Snieder, 2009; Hillers et al., 2012], and the Green’s function is approximated well. Non-uniformities in the geographic distribution of noise sources still allow to estimate the velocity of surface wave propagation, but greatly complicate phase and amplitude measurements [Froment et al., 2011; Tsai, 2009, 2010], and, in general, the reconstruction of the complete Green’s function including surface waves, body waves and reflected waves. The length of the cross-correlation time window is often regarded as alternative to the sources uniformity, but the validity of this assumption and the trade off between the two have not been sufficiently studied.

Using flexural waves on a thin plate we propose an analysis, supported by laboratory and numerical experiments, that aims at disentangling the relative roles of reverberation, cross-correlation time window and source distribution in giving rise to a wave field diffuse enough for cross-correlations to approximate well the Green’s function, beyond the often observed, direct surface-wave peak. Because of their dispersive nature, flexural waves in a thin plate are well suited to mimic the behaviour of Rayleigh waves in the Earth Larose et al. [2007].

The article is divided into two main sections. After a theoretical example showing the benefit of a uniform distribution of sources when phases other than the direct one are sought (Sec. 2), a spectral element simulation of the plate motion is presented and followed by a benchmark of various source distribution layouts and cross-correlation lengths. We then (Sec. 3) illustrate how the receiver-receiver Green’s function is retrieved from ensemble-average cross-correlation in a laboratory experiment, and evaluate how the performance of interferometry is affected by the nature and distribution of sources.

5.1.1 Spatially- vs. azimuthally-uniform source distribution

The theory of diffuse wave-field interferometry is based on the finding that, by (i) cross-correlating the signal generated by a point source at two receivers, (ii) iterating over a sufficiently large set of more or less uniformly distributed sources, and (iii) stacking (“ensemble-averaging”) the cross-correlations, an average trace is found that approximates the Green’s function associated with the locations of the two receivers [Boschi et al., 2012]. Mathematically, this is most generally expressed by the following expression at frequency $\omega$:

$$G_{12} - G_{21} = \frac{4i\omega\kappa}{c} \int_V G_{1x}G_{2x}^* d^3x + \int_{\partial V} (G_{1x}\nabla G_{2x}^* - \nabla G_{1x}G_{2x}^*) d^2x,$$  (5.1)

where $G_{ij}$ denotes the Green’s function associated with source location $i$ and receiver location $j$, $c$ is phase velocity and $\kappa$ attenuation. After Fourier transform back to the time domain the two terms at the left-hand side of (5.1) are the “causal” and “anticausal” parts of the Green’s function, i.e. the Green’s function corresponding to a source at the location of receiver 1, recorded at receiver 2, and the reciprocal Green’s function (source at the receiver 2, recorded at 1), respectively. The volume integral extends to the volume $V$ occupied by sources, and the surface integral is conducted along the boundary of such volume, which is assumed to be far from any sources or obstacles [?]. In practice
we can hardly imagine such an even source distribution. Since the available sources (active sources or sources of ambient noise) are located at the surface of the Earth, it is tempting to view the problem of correlations as a reduction of Eq. 5.1 to the surface integral term. Furthermore, in practice it would be difficult to measure gradient, it is generally assumed that the surface integral can be reduced to a form [e.g. ?]:

\[ G_{12} - G_{21}^* = \frac{2i\omega}{c} \int_{\partial V} G_{1x}G_{2x}^* d^2x. \] (5.2)

This is a valid approximation if the surface is in the far field of the receivers and of the heterogeneity of the medium. In this case the integrand refers to correlation of direct observables. The source averaging of cross-correlations is the processing strategy that is followed in the applications, and this is the strategy we choose here too in order to evaluate the pertinence of this approach. In the following we have to keep in mind the approximation made when choosing our processing. Note that in the 2D experiments we present, the volume and surface integrals of Eq. (5.1) reduce to surface and line integrals, respectively.

Many sources (or, alternatively, many scattering obstacles) are needed for the wave field to be diffuse, which is essential for the Green’s function to be retrieved from a stack of cross-correlations. In practice, if the medium of propagation is simple, i.e. homogeneous, non-scattering and non attenuating, a simple layout of point sources such as a circle or an ellipse enclosing the receivers may be sufficient to reproduce \( G_{12} - G_{21}^* \) [Froment et al., 2011; Snieder, 2004]. If we are simply interested in reconstructing the “first arrival”, i.e. the earliest portion of the Green’s function, it might be enough to have sources in the so-called “stationary-phase regions”, i.e. aligned with the azimuth defined by the receiver pair [Curtis et al., 2012; Fan and Snieder, 2009; Roux et al., 2005]. If the medium is more complex, including scatterers, boundaries, interfaces and/or smooth heterogeneities, the Green’s function results from the superposition of a variety of arrivals, and is harder to reconstruct. In this case, it becomes necessary to illuminate the medium with a uniform, dense distribution of sources, if the complete Green’s function is to be reconstructed [Sato, 2010].

Numerical and laboratory experiments on scattering reconstruction [Fleury et al., 2010; Mikessell et al., 2012; Snieder and Fleury, 2010] have been carried out upon a source-receiver layout where sources are located along a line surrounding the receiver pair, never evenly distributed over the whole target area. This is qualitatively equivalent to neglecting the volume integral at the right-hand side of Eq. (5.1). Using a simple 2-D example we demonstrate how the presence of only one reflecting boundary on a thin plate, responsible of a second arrival in the Green’s function, requires the source distribution to be uniform over the medium’s volume, for the Green’s function to be accurately reconstructed. Fig. 5.1a, b show our circular and uniform source layouts, respectively. The receivers, respectively R1 and R2, are 60 cm away from one another, while the wall is located at a distance of 3 m from both R1 and R2, in the “North” direction. In this first, “toy” experiment, we model wave propagation via a simple ray-theory approximation: a sinusoid modulated with a Gaussian propagates along straight ray paths from a point (geometrical spreading is accounted for), with the phase velocity found on our plate at the selected central frequency.

The cross-correlation gather in Fig. 5.1a shows how the arrival time of each phase in the cross-correlation depends on the azimuth of the source with respect to the azimuth of the two receivers. The gather is dominated by the “ballistic” term, i.e. the arrival time of the cross-correlation maximum changes smoothly with azimuth, is largest (in absolute value) for sources aligned with the receivers, and 0 when the source is equally distant from the receivers. The stacked cross-correlation in Fig. 5.1c
is dominated, as expected, by the “direct” signal, propagating from one receiver to the other, and by the “reflected” signal propagating from one receiver to the wall and, after reflection, to the other receiver. These two phases result from the positive interference between cross-correlations of sources in the stationary-phase area when they are stacked [Roux et al., 2005; Snieder, 2004] i.e., when the slope of the cross-correlations maxima changes in the gather plot [Fan and Snieder, 2009], and are clearly visible in both the causal (positive-time) and anti-causal (negative-time) portions of the cross-correlation, at ±0.7 ms and ±6 ms, respectively. Fig. 5.1c also shows, however, that a number of stationary-phase points result from the circular geometry of the source distribution, giving rise, in the stacked cross-correlation, to a set of seismic phases whose arrival time depends on the radius \( r_i \) of each circle of sources. These arrivals are not part of the Green’s function associated with the receiver locations, whose form depends only on the medium properties and interface geometry. We call such phases “spurious”: if the correct Green’s function is to be retrieved by interferometry, they have to be eliminated by improving the source distribution. We have found that increasing the distance of the sources \( r_i \) with respect to the receivers separation \( d \) is not sufficient to remove the spurious arrivals.

The gather and stack in Fig. 5.1d result from the uniform source distribution of Fig. 5.1b. Although the total number of sources used is lower than in Fig. 5.1a or c, there are no stationary-phase points other than those associated with arrivals in the true Green’s function, and the cross-correlation consequently does not include any spurious maxima. We infer that spurious oscillations are cancelled more efficiently by a spatially, rather than azimuthally uniform source distribution. The “ballistic” peak associated with the reflected wave in the cross-correlation gather of Fig. 5.1d is characterized by a sudden amplitude drop around the stationary-phase region. This is explained by the nature of the algorithm used to calculate the gather: cross-correlations are grouped in 0.5° bins, and traces forming the gather plot already result from stacking the signal within each bin. Away from the receiver-receiver azimuth, even small changes in azimuth give rise to significant changes in the recorded signals, which interfere destructively when stacked.

In the following, we shall employ numerical simulations to further compare uniform and circular source distribution, in more complex and realistic scenarios that include dispersion and multiple reverberations.

### 5.2 Numerical simulations of flexural waves

Flexural waves \( A_0 \) Lamb’s mode [Lamb, 1904]) generated in a thin plate are a good proxy for Rayleigh waves in the Earth [Larose et al., 2007]. We model numerically the 1.5 × 1.5 m aluminium thin plate (2 mm thickness) with free boundaries depicted in Fig. 5.2. The material, aluminium 1050, is characterized by a density \( \rho = 2710 \text{ kg/m}^3 \), a compressional wave speed of \( V_p = 6300 \text{ m/s} \), and a shear wave speed of \( V_s = 3100 \text{ m/s} \). We assume the material to be isotropic and homogeneous. Some difficulties arise (computational cost) but the flexibility of the spectral-element method [Padovani et al., 1994] (SEM) we employ makes it easier to disentangle the relative contributions of different aspects of the experiments: in particular, reverberation and (non)uniformity of the source distribution, which can be turned on and off by editing a parameter file.

Our approach differs from other works where numerical simulation has been used [Snieder et al., 2008] in that we allow for a much longer propagation time within a closed, reverberating cavity; there is time for multiple border reflections, resulting in a very diffuse field.
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Figure 5.1: (c) Cross-correlation gather calculated using ray theory and geometrical spreading factor for the configuration in (a), ordered along the $y$-axis upon the azimuth for increasing radius starting from the bottom with the innermost circle. The $x$-axis represents time in [s]. (d) Same as (c) but for the configuration in (b) ordered along the $y$-axis upon the azimuth. (a-b) The sources (red)-receiver (blue) layout for the two cases. The size of the domain is $6 \times 6$ m in both examples, receivers are 0.6 m separated and aligned with the centre. The impulse used has a central frequency of 10 KHz. N-side stands for the north boundary, the one responsible for the reflections. Dashed black lines, sketch the approximate position of the sources and the associated cross-correlations.
5.2.1 Simulation setup

We make use of the latest release of SPECFEM3D [Peter et al., 2011], in combination with the meshing tool CUBIT (http://cubit.sandia.gov/), to simulate the propagation of elastic waves on our plate. After decomposing the mesh in a load-balanced fashion, the simulation is executed in parallel on 2048 CPUs for ~2 hrs to simulate a ~25-ms-long accelerogram. In such a short time, a wave at 10 KHz bounces back and forth from the sides of the plate more than 20 times. Since each simulation has a considerable cost, proportional to the accelerogram length, we use the source-receiver reciprocity theorem [Aki and Richards, 1980; Curtis et al., 2012] which allows to swap the roles played by sources and receivers: to simulate how a diffuse field (generated by the combined effect of multiple sources) is measured at a receiver pair, only two simulations need to be conducted, each initiated by a source placed at the location of one of our receivers, R1 and R2. The signal is then “recorded” at source locations, which, in analogy with section 5.1.1 above, are alternatively distributed along a circle around R1 and R2 (Fig. 5.3a), or uniformly over the surface of the plate (Fig. 5.3b). This simplification does not change the physics of the problem, and it is common practice in this type of numerical experiments [Mikesell et al., 2012]. The piezoelectric point source that would be used in reality to excite the plate is emulated by a numerical Dirac’s function in time and space, acting on the vertical direction, the “receivers”, located w record z-component of the acceleration. The spectrum
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(a) Circular distribution

(b) Uniform distribution

Figure 5.3: (a) The plate with sources arranged in a circle around the receivers. The whole circle contains approximately 600 sources, the azimuth is computed according to the convention $[-\pi, \pi]$ from the midpoint between the two receivers as shown by the arrows. (b) The plate with the sources uniformly distributed over the surface 0.06 m spaced, for approximately 600 sources in total. The same convention is used for the azimuth.

Figure 5.4: The first 2 ms of the normalized Green’s function filtered between 10 and 25 KHz containing direct arrival, and the main first reflections from the boundaries label after a travel-time analysis according the source-boundary-receiver distance.

of the source, being flat, requires the accelerogram to be filtered in the $10 - 25$ KHz frequency band. Importantly, attenuation is neglected in our simulations; the coupling of our system with air (part of the signal emitted by a piezoelectric transducer propagates as sound), and of the plate with the supporting structure and with the accelerometer is likewise not modeled. As a result, we do not expect to match laboratory results exactly.

5.2.2 First arrival analysis

Prior to the reconstruction by cross-correlation, we verify that the response to an impulsive source, i.e. the Green’s function recorded at a given position of the plate, contains, besides the first arrival, other secondary phases due to reverberation. We calculate numerically the wave field generated by an impulsive point source in R1, and show in Fig. 5.4 the corresponding signal at R2, i.e. the reference Green’s function between R1 and R2. In Fig. 5.4 we have attempted to explain each peak in terms of a reflection from one of the four sides of the plate. The main difficulty in this exercise is to isolate single phases when the medium is dispersive and reverberant. Three main wave packets are distinguishable after the direct arrival, each containing reflected phases. We compute the travel-time using the wave-speed calculated from the main wiggle of the direct arrival (thus at 0.5 ms), resulting in a speed of $\sim 1200$ m/s. The other travel-times are derived easily from a geometric analysis of each
source-boundary-receiver configuration using the blueprint in Fig 5.2. Any arrival after these four phases results from interfering paths because of multiple reflections on the plate boundaries.

5.2.3 Circular vs. uniform distribution of sources

We show in Fig. 5.5 and Fig. 5.6 the results of generating diffuse-like wave fields from the source distributions of Fig. 5.3b and a, respectively. In both cases, we filter the signal between 10 and 25 KHz, cross-correlate it over two different time windows and compare the results. The cross-correlation gather and corresponding stack in Fig. 5.5a are obtained after selecting a 2 ms time-window starting from 0-time, which contains the direct phase and the first coherent later arrivals discussed in Fig. 5.4. The gather plot in Fig. 5.5a is qualitatively analogous to that of Fig. 5.1d, dominated by the ballistic term. The constructive interference which results in the direct arrival in the cross-correlation stack corresponds to the time at which the ballistic maximum in the gather has a slope change, i.e. the stationary-phase region at $\pm 0.5$ ms [Fan and Snieder, 2009]. The stack matches fairly well the portion of the reference Green’s function that corresponds to the direct arrival, but the fit deteriorates before and after.

If we cross-correlate over a longer time window (Fig. 5.5b), the gather is no longer characterized by the ballistic signature, but rather by vertical, constant-arrival-time stripes that can be associated to the predicted arrival times of, (i) at $\pm 0.5$ ms, the direct phase from R1 to R2 and vice versa, and, (ii) at $\pm 0.15$ ms, the phases traveling from R1 (R2) to the two closest reflecting sides, and then, after reflection, to R2 (R1). Importantly, the stacked cross-correlation practically coincides with the reference Green’s function, except for the 0-time where (weak) spurious oscillations pollute the trace.

Many authors [Fan and Snieder, 2009; Wapenaar et al., 2010] employ virtual or real rings of sources to generate diffuse wave fields and to study the role of azimuthal source density on the ensemble-averaged cross-correlation [Froment et al., 2011]. We show in Fig. 5.6 the results of applying this approach, with the source-receiver configuration of Fig. 5.3a. The cross-correlations in Fig. 5.6a were conducted over a time window as short as that of Fig. 5.5 (2 ms); yet, the gather plot is much more complicated, with the superimposed ballistic signature of numerous phases other than the obvious, “direct” one. If we consider just the direct arrival, plus the 4 boundary reflections we expect 25 patterns in total of which: 10 are physical while 15 are due to spurious oscillations. In analogy with Fig. 5.5, the ballistic signature is lost by increasing the length of the cross-correlation window. The gather plot of Fig. 5.6b is characterized by causal and anti-causal (i.e., positive- and negative-time) constant travel-time arrivals that sum up constructively in the stack, corresponding to the causal and anti-causal direct and the side reflections arrivals also seen in Fig. 5.5b. Yet, vertical stripes of high-cross-correlation in the gather plot of Fig. 5.6b are less clearly visible than in the corresponding plot of Fig. 5.5b, and the fit between the stack and the reference Green’s function is accordingly not as good.

We explain this effect on the basis of Fig. 5.1 and the corresponding discussion. A circular source distribution interacts with an obstacle in a complicated medium, giving rise to a coherent, “ballistic” arrival in the cross-correlation gather that contributes constructively to the cross-correlation stack, but does not appear in the medium Green’s function (i.e. it is “spurious”). In Fig. 5.1c, the gather plot was relatively simple because the medium (a uniform half space) only included a single obstacle (the reflecting boundary on the north side of the plate). In Fig. 5.6a, where flexural waves are reflected...
Figure 5.5: Cross-correlation gathers (top) and stacks (bottom) for the uniform source distribution in Fig. 5.3b filtered over a frequency band of 10-25 KHz. (a) Cross-correlations computed over a 2 ms time window, which includes only the first arrival and the secondary reflections; stacked cross-correlation (blue) compared to the reference Green’s function (green). (b) Same as (a) but for a time window of 25 ms starting from the 0-time. We have muted the signal coming from sources too close to the receivers because they pollute the signal.
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Figure 5.6: Cross-correlation gathers and stacks for circular source distribution in Fig. 5.3a filtered over a frequency band of 10-25 KHz. (a) Cross-correlations gather for a 2 ms time window including only first arrival and secondary reflections. Below, the stacked cross-correlation in blue, while the reference Green’s function in green. (b) Same as (a) but for a time window of 25 ms starting from the 0-time.

from four sides, the number of phases quickly grows and so does the number of spurious arrivals in the cross-correlation stack.

We infer that a circular source distribution, very useful to highlight azimuthal dependencies and spurious terms in each cross-correlation, is not ideal for extracting the Green’s function if the medium is relatively complex and arrivals other than the direct one are expected. In the presence of reflection and reverberation, spatial uniformity in the source distribution is necessary to sample all possible stationary-phase regions.

5.3 Laboratory experiments

The characteristics of diffusivity of the noise source are one of the key factor to extract the Green’s function using seismic interferometry in experiments and actual scale applications. One limit of numerical simulation is the difficulty (if possible at all) of implementing an actual diffuse source [Peter et al., 2011]. On the contrary, this can be achieved in the laboratory e.g. by means of air-jet forcing [Larose et al., 2007]. Compared to a traditional point source typical of laboratory experiments [Mikesell et al., 2012], air-jet forcing has the advantage of being intrinsically diffuse, and so of more rapidly generating a diffuse field in the target area.
5.3.1 Experimental set-up

We propagate flexural waves on the actual $1.5 \times 1.5 \times 0.002$ m aluminium plate described at the beginning of sec. 5.2 and in Fig. 5.2. The plate stands on a metallic frame that keeps it 70 cm above ground. The coupling between plate and frame is damped by means of small absorbing-elastic patches that limit resonance effects. Two broad-band Br"uel & Kjær accelerometers are attached to the central area of the plate through a thin layer of bees-wax (Fig. 5.2). They ensure flat response between 1 Hz and 80 KHz. Their relative azimuth is roughly parallel to the sides of the plate and they are 61 cm distant. The sampling frequency of both accelerometers is set at 100KHz. Using either a piezoelectric transducer (section 5.3.3) or an air-jet injected by an air-nozzle (section 5.3.2), $A_0$ Lamb waves [Lamb, 1904] are generated in the plate.

5.3.2 Excitation by air-jet sources

The performance of the air jet is explained by the nature of the excitation it produces. Acting at 10-20 cm of the surface it results in a wide (tens of cm) zone where a pressure field is generated by the turbulent airflow. Moreover it moves few cm around a given position. It corresponds therefore to a continuous incoherent extended source. According to the numerical results present previously, a surface distribution is a more favorable situation than a point source. Comparing Fig. 5.2b and Fig. 5.2c, it is not hard to see that the wave-field thus generated is profoundly different from that obtained using point sources. The nozzle is also displaced along an ellipse similar to that of Fig. 5.2. The total time of recording is about 250s divided into 5s long time windows: each 5s interval corresponds to a different mean position of the air nozzle, roughly along the ellipse of Fig. 5.2. The recorded signal is band-passed in the 0.5-5 KHz frequency range, and no further processing is applied (i.e. no whitening or “one-bit” filtering).

Following common practice in ambient noise seismology Poli et al. [2012], we compute cross-correlations over the largest available time window for which continuous recordings are available (i.e., 5s), regardless of the expected length of the sought Green’s function. The gather in Fig. 5.7, obtained cross-correlating each 5s record, is quite different from those seen so far in this study (Fig. 5.1, Fig. 5.5, Fig. 5.6), in that no ballistic signature is clearly visible, while maxima of constant arrival time are dominant. These maxima can be associated to the direct ($\pm 1$ms) and reflected arrivals of the Green’s function. We infer that a single realization of our experiment (a single cross-correlation in the gather) is sufficient to generate a wave field diffuse enough for the Green’s function to emerge.

The stack in Fig. 5.7 also shows that the causal anti-causal branches are very close to be symmetric. Symmetry with respect to time is an essential property of the Green’s function, and we use it here as an heuristic, but effective measure of effectiveness of Green’s function’s retrieval (measuring the actual Green’s function of the medium would require a complex, and possibly not entirely accurate, deconvolution of the source). It appears from Fig. 5.7 that not only the first-arrival section of the Green’s function has been reproduced, but also later arrivals ($\pm 3$ms) are visible. With an analysis analogous to that of Fig. 5.4 it is possible to attribute each peak to a boundary reflection. The results from this section highlight the robustness of cross-correlation measurements when used with a diffuse source and sufficiently long time window.
Figure 5.7: (Top) Cross-correlation gather as a function of time using the air-jet forcing for a signal filtered between 500Hz and 5KHz. (Bottom) Stack (blue) of the fifty, 5-s long records, giving a ~250 s long cumulated signal; (red) same stack, flipped with respect to 0-time. The symmetry of stacked cross-correlation can be seen as a measure of how well it approximates the Green’s function. The time window is sufficiently long to contain the first arrival and the first reverberations from the plate boundaries.
5.3.3 Point-source results

In our experiment, point sources consist of piezoelectric transducers, which are coupled with the plate by applying a small weight. Any signal can be sent from the audio interface of our computer to the transducer. We select a sinusoid modulated with a Gaussian defined upon its central frequency which is set at 10 KHz. After each pulse we record a ~60 ms accelerogram as shown in Fig. 5.2c, sufficient for a flexural wave to propagate ~40 times back and forth on the 1.5 m-wide plate for a 10 KHz pulse. The signal recorded after each pulse is then averaged over 100 realizations at the same location, which eliminates, along with filtering, most electric noise. We shift our transducer along two closed curves of approximately elliptical shape (Fig. 5.2). As in the previous example, we employ the symmetry of the causal and anti-causal branch to benchmark the quality of the reconstructed Green’s function.

In Fig. 5.8a the cross-correlation is shown for a 3ms time-window including only direct arrival and first border reflections, while in Fig. 5.8b 40ms of signals (i.e. including the coda) are cross-correlated. Results from the shorter time window (Fig. 5.8a) are clearly dominated by the ballistic direct arrival (and other not well identifiable patterns) as confirmed by the two clear maxima visible in the stack. Similar to other point-source results illustrated above, the arrival times of the causal and anti-causal direct wave correspond to the extremes drawn by the direct wave curve in the gather at a time of approximately ±0.7ms. The stack, in this short window case, is not symmetric. For the longer time window case depicted in Fig. 5.8b, the stack is of greater quality although spurious terms do not disappear completely leaving a residual asymmetry. Later arrivals are not clearly visible in either gather or stack.

We conclude that, in the case of point sources distributed along a ring, cross-correlations strongly depend on the azimuth of the source. A single shot from the transducer does not generate a wave-field diffuse enough despite the numerous reverberations from the borders. The recovery of the direct arrival is only possible by stacking the cross-correlations, and a sufficient number of realizations located on a curve enclosing the receivers is necessary. The recovery of secondary arrivals seems to be not possible even with the use of a long coda since spurious oscillations do not cancel out polluting the stacked signal.

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5.4 Conclusions

Using flexural waves on a thin plate we propose an analysis supported by laboratory and numerical experiments that aim at disentangling the relative roles of scattering, reverberation and source distribution in giving rise to a diffuse wave field. We consider a wave field to be “sufficiently diffuse” when the (stacked) cross-correlation of recorded signal approximates well the Green’s function of the medium, including phases other than the direct one.

We have found that the way the plate is excited is critical to the “diffuseness” of the generated wave-field. For individual point sources, the “ballistic” signature is dominant in the cross-correlation
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Figure 5.8: (a) Cross-correlations gather as a function of time (horizontal axis) and azimuth (vertical axis) for the point sources. Below the gather we plot in blue the stacked cross-correlations. In red we show the stack flipped about the vertical axis (red line). The azimuth is calculated in degrees with respect to the midpoint between the receivers (Fig. 5.2). Starting from the top, the values of the angle correspond to the outer ellipse, while the second loop (right axe) corresponds to the inner ellipse. The time window used in the cross-correlation is 3 ms. (b) Same as (a) but for a cross-correlation time window of 40 ms.
gather when short time windows are considered, and the wave-field is clearly not sufficiently diffuse for the Green's function to be adequately reproduced by a single (or a stack of just few) cross-correlations. Only after a large number of realizations, with associated point sources uniformly covering the target area, and using a long time window for the cross-correlation including many reverberations from the borders, the reconstruction is nearly complete. In general, increasing the length of the cross-correlation time window, hence including reverberations and coda, drastically improves the results both for direct and secondary arrivals.

For cross-correlation of ambient signal to approximate well the Green’s function, it is essential that a broad area is covered by sources. We have found experimentally that an air-jet exciting a finite area of an aluminum plate is much more effective than the combination of few point sources in giving rise to a sufficiently diffuse wave field. We have proved numerically that a spatially uniform distribution of noise sources is accordingly more effective than an azimuthally uniform distribution along a close line, even if the total number of sources is the same. In its most general form, the correlation theorem \[\text{(Eq. (5.1))}\] states that the Green’s function associated with the locations of two receivers is obtained by combining a volume and a surface integral, over the region populated by sources of seismic noise, and its boundary. We have found that, in our experimental setup, the volume integral plays a dominant part in the reconstruction of the complete Green function, while the surface integral can be neglected in practice. Further theoretical work, beyond the present study, will be needed to explain this result analytically.

In the limit of a very diffuse source, i.e. an air-jet randomly displaced on the plate, and by using a long cross-correlation window including thousands of reverberations, we proved that the Green’s function, including several reflected arrivals, emerges quite clearly from the stacked cross-correlation.
Core mantle boundary topography tomography and waveform sensitivity. The core-mantle boundary (CMB) is one of the most important global interfaces of the Earth, separating the solid silicate mantle from the fluid iron core. Its topography has not been characterized well yet, although it could provide precious insights about dynamics and thermal profile of the surrounding regions. Complex structures above and below are keys to understand past and future evolution of our planet through geodynamics and Earth magnetism analysis. In the first 2 chapters of this manuscript, we aim to characterize the sensitivity of seismic waves due to CMB topography in terms of forward and inverse seismic modeling. In the first part of chapters 2 and 3, using full 3-D wave propagation, we computed a large ground-truth database to examine the parameter space spanned by CMB topography, mantle model, geometry, epicentral distance, seismic phase, and frequency on seismograms. This is to be seen as a guide for optimal data configurations to illuminate such topography or for inversion algorithm benchmark. In particular, $PcP, ScS$ and $PKP$ phases are, as expected, useful to detect CMB topography, whereas $P_{diff}$ are less sensitive to such undulations.

In chapter 3 we formulate the inverse problem for boundary topography based on waveform inversion. The algorithm relies on boundary sensitivity kernels using 1st order perturbation theory, computed with an axisymmetric spectral-element code. The theory and the procedure have been accurately described in the second half of chapter 2. This methodology allows to model frequencies as high as required by the database analysis, even in the framework of large-scale tomographic datasets. Those kernels, representing the Fréchet derivatives of perturbations of data with respect to topography, account for finite-frequency effects and can be used in waveform inversion to invert for boundary perturbation.

In the second part of chapter 3, through cross-correlation measurements from the synthetic database, we test the inversion algorithm. Later we apply it to real global seismic datasets of both compressional and shear waves to map the CMB topography. By means of synthetics data, we demonstrate that with adequate data coverage and known 1-D or 3-D mantle models, the reconstruction of the CMB topography by waveform, finite-frequency tomography, converges to the input model both for reflected ($PcP, ScS$) and transmitted waves ($PKP$) although the signature of the topography is very small compared to that due to mantle heterogeneities. When we move to real data sets, the assumptions about coverage and data quality are more sketchy and the reliability of the solution controversial (chapter 4). Starting from a 1-D CMB model we separately invert ISC data and cross-correlated travel-time data obtaining diverging results. Although other studies reported a similar behaviour, it should in principle not happen. Most likely the way mantle corrections are
implemented bias our maps. In addition to that, the frequency at which ISC data are calculated is unknown, and the travel-time measures are calculate from onset time. The problem of the mantle correction can be solved either from using differential travel-times or, as shown in chapter 3, using a joint inversion with two parameters: mantle velocity and CMB topography. The data problem remains however unsolved in this study and it remains the main challenge for the future. Unfortunately the success of tomography through waveform sensitivity and finite frequency, is closely linked to the availability of cross-correlation measurements or other forms of waveform misfit. Yet, it is not easy to find in literature authors who compiled such data-bases for deep mantle and in particular for the CMB. This is a big limitation, if we consider that for other regions of the upper mantle or the crust, wave-from inversion has demonstrated high capabilities and it has delivered models at unprecedented resolution. We would like to repeat such a study using a database that only covers regions where the sampling is good enough. This would not imply big changes in the code, an increased complexity due of the higher frequency of the wave-form would be compensated by the reduced computational domain required from the regional studies. This could be done along with a joint inversion. Other disciplines such as geodynamics and Earth magnetism are waiting for an appropriate model of CMB topography to explain the evolution and the dynamics of the core and the deep mantle.

**Ambient seismic noise reconstruction on the plate: conclusion and outlook** In chapter 5 we move from the Earth scale to the laboratory scale showing another application of the spectral element method coupled with a laboratory acoustic experiment. In a setting similar to the solid Earth, we show how ambient noise seismic interferometry can successfully extract the Green’s function featuring, besides the direct arrival, reverberation. In the past years, seismic interferometry moved quickly from an embryonic stage to the actual application stage, and many authors obtained results which are consistent or outstanding compared to those obtained traditional active source seismology. Here we use spectral elements as complementary method to an actual experiment where we apply the ambient noise technique on recording the motion of flexural waves in a thin aluminium plate. More in detail, in the laboratory part we test the influence of the source type (diffuse or not diffuse) with respect to the quality of the Green’s function reconstruction. An intrinsic diffuse source such as an air-jet is very efficient in extracting the response with respect to the stacking of multiple ballistic signals generated by time-space point sources. We further develop our study modelling the plate with a spectral element software. There we prove that the use of the coda (i.e., a long time window when computing the cross correlation), made of reverberated waves, allows a very good reconstruction of the entire Green’s functions. We prove that a spatially uniform distribution of point sources improves the quality of the reconstruction (when reverberations are present) when compared to a distribution only azimuthally uniform but not spatially. The quality of the reconstruction is such that it might allow the use of not only the phase information (i.e., travel-time tomography) but also the amplitude, very important when attenuation has to be constrained. Future studies might for instance investigate the ratio of the reconstructed signal with respect to cross correlation time window as functions of the diffusivity of the field, or try to measure the intrinsic attenuation using the methodology developed by Weemstra et al. [2012]. As a short term goal, we wish to apply a similar methodology to study the reconstruction on an actual data set coming from the Japanese seismic arrays which has a very dense and uniform coverage. This will tell us more about how close the conditions of our experiment are with respect to the Earth’s diffuse field.
Outlook for future core mantle boundary studies  Upon the results collected in this work, we propose two approaches that should improve the robustness of the CMB study. Both the approaches starts from the common requirements that a global study using body waves is at the moment not possible due to the lack of coverage. Therefore we would like to use USArray recording to map the portion of the CMB illuminated by those data. Given the density of the net, we are confident to find a sufficiently large set of measurements. The first possible test requires the usage of differential travel-time measurements to solve the bias generated by the mantle. It is technically very easy to handle but it requires the availability of this type of cross-correlation measurements. Ideal data for this study can be $PcP - PKP$. This type of measurement would fit appropriately the aperture size of the USArray. If such a database has not been compiled yet, than the first task would be its creation. The second approach requires the implementation of a joint inversion. The best mix of data would be in this case $P, PP$ and/or $S, SS$ for the mantle while $PcP$ and $PKP$, or their $S$ component. The combined usage of reflected and transmitted wave may help to de-couple the surrounding mantle from structure and topography. Transmitted waves in particular have same type of sensitivity for fast anomaly and depressed mantle, while reflected phases have sensitivity of opposed sign, and hence those latter may underestimate the anomaly. The practical implementation can be realized through few steps:

- Cross correlated residuals for difference frequency bands have to be measured for the requested data. The target frequency band should be approximately between 40s and 5s to best constrain medium and small scale features. Standard ellipticity and crust corrections have to be applied to the residuals.

- First we perform a mantle inversion using only mantle data and we then compare the results with other study featuring waveform inversion. Notice that if $PKP$ phases are to be used for the joint inversion, a global mantle coverage must be accounted. Eventual resolution test on synthetic data might be included in the analysis.

- A regional study with reduced numerical cost can be executed at a first stage. The use of only $PcP$ or $ScS$ limit the computational domain to the region illuminated by those data.

- Increasing the numerical complexity we can include $PKP$ data and a global mantle tomography to account for mantle effect.

- Eventually inner core radial anisotropy can be taken into account in the joint inversion.

This work-flow ensures that at each step we progressively add data and complexity to the inversion while at the same time we keep under control the quality of the mantle correction. Said so, we should keep in mind that there may be the eventuality that the signal that we can extract from CMB anomaly is simply too small with respect to other mantle features. And an accurate mapping, above the degree 2-3 will not be possible.

Possible ways to improve the $P_{a\text{ff}}$ signal. The low sensitivity shown by $P_{a\text{ff}}$ wave is certainly surprising and raise questions about the reliability of previous and current studies with this data. Before discarding completely this kind of measurements we can try to change the way the travel-time difference is quantifies (cross-correlation in this study). By using the tool provided either by Fichtner et al. [2008] or Bozdag et al. [2011] we can track the perturbation in the time-frequency domain. Another possible approach is to measure $P_{a\text{ff}}$ at a much higher frequency, such that sensitivity
region becomes much smaller. This is clearly bounded by the frequency band in which $P_{\text{diff}}$ is observed (down to 5 s at most).

The role of ambient-noise measured data. While for surface waves the ambient noise measured data produced a significant amount of observation, the extraction of body waves is not as simple. Studies such as Poli et al. [2012] show that the signal of body waves (transmitted and reflected) is clearly present in the Green’s function extracted by cross-correlation. Now the main difficulty relies in the quantification of the average error during phase measurements, the starting point for any type of travel-time tomography. In the case of surface waves, the velocity variation in the crust are so high that the error on the phase velocity measurements is negligible. Such an error is typically due to insufficient equipartition of noise sources in the crust Hillers et al. [2012]. As this study shows, the variations at the CMB are small and the bias in phase measurements must be very small. Seismologists of the research group in Grenoble are currently evaluating this problem, by compiling the first global database of ambient noise $PcP$ and $PKP$ phases (Fig 6.1) which will eventually be included in future inversions.

Figure 6.1: Global seismic section showing the teleseismic body waves from the ambient noise correlations taken from Boue et al. [2013]. Numbers on the synthetic section (right) help to distinguish each seismic phase.


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Axial symmetry and Cartesian reference frame

Going from the 2-D semi-disc quantities given by AXISEM to general 3-D cylindrical coordinates requires some multiplicative factor to be applied:

\[ \mathbf{u}^{3D}_{cyl}(s, \phi, z) = \left( f_1(\phi) \mathbf{u}^{2D}_x, f_2(\phi) \mathbf{u}^{2D}_\phi, f_1(\phi) \mathbf{u}^{2D}_z \right), \]  
\[ \mathbf{E}^{3D}_{cyl}(s, \phi, z) = \mathcal{F} \otimes \mathbf{E}^{2D}, \]

where \( \mathcal{F} \) contains the azimuthal pre-factors \( f_1 \) and \( f_2 \):

\[ \mathcal{F} = \begin{pmatrix} f_1(\phi) & f_2(\phi) & f_1(\phi) \\ f_2(\phi) & f_1(\phi) & f_2(\phi) \\ f_1(\phi) & f_2(\phi) & f_1(\phi) \end{pmatrix}, \]  

and \( \otimes \) stands for element-wise product. The values of the azimuthal pre-factors \( f_i \) depend on \( \phi \), source type and moment tensor component. The following table summarizes the dependencies.

<table>
<thead>
<tr>
<th>Source type</th>
<th>M component</th>
<th>Prefactor</th>
<th>( f_1(\phi) )</th>
<th>( f_2(\phi) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monopole</td>
<td>( \frac{1}{2} M_{zz} )</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \frac{1}{2} (M_{xx} + M_{yy}) )</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Dipole</td>
<td>( \frac{1}{2} M_{zz}, p_x )</td>
<td>( \cos \phi )</td>
<td>( -\sin \phi )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \frac{1}{2} M_{yz}, p_y )</td>
<td>( \sin \phi )</td>
<td>( \cos \phi )</td>
<td></td>
</tr>
<tr>
<td>Quadrupole</td>
<td>( \frac{1}{2} (M_{zz} - M_{yy}) )</td>
<td>( \cos 2\phi )</td>
<td>( -\sin 2\phi )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( M_{xy} )</td>
<td>( \sin 2\phi )</td>
<td>( \cos 2\phi )</td>
<td></td>
</tr>
</tbody>
</table>

The angle \( \phi \) is known for each of the kernel grid-points \( \mathbf{x} \), projecting its components onto the x-y plane and calculating the angle with the \( \text{atan2} \) function. The Cartesian reference frame is assumed to have the z-axis oriented towards the source (Fig. 3.11). The values of \( \phi \) have to be recalculated for every source-receiver configuration. The easier case happens when all sources are monopole and therefore azimuth-invariant such that this operation can be avoided. If we denote with \( B \) the matrix that maps
the Cartesian reference frame into the cylindrical reference frame, then the following transformations hold:

\[ \mathbf{u}_{\text{cart}} = \mathbf{B}^T \mathbf{u}_{\text{cyl}}^{3D} \quad \text{tensors:} \quad \mathbf{E}_{\text{cart}} = \mathbf{B}^T \mathbf{E}_{\text{cyl}}^{3D} \mathbf{B}, \]

where the \( b_{ij} \) entries of the change of basis matrix \( \mathbf{B} \) are:

\[ \mathbf{B} = \begin{pmatrix} \cos \phi_r & -\sin \phi_r & 0 \\ \sin \phi_r & \cos \phi_r & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (A.5) \]

For example, the cylindrical coordinates of the kernel mesh are converted to Cartesian with:

\[ \mathbf{x}_{\text{cart}} = \mathbf{B}^T \mathbf{x}_{\text{cyl}}^{3D}. \]

The coefficients for the rotation matrix \( \mathbf{R} \) in eq. (3.20) are:

\[ \mathbf{R} = \begin{pmatrix} \cos \theta_{r,s} \cos \phi_{r,s} & -\sin \phi_{r,s} & \sin \theta_{r,s} \cos \phi_{r,s} \\ \cos \theta_{r,s} \sin \phi_{r,s} & \cos \phi_{r,s} & \sin \theta_{r,s} \sin \phi_{r,s} \\ -\sin \theta_{r,s} & 0 & 0 \end{pmatrix}. \quad (A.6) \]

Here \( \mathbf{R} \) is uniquely defined for all the mesh grid-points \( \mathbf{x} \) depending on the source and receiver coordinate \( (\theta_s, \phi_s) \) or \( (\theta_r, \phi_r) \). Note that \( (\theta_r, \phi_r) \) are not the initial receiver coordinates, but rather those defined within the coordinate frame attached to the kernel mesh.

Finally, the geometrical relationships between Cartesian 3-D grid \( (x, y, z) \) and 2-D semi-disc in cylindrical coordinates \( (\phi, z) \) are:

\[ s = \sqrt{x^2 + y^2}; \quad (A.7a) \]

\[ \phi = \tan^{-1}(y/x); \quad (A.7b) \]

\[ z = z. \quad (A.7c) \]

We compute the gradient of the displacement on-the-fly inside AXISEM via

\[ \nabla \mathbf{u} = \begin{bmatrix} \frac{\partial u_s}{\partial s} & \frac{1}{s} \frac{\partial u_s}{\partial \phi} & \frac{\partial u_s}{\partial z} \\ \frac{\partial u_s}{\partial r} & \frac{1}{s} \frac{\partial u_s}{\partial \phi} + \frac{u_s}{s} & \frac{\partial u_s}{\partial z} \\ \frac{\partial u_s}{\partial \phi} & \frac{1}{s} \frac{\partial u_s}{\partial \phi} & \frac{\partial u_s}{\partial z} \end{bmatrix}, \quad (A.8) \]

keeping always in mind that multiplicative pre-factors have to be applied once the geometry of the kernel mesh is known.
APPENDIX A. AXIAL SYMMETRY AND CARTESIAN REFERENCE FRAME

Figure A.1: A visual interpretation of the projection defined in (A.7). The point on the semi-disc is chosen to be the closest to the actual projection.

Figure A.2: The kernel mesh with $\phi$ values superimposed. Left: values of $\phi$ for the forward field located at north pole. Right: the backward field rotated 170° towards south. The $z$-axis in both plots points outward from the page.
Algorithmic optimization and accuracy

To compute $K_d$ in (3.15) for a given database including $N_r$ receivers and $N_s$ sources we proceed as follows:

- Forward fields for every source depth $s$ are computed via AXISEM, saving the necessary wavefields 10 times per dominant period of the source time function $\hat{m}(t)$ i.e., re-sampling using a larger time-step, then imposed by the numerical CFL condition. This value, ensures sufficient time sampling to avoid both aliasing and reduce the computational cost and storage size [Fichtner et al., 2009].
- By virtue of axial symmetry and the seismic representation theorem, only two simulations for all the observations are sufficient to compute the backward field.
- The kernel code computes Eq. (3.11) according to section 3.3.2 for every given receiver $r$ associated to each source $s$.
- Results are stored and the procedure is repeated for all the sources in the database. Eventually, once one has the inversion grid available, inversion matrix entries may be given as output.

The parallelization of the forward solver AXISEM is discussed in Nissen-Meyer et al. [2007b, 2008], therefore we do not discuss it here, but depict the domain decomposition in Fig. B.1.

B.1 Parallelization and in-core optimization

In our formulation, computing kernels is a task involving wave-field rotations and time domain convolution, hence the parallelization is straightforward. We set up the domain decomposition along the $\phi$ direction assigning to each processor a vertical slice spanning a given interval. The decomposition ensures perfect load balancing for best scalability on large parallel machines. In order to calculate only the kernel there is no need for intra-node communication, so that convolution, once the domain is split, is handled independently by each processor. Every processor simply needs to know the $\delta\phi$ spanned by the assigned slice and the permutation array to remap for actual source or receiver locations. A significant gain in performances, was obtained by embedding a GPU-accelerated region of the code that handle this task with extremely high efficiency. This has proven to be particularly useful to calculate $G_i$ in Eq. (4.3). This feature remains for now strictly experimental. "In-core" optimizations were obtained designing the convolution as 1-D array operations compliant to the
Figure B.1: Domain decomposition for the kernel mesh (a) and for AXISEM spectral element mesh (b) for 8 processors as an example. Each slice is handled by a different processor. The number of processor is defined by the users according to memory/wall-clock time desired.

Fortran-like memory layout. Wherever possible we avoid nested for-cycles or control statements. The code is designed to exploit the most recent compiler optimization especially those of PGI with GPU accelerators (www.pgroup.com).

B.2 I/O optimization

For every source depth $s$, AXISEM saves vector fields that are used to compute kernels. For I/O performance, we mean all the operations transferring data back and forth from the central memory (RAM) to the hard disk. A few best practices have been followed when designing this I/O intensive code for parallel machines.

- Use single precision whenever double is not necessary (almost always true in numerical wave propagation). This countermeasure simply halves storage requirements.

- I/O infrastructures are designed to handle large files. I/O of small files is never optimized, thus it is better to reduce the number of total disk access (disk latency time is several orders higher than RAM access). Maximize bandwidth usage for disk I/O building memory buffers inside RAM memory. To compute one boundary kernel with AXISEM, only a one-dimensional, time dependent collection of points is required (aligned along the interface) and it is therefore possible to fit all the necessary field values inside a node memory. In such a way, input fields are read from disk once-and-for-all at the start-up.

- Use a portable format which can be written/read from heterogeneous system. For example, data from the forward simulation can be computed on specifically designed machines and then the output fields need to be read from another machine which may have a different hardware structure to specifically enhance performance of the algorithm calculating kernels. We use the NetCDF data library (www.ucar.org), a self describing, meta-data format widely supported and optimized for data intensive application.
Figure B.2: The inversion work-flow set-up on our institute cluster Brutus. The synthetic database is compressed to occupy few hundreds of GByte. Data are processed on the cluster nodes and the residual for the desired stored. The wave-field values computed only once are stored on the disk and they are re-used for every kernel because the event characteristic does not change (see Colombi et al. [2012] for the details). The kernel computation, is parallelized by the cluster scheduling system without needs of MPI.

- We embed data visualization in the output data format using the CF convention (http://cf-pcmdi.llnl.gov/), natively supported by software like Paraview or GMT.

B.3 Technical implementation of the inversion workflow

The computation of forward and backward quantities with the software of Nissen-Meyer et al. [2007b] is not sufficient to make this tomographic inversion affordable, a wise optimization on some aspects has been necessary. Waveform treatment to extract travel-time, forward and backward field computation, kernel computation and matrix inversion have been carried out on the institute cluster "Brutus" at ETH Zurich. The most interesting aspect was to optimize the kernel computation for thousands of events, not with MPI, but leaving to the batch system of the cluster the parallelization. Each kernel computation was seen as a single job over the whole database nothing else than exploiting another dimension of parallelism of the seismic inverse problem. This trick increases the throughput (2-3 times) on that machine. It can be done as long as the memory required by dynamic allocation does not exceed the RAM available on each CPU. Specification about the kernels algorithm can be found in Colombi et al. [2012]. Fig. B.2 shows the conceptual scheme we put in place to carry on inversions. For the kernel computation, roughly 0.5 mln of computing hours have been used. The cost for computing the synthetic seismogram database with the software SPECFEM3D GLOBE reached 1 mln of computing hours.

B.4 Spatial and temporal derivatives accuracy test

The accurate solution computation of spatial derivative is the key advantage of SEM. A reliable calculation of the tensor or the velocity field either inside fluid domain or solid is extremely important
Figure B.3: The left plot shows the period function discretized on a two element per period grid. The picture on the right shows the relative error between numerically computed derivative of \( f \) and its analytical expression:

\[
\frac{\partial f(s,z)}{\partial s} = 50\pi \cos\left(50\pi s\right) \cos\left(50\pi \frac{z}{R}\right)
\]

to get reliable sensitivity kernel. A quick test to verify spatial accuracy consist in discretizing a double valued sine \( f = \sin(\omega \pi s) \cos(\omega \pi s) \) function and calculating its derivatives on the semi-disc and comparing the results with analytical expression:

\[
\frac{df}{ds} = \omega \pi \cos(\omega \pi s) \cos(\omega \pi s).
\]

The function and the relative error are shown in figure B.3: The interface condition: (3.2b) are tested comparing the traces of \( u \) and \( T \) from the two side of the interface \( \Sigma \). There is no need to test condition (3.2b) as they are naturally embedded in the assembly procedure of the stiffness matrix of the SEM solver.
Using the simpler acoustic model we revise the derivation of wave sensitivity to mechanical property perturbations. The derivation is based on 1st order perturbation theory, or Born modelling and it is taken from Tarantola [2005].

C.1 Integral theorems

Integration by parts for single valued functions:

\[ \int_{a}^{b} u \frac{dv}{dx} = uv|_{a}^{b} - \int_{a}^{b} v \frac{du}{dx}. \]  

(C.1)

We shall denote the domain \( \Omega \in \mathbb{R}^{3} \) and its boundary with \( \Gamma \). The interface between two regions with different physical properties is denoted with \( \Sigma \). The generalized Gauss and Stokes theorems for \( \Phi \), either a scalar or tensor function, and \( \ast \) the algebraic operation according to the set of definition of \( \Phi \):

\[ \int_{\Omega} \nabla \ast \Phi \, d\Omega = \int_{\Gamma} \mathbf{n} \ast \Phi \, d\Gamma. \]  

(C.2)

Integration by parts with \( u \) scalar and vector function \( \mathbf{v} \):

\[ \int_{\Omega} \nabla u \cdot \mathbf{v} \, d\Omega = \int_{\Gamma} (uv) \cdot \mathbf{n} \, d\Gamma - \int_{\Omega} u \nabla \cdot \mathbf{v} \, d\Omega. \]  

(C.3)

C.2 General procedure in inverse problem theory

When solving the direct problem we deal with two sets of elements: data \( \mathcal{D} \) and model parameters \( \mathcal{M} \). The eventual aim is the definition of a unique mapping \( \mathbf{G} : \mathcal{M} \rightarrow \mathcal{D} \) that associates to our model parameters \( \mathcal{M} \) (physical property) the observed physical quantities \( \mathcal{D} \). Such unique relationship exists in most of the cases for direct problems.
and continuous dependency from data. In this case, the problem is said to be "well posed" and it can be written as follow:

\[\kappa^{-1}(x)\ddot{p} - \nabla \cdot (\rho^{-1}(x) \nabla p(x, t; x_s)) = F(x, t; x_s) \quad \text{on } \Omega; \]  
\[p(x, t; x_s) = 0 \quad \text{on } \partial \Omega; \]  
\[p(x, 0; x_s) = 0; \]  
\[\dot{p}(x, 0; x_s) = 0. \]  
(C.4a)

The opposite cycle, \(G^t : D \rightarrow M\), going from data to model parameters does not enjoy the same properties and to obtain the best solution we are to explore the parameters space by setting an optimization problem. For instance we can tackle it by minimizing the following cost function:

\[\min \frac{1}{2} \| g(m) - d_{obs} \|^2. \]  
(C.5)

The typical approach exploits information from the directional derivatives to reach the minimum point. Non-linearities nested in the formulation prevent us from a safe convergence to a global minimum when we start too far away from it. A point-wise evaluation of the derivatives would require an infeasible amount of computation power that is likely to be never available. The trick resides in defining derivatives from a functional framework which directly embeds the direct propagation problem.

**Iterative solvers**  In numerical analysis one often faces the resolution of a linear system of equations \(Ax = b\). A gradient method exploits local properties of the cost function to set in which direction model parameters must be modified to reach the minimum. If we are using a steepest descend method, we are following the steepest path leading to such minimum point. We must always keep in mind that since the problem is non linear, this minimum point might just be a local minimum or a saddle point (if just first order derivatives are computed).

The iterative scheme updates the model parameter at every step \(n\), with the structure: \(m_{n+1} = m_n + \Phi \delta m\) where \(\Phi\) is the parameter leading the descend direction. The steps of an iterative algorithm may look as follow:

\[\delta d_n = g(m_n) - d_{obs}; \]  
(C.6a)

\[\delta m_n = G^t_{d_n} \delta d_n; \]  
(C.6b)

\[m_{n+1} = m_n + \Phi \delta m_n; \]  
(C.6c)

We first solve the direct problem with parameters \(m_n\) to obtain the artificial data. Then we calculate residuals against the measured data. In the second step, with the help of the transpose operator, we convert residuals into model variations. The third and last step updates the model parameters so that another cycle can start. The stopping criteria is normally taken when residuals are small enough or a given number of iterations has been reached.
C.3 Metrics and operator

Derivative over functional spaces  Let $m$ be the model parameters ($\rho$, $\mu$, $\lambda$, ...) and $d$ our data (seismogram). The derivative of the operator $g$ linking $d$ to $m$ is defined as:

$$g(m_0 + \delta m) = g(m_0) + G_0 \delta m + O(\delta m^2),$$

simply, the Taylor expansion. When the space $M$ and $D$ are functional space the term $G_0$ is named Frechet derivative. For 1-D case it would just be the slope of the tangent at $m_0$. If $M$ and $D$ are discrete spaces, $G_0$ is a matrix defined as:

$$(G_0)_{i,j} = \frac{\partial g_i}{\partial m_j}|_{m_0};$$

where the discrete sets are defined as:

$$d_i = g_i(m_1, m_2, ..., m_j) \quad (j \in I_M, i \in I_D).$$

The first order term $G_0 \delta d$ appears naturally when governing equations are perturbed. This approach resembles the so called perturbation theory (Born’s) which has several common points with the method here described. When we approach full waveform inversion, we cannot (and we do not want) calculate explicitly the matrix $G_0$. We prefer to stay with the functional settings strictly tight to the direct problem.

Scalar product  Being $M$ and $D$ functional spaces we must define the usual operation in a more ample sense.

Let $x$ denote a point of an Euclidean $n$-dimensional space with cartesian coordinates $x = (x_1, x_2, ...)$. The function $f(x)$ is a vector valued function (it takes value in $\mathbb{R}^n$). The scalar product between two functions is defined as:

$$(f, g) = \sum_{i=1}^{n} \int_{\Omega} f_i g_i \, d\Omega \quad \text{or} \quad (f, g) = \sum_{i=1}^{n} \int_{\Omega} f_i g_i \, d\Omega.$$ (C.10a)

The action of $s_i$, positive weighting function, can be ignored. The application of the scalar product $(\cdot, \cdot) \in \mathcal{R}$, produces a real number. To the scalar product is hinged the definition of the derivative with respect to the model parameters in a functional settings (see (C.7)).

Adjoint operator  The following definition of the adjoint of an operator $G$ will allow us to calculate analytically the transpose of the derivative operator $G^t$ required by our iterative solver. The adjoint of $G$, termed $G^* : \mathcal{D} \to \mathcal{M}$, is the linear operator mapping data into model parameter space:

$$(G^* d, m)_D = (d, Gm)_M.$$

In the next paragraph we draw the connection between adjoint and transpose operator. An applicative usage of the scalar product and adjoint can be found in the example. For now we can clarify see that: if we know how $G$ looks like, by means of (C.10a) we also know from where $G^*$ will come.
Kernel

With the word *kernel* we refer to the inner part of a linear operator:

\[ d_i = \sum_{j=1}^{n} G_{ij} m_j \quad (j \in I_M, i \in I_D); \]  
\[ d_i = \int_{\Omega} G_i(x) m(x) d\Omega \quad (i \in I_D, x \in V). \]  
(C.12a)  
(C.12b)

The matrix $G_{ij}$, the vector of functions $G_i(x)$ are called *kernel* of the linear operator $G$.

Adjoint and transpose

On generic functional space the adjoint term is called transpose but a (complete) derivation starting from a the transpose operator would require too much time and it goes beyond the scope of this brief introduction. Furthermore, the transpose operator applies on dual spaces, concept which are too abstract for a mechanical and applicative engineering’s mind. For this time it suffices to assume that on the field $D$ the scalar product (C.10a) is defined and that $G^t = G^*$ holds. The simplest case is when the spaces are discrete:

\[ d_1 = Gm_1 \quad \text{or} \quad (d_1)_i = \sum_{j=1}^{n} G_{ij}(m_1)_j; \]  
(C.13)

where matrix $G_{ij}$ is the kernel of $G$. Then, its transpose is just the usual transpose of a matrix:

\[ m_1 = G^t d_1 \quad \text{or} \quad (m_1)_j = \sum_{i=1}^{n} (G^t)_{ji}(d_1)_i; \]  
(C.14)

therefore:

\[ (G^t)_{ij} = G_{ji}. \]  
(C.15)

Nothing else than the transpose of the matrix (the kernel). The index 1 stems from model parameter set $m_1$. If the spaces considered are more general, functional space for example the definition of $d = Gm$ needs a generalization:

\[ d_{ij}(u,v,...) = \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} \cdots \int dx \int dy \cdots G_{ij \cdots \alpha \beta \cdots}(u,v,...,x,y,...) m_{\alpha \beta \cdots}(x,y); \]

and the linear equation $m = G^t d$ becomes:

\[ m_{\alpha \beta}(x,y,...) = \sum_{i=1}^{n} \sum_{j=1}^{n} \cdots \int du \int dv \cdots (G^t)_{\alpha \beta \cdots ij \cdots}(x,y,...,u,v,...) d_{ij \cdots}(u,v); \]

The relationship between $G^t$ and $G$ is generalized as:

\[ (G^t)_{\alpha \beta \cdots ij \cdots}(x,y,...,u,v,...) = G_{ij \cdots \alpha \beta \cdots}(x,y,...,u,v,...); \]  
(C.16)

Quoting Tarantola’s book we have the following rule for the variable transposition:

**Definition 1.** (Variable transposition) If the kernel of a linear operator is $G_{ij \cdots \alpha \beta \cdots}(u,v,...,x,y,...)$, and the application of $G$ implies sums or integrals over the variables $\alpha \beta \cdots, x, y \cdots$, then, the kernel of the transpose operator is essentially the same and the application of $G^t$ implies sums, integrals over the other variables $i, j \cdots, u, v \cdots$. 


C.4 Applications

Example 1 (Acoustic waveform inversion). The waves propagating in an acoustic media characterized by bulk modulus $\kappa(x)$ and density $\rho(x)$ are described by the scalar wave equation:

$$\kappa^{-1}(x) \ddot{p} - \nabla \cdot \left( \rho^{-1}(x) \nabla p(x, t; x_s) \right) = F(x, t; x_s) \quad \text{on } \Omega; \quad (C.17a)$$
$$p(x, t; x_s) = 0 \quad \text{on } \partial \Omega; \quad (C.17b)$$
$$p(x, 0; x_s) = 0; \quad (C.17c)$$
$$\dot{p}(x, 0; x_s) = 0; \quad (C.17d)$$

At time $t > 0$ we trigger one of the $n_s$ source located at $x_s$ and we record the pressure field at $n_r$ point located at $x_r$. The source is always exactly known. We repeat the acquisition process once that all the source has been triggered. Recordings from this experiment establish the $d_{obs}$ term.

Our aim is to extract the operator $G^t$ needed in algorithm (C.6a) to reconstruct $\kappa(x)$ of the media which matches the observed pressure field.

Owing to probability issue we better reformulate (C.17a) in terms of logarithmic bulk modulus.

$$m = -\log \frac{\kappa}{\kappa_0} \quad \rightarrow \quad \frac{1}{\kappa} = e^{m}. \quad \text{(C.18)}$$

The reasons are mainly two: the metric over $\mathcal{M}$ gets simpler, and negative values of $\kappa$ are no longer allowed because of the exponential function used to get $\kappa$ back.

The computation of the direct problem is as usual $d = Gm$ and we look for the transpose operator $m = G^t d$. In particular we want such an operator that links model perturbation to data residuals:

$$\delta d = G \delta m \quad \text{and} \quad \delta m = G^t \delta d. \quad \text{(C.19)}$$

Let the scalar product on the spaces $\mathcal{M}$ and $\mathcal{D}$ be defined according to (C.10a) for $p$ we have:

$$\langle \delta p_1, \delta p_2 \rangle = \sum_{s=1}^{n_s} \int_0^T \int_0^{n_r} \delta p_1(x_r, t, x_s) \delta p_2(x_r, t, x_s) \, dt, \quad \text{(C.20)}$$

the operators are applied according to the order of appearance of the variables. For $m$ we have:

$$\langle \delta m_1, \delta m_2 \rangle = \int_\Omega \delta m_1(x) \delta m_2(x) \, d\Omega. \quad \text{(C.21)}$$

The relationship connecting forward to inverse problem is the following definition of adjoint operator (we assume again that $G^t = G^*$):

$$\langle G^t \delta p, \delta m \rangle_\mathcal{D} = \langle \delta p, G \delta m \rangle_\mathcal{M} \quad \text{for any } \delta p \text{ and } \delta m . \quad \text{(C.22)}$$
Now that all the tools have been introduced we can begin with the actual computations. The governing equation with model parameter \( m_n \), pressure field \( p_n \) and source term \( F \) reads:

\[
\frac{e^{m_n}}{\kappa_0} \ddot{p}_n - \nabla \cdot (\rho^{-1} \nabla p_n(x, t; x_s)) = F(x, t; x_s) \quad \text{on } \Omega; \tag{C.23a}
\]

\[
p_n(x, t; x_s) = 0 \quad \text{on } \partial\Omega; \tag{C.23b}
\]

\[
p_n(x, 0; x_s) = 0; \tag{C.23c}
\]

\[
\dot{p}_n(x, 0; x_s) = 0. \tag{C.23d}
\]

Boundary and initial condition ensure solution’s uniqueness and simplify boundary terms when integrated. The Green’s function \( \phi_n(x, t; x_s, \tau) \) is as usual the solution of the following propagation problem:

\[
\frac{e^{m_n}}{\kappa_0} \ddot{\phi}_n - \nabla \cdot (\rho^{-1} \nabla \phi_n(x, t; x_s, \tau)) = \delta(x - x_s) \delta(t - \tau) \quad \text{on } \Omega; \tag{C.24a}
\]

\[
\phi_n(x, t; x_s, \tau) = 0 \quad \text{on } \partial\Omega; \tag{C.24b}
\]

\[
\phi_n(x, 0; x_s, \tau) = 0 \quad \text{for } t < \tau; \tag{C.24c}
\]

\[
\dot{\phi}_n(x, 0; x_s, \tau) = 0 \quad \text{for } t < \tau. \tag{C.24d}
\]

We now perturbs equation (C.23a) with \( m_n + \delta m \). To the perturbation of \( m \) follows the perturbation on \( p_n + \delta p \):

\[
\frac{e^{m_n}}{\kappa_0} \ddot{\delta p}_n - \nabla \cdot (\rho^{-1} \nabla (\delta p_n(x, t; x_s) + \ddot{p}_n(x, t; x_s))) = F(x, t; x_s) \quad \text{on } \Omega; \tag{C.25a}
\]

\[
p_n(x, t; x_s) + \delta p_n(x, t; x_s) = 0 \quad \text{on } \partial\Omega; \tag{C.25b}
\]

\[
p_n(x, 0; x_s) + \delta p_n(x, 0; x_s) = 0; \tag{C.25c}
\]

\[
\dot{p}_n(x, 0; x_s) + \delta \dot{p}_n(x, 0; x_s) = 0. \tag{C.25d}
\]

The term \( e^{\delta m} \) is expanded in a Taylor series truncated at first order giving \( e^{\delta m} \equiv \delta m \). Applying all the products and discarding second order terms \( \delta m \delta p \) we can plug (C.23a) such that the forces \( F \) cancels out. After simplifying we get:

\[
\frac{e^{m_n}}{\kappa_0} \frac{\partial^2 p_n(x, t; x_s)}{\partial t^2} - \nabla \cdot (\rho^{-1} \nabla \delta p_n(x, t; x_s)) =
\]

\[
= -\frac{\partial^2 p_n(x, t; x_s)}{\partial t^2} \frac{e^{m_n}}{\kappa_0} \delta m \quad \text{on } \Omega; \tag{C.26a}
\]

\[
\delta p_n(x, t; x_s) = 0 \quad \text{on } \partial\Omega; \tag{C.26b}
\]

\[
\delta p_n(x, 0; x_s) = 0; \tag{C.26c}
\]

\[
\delta \dot{p}_n(x, 0; x_s) = 0 \tag{C.26d}
\]

Making use of the representation theorem, and the Green’s function \( \phi_m \) characterizing the media, we know the solution at every point \( x \in \Omega \). The representation theorem for equation (C.23a) is:

\[
p_n(x, t; x_s) = \int_{\Omega} \phi_n(x, t; x_s, 0) * F(x, t; x_s) \, d\Omega. \tag{C.27}
\]
The star operator indicates convolution of the two signals. If we apply it to our problem we obtain:

\[ p_n(x,t;x_s) = \int_{\Omega} \phi_n(x_s,t;x_0) \ast \frac{\partial^2 p_n(x,t;x_s)}{\partial t^2} \frac{e^{m_n}}{\kappa_0} \delta m \, d\Omega. \] (C.28)

We have just obtained the sought operator that solves the direct problem \( \delta p = G \delta m \). Invoking the adjoint definition ((C.22)) and the scalar product ((C.20)) we write:

\[ \sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r,t;x_s)(G_n \delta m)(x_r,t;x_s) \, dt = - \int_{\Omega} (G_n' \delta p)(x) \delta m(x) \, d\Omega. \] (C.29)

Expanding all terms:

\[ \sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r,t;x_s) \int_{\Omega} \phi_n(x_s,t;x_0) \ast \tilde{p}_n(x,t;x_s) \frac{e^{m_n}}{\kappa_0} \delta m \, d\Omega \, dt = \int_{\Omega} (G_n' \delta p)(x) \delta m(x) \, d\Omega. \] (C.30a)

finally, rearranging:

\[ \int_{\Omega} \delta m \left( \frac{e^{m_n}}{\kappa_0} \sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r,t;x_s) \phi_n(x_s,t;x_0) \ast \tilde{p}_n(x,t;x_s) \, dt \right) d\Omega = 0; \] (C.31a)

which must hold for every \( \delta m \). Finally we arrive to the sought result:

\[ (G_n' \delta p)(x) = \frac{e^{m_n}}{\kappa_0} \sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r,t;x_s) \phi_n(x_s,t;x_0) \ast \tilde{p}_n(x,t;x_s) \, dt \] (C.32)

At this point, we can consider the derivation of the \( G' \) theoretically done. However to further simplify the overall methodology we proceed introducing the so called adjoint source.

**Example 1** (Adjoint source). We introduce the field \( \psi(x_r,t;x_s) \) defined by the differential system for \( x \in \Omega \) and \( t \in [0,T] \):

\[ \frac{e^{m_n}}{\kappa_0} \psi_n - \nabla \cdot (\rho^{-1} \nabla \psi_n(x,t;x_s)) = S(x,t;x_s) \quad \text{on} \ \Omega; \] (C.33a)

\[ \psi_n(x,t;x_s) = 0 \quad \text{on} \ \partial \Omega; \] (C.33b)

\[ \dot{\psi}_n(x,T;x_s) = 0; \] (C.33c)

\[ \dot{\psi}_n(x,T;x_s) = 0; \] (C.33d)

notice that we ask the solution to satisfy final condition instead of initial. The (adjoint) source term is defined as the sum of the distributed source at receiver’s locations:

\[ S = \sum_{r=1}^{n_r} \delta(x - x_r) \delta p(x,t;x_s). \] (C.34)
The magnitude depends on the residuals at each station. Using time reciprocity of the green function, \( \phi(x, t; x_r, t') = \phi(x, t + \tau; x_r, t' + \tau) \). The convolution in the representation theorem means integration reversed in time:

\[
\psi(x, t; x_s) = \int_0^T \int_0^T \phi_n(x, 0; x_s, t - t') \sum_{r=1}^{n_r} \delta(x - x_r) \delta p(x, t'; x_s) \, dt' \, d\Omega \quad \text{(C.35)}
\]

Integration over point sources amounts to a sum over the sources:

\[
\psi(x, t; x_s) = \sum_{r=1}^{n_r} \int_0^T \phi_n(x, 0; x_r, t - t') \delta p(x, t'; x_s) \, dt' \quad \text{(C.36)}
\]

Using reciprocity and keeping in mind that only the green function is dependent on \( t \) we take the time derivative of \( \psi \):

\[
\psi_n(x, t; x_s) = \sum_{r=1}^{n_r} \int_0^T \phi_n(x, t' - t; x, 0) \delta p(x, t'; x_s) \, dt' = - \sum_{r=1}^{n_r} \int_0^T \phi_n(x, t - t'; x, 0) \delta p(x, t'; x_s) \, dt' \quad \text{(C.37a)}
\]

Exploiting initial and final conditions in (C.24a) and (C.33a), it is trivial to demonstrate that:

\[
\phi_n(x_r, t; x, 0) \ast \tilde{p}_n(x, t; x_s) = - \dot{\phi}_n(x_r, t; x, 0) \ast \tilde{p}_n(x, t; x_s) \quad \text{(C.38)}
\]

We can plug into the expression of \((G^p_n \delta p)\) the last 2 relationships retrieved:

\[
\sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r, t; x_s) \phi_n(x_r, t; x, 0) \ast \tilde{p}_n(x, t; x_s) \, dt = \quad \text{(C.39a)}
\]

\[
= - \sum_{s=1}^{n_s} \int_0^T \sum_{r=1}^{n_r} \delta p(x_r, t; x_s) \dot{\phi}_n(x_r, t; x, 0) \ast \tilde{p}_n(x, t; x_s) \, dt = \quad \text{(C.39b)}
\]

\[
= - \sum_{s=1}^{n_s} \int_0^T \int_0^T \sum_{r=1}^{n_r} \delta p(x_r, t, x_s) \dot{\phi}_n(x_r, t - t'; x, 0) \, dt \, \tilde{p}_n(x, t'; x_s) \, dt' = \quad \text{(C.39c)}
\]

\[
\sum_{s=1}^{n_s} \int_0^T \int_0^T \psi(x, t; x_s) \, dt = \quad \text{(C.39d)}
\]

We have now obtained the final form of the transpose operator:

\[
(G^p_n \delta p)(x) = \frac{c_{\text{mo}}}{k_0} \sum_{s=1}^{n_s} \int_0^T \psi_n(x, t; x_s) \, \tilde{p}_n(x, t; x_s) \, dt. \quad \text{(C.40)}
\]

The term inside the integral is the bulk modulus kernel. The magnitude of the adjoint wave-field depends on the residual magnitude. Where no wave passes the contribution will be zero, where the wave-field has high value and the adjoint wave-field will also be high. If the computational domain has been discretized, \((G^p_n \delta p)(\mathbf{x})\) inherits the same spatial discretization.
I left this section as the very last, writing it only few hours before handing in the final version. Time was needed to properly prepare this tiny but important paragraph. The protocol suggests to thanks first collaborators so lets start from them. Thanks Lapo, you above the others, inspired and supported my research, and turned my mediocre articles into masterpieces. I hope you got something back from me as well by improving your proficiency with mechanical tools and learn how to fasten screws properly! Tarje, stop with writing proposals, revising articles, editing articles, preparing presentations and teaching classes. Take 2 minutes to breath and read this. Thanks for the help and the encouragement throughout these years, you as much as Lapo has contributed to teaching me how to become a scientist. I am sorry for the many times you had to bear my complaints and scepticism towards "deep Earth stuff"! Thanks to Domenico for offering me the possibility of measuring myself with this challenge and for the advise and support throughout the project.

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