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Boundary-aware Poisson-based P–S separation of elastic wave-fields in isotropic media

TESI DI LAUREA MAGISTRALE IN
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Abstract

Elastic seismic imaging relies on the simulation and analysis of wave-fields in which compressional (P) and shear (S) contributions are superposed. Thus P–S separation helps analyze wave propagation and reduce modal cross-talk in imaging and inversion workflows. Among existing strategies, Poisson-based formulations are attractive because they recover the compressional component through a scalar Poisson equation. However, in bounded domains, this equation does not define a unique separation unless suitable boundary conditions are prescribed. This thesis investigates these boundary conditions by interpreting Poisson-based P–S separation within the Helmholtz–Weyl decomposition framework. The Poisson–Neumann and Poisson–Dirichlet formulations are analyzed as distinct realizations of the irrotational/solenoidal decomposition in a bounded domain. Fast transform-based Poisson solvers, consistent with the boundary closures and the staggered grid of the elastic solver, are developed and tested on wave-fields of increasing complexity. The numerical experiments show that boundary artifacts are reduced by extending the separation domain to include absorbing layers. In effectively unbounded configurations, this makes the Poisson–Neumann and Poisson–Dirichlet formulations practically equivalent in the interior physical region. The situation changes in the presence of a free surface. In fluid free surface configurations, the Poisson–Neumann formulation better reflects the absence of shear waves in the fluid, whereas the Poisson–Dirichlet formulation may generate spurious P-to-S leakage near the surface. This motivates a mixed formulation, imposing non-homogeneous Neumann conditions at the free surface and homogeneous Dirichlet conditions on artificial boundaries. Finally, the thesis investigates the use of P–S separation in Elastic Full Waveform Inversion to reduce $V_P - V_S$ coupling. A separated-gradient strategy is introduced to modify the modal interactions entering the adjoint-state gradients. The formulation is interpreted as a targeted mitigation of the volumetric pathway of $V_P \rightarrow V_S$ cross-talk, rather than as a complete decoupling of the multiparameter inverse problem.

Keywords: P–S wave-field separation; Poisson-based methods; boundary conditions; Elastic Full Waveform Inversion.

Abstract in lingua italiana

L'imaging sismico elastico si fonda su simulazione e analisi di campi d'onda in cui contributi compressionali (P) e di taglio (S) sono sovrapposti. La separazione P-S aiuta ad analizzare la propagazione d'onda e a ridurre il cross-talk modale nei flussi di imaging e inversione. Tra le esistenti, le formulazioni basate su Poisson sono interessanti perché recuperano la componente P tramite un'equazione di Poisson scalare. Tuttavia, in domini limitati, tale equazione non definisce univocamente una procedura di separazione senza opportune condizioni al contorno. La tesi studia tali condizioni al contorno interpretando la separazione P-S basata su Poisson nel quadro della decomposizione di Helmholtz–Weyl. Le formulazioni Poisson–Neumann e Poisson–Dirichlet sono analizzate come diverse realizzazioni della decomposizione irrotazionale/solenoidale in un dominio limitato. Solutori di Poisson basati su trasformate veloci, coerenti con le chiusure al contorno e con la griglia sfalsata del solutore elastico, sono sviluppati e testati su campi d'onda di complessità crescente. Gli esperimenti numerici mostrano che gli artefatti di bordo si riducono includendo gli strati assorbenti nel dominio di separazione. In configurazioni di fatto illimitate, ciò rende le formulazioni Poisson–Neumann e Poisson–Dirichlet praticamente equivalenti nella regione fisica interna. La situazione cambia con superficie libera in cui la formulazione Poisson–Neumann risulta più coerente con l'assenza di onde di taglio nel fluido, mentre la formulazione Poisson–Dirichlet può generare contaminazione spuria da P a S vicino alla superficie. Ciò motiva una formulazione mista, con condizioni di Neumann non omogenee alla superficie libera e di Dirichlet omogenee ai bordi artificiali. Infine, si indaga l'uso della separazione P-S nell'Elastic Full Waveform Inversion per ridurre l'accoppiamento $V_P - V_S$. Si introduce una strategia a gradiente separato per modificare le interazioni modali che entrano nei gradienti adjoint-state. La formulazione è interpretata come mitigazione mirata del canale volumetrico di cross-talk $V_P \rightarrow V_S$, piuttosto che come disaccoppiamento completo del problema inverso multiparametrico.

Parole chiave: separazione P-S del campo d'onda elastico; metodi basati su problemi di Poisson; condizioni al contorno; Elastic Full Waveform Inversion.

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1 | Introduction

Seismic imaging is a fundamental tool for investigating the structure and physical properties of the subsurface from recorded wave data. In elastic media, the interpretation of these data is complicated by the coexistence and interaction of compressional and shear wave modes. This thesis focuses on this modal structure by studying Poisson-based P-S wave-field separation in bounded computational domains, with particular attention to the role of boundary conditions, numerical realization and application to Elastic Full Waveform Inversion.

1.1. Elastic wave-field separation in seismic imaging

Elastic seismic imaging relies on the numerical simulation and analysis of elastic waves propagating through the subsurface. In linear elastic and isotropic media, the elastic wave equation supports different propagation modes, associated with different types of mechanical motion. Compressional waves, usually referred to as P-waves, are related to volumetric deformation and particle motion along the direction of propagation, whereas shear waves, usually referred to as S-waves, are related to distortional deformation and particle motion orthogonal to the direction of propagation. The coexistence of compressional and shear contributions is one of the distinctive features of elastic wave propagation. It enriches the physical information carried by the wave-field, but it also makes its analysis more involved. Indeed, the displacement or velocity field obtained from an elastic simulation is generally observed as a total vector field, in which the different modal contributions are superposed and, in heterogeneous media, interact with each other.

In an unbounded, homogeneous and isotropic medium, this modal distinction has a precise mathematical characterization. The canonical time-harmonic plane-wave analysis of the elastic wave equation shows that the so-called *acoustic tensor* admits one longitudinal eigenmode, associated with the P-wave, and transverse eigenmodes, associated with S-waves. In two space dimensions, the in-plane shear mode is referred to as SV. In realistic seismic configurations, however, this ideal modal picture is complicated by the presence of heterogeneities, material interfaces and boundaries. At material contrasts, incident

waves may be reflected, transmitted and converted from one mode to another, so that compressional and shear contributions are continuously redistributed within the wave-field (see, e.g., [1, 26]). Moreover, free surfaces and interfaces may support coupled wave modes, such as Rayleigh, Love, Stoneley and Scholte waves (see, e.g., [2, 31, 33]). The total elastic wave-field is therefore a superposition of direct, reflected, transmitted, converted and boundary-related events, whose modal content and physical nature are often difficult to identify from the total field alone.

P–S wave-field separation addresses this difficulty by decomposing the total elastic wave-field into compressional and shear contributions, thus reorganizing the information contained in the total wave-field according to its dominant modal character. In the two-dimensional setting considered in this thesis, this means separating the in-plane displacement field into a P component and an SV component. From this perspective, wave-field separation is first of all a tool for the physical analysis of elastic wave propagation. By inspecting the separated components, one can better distinguish direct P and S arrivals, identify converted events generated at material interfaces, and analyze boundary-related phenomena such as free-surface effects.

Beyond the analysis of wave propagation itself, P–S separation plays an important role in elastic seismic imaging workflows. In elastic reverse-time migration, imaging conditions are typically based on time cross-correlations between the so-called source and receiver wave-fields, respectively obtained by forward propagation of the source and by back-propagation of the recorded data. If applied directly to the total elastic wave-fields, this procedure may generate images affected by the mixing of contributions associated with different propagation modes. In this context, P–S separation has been successfully employed by applying the imaging condition separately to the P and S components of the source and receiver wave-fields. This leads to mode-separated P–P, P–S, S–P and S–S migrated images, which carry complementary subsurface information and are less affected by inter-mode cross-talk artifacts (see, e.g., [40, 44]).

A similar motivation arises in Elastic Full Waveform Inversion (E–FWI), where the objective is to reconstruct the subsurface properties by iteratively minimizing the discrepancy between observed and simulated data (see, e.g., [39]). In the isotropic multiparameter setting, E–FWI involves the simultaneous reconstruction of the P-wave velocity V_P , the S-wave velocity V_S and, possibly, the density ρ . A well-known difficulty of this inverse problem is the coupling between the different parameters, especially between V_P and V_S (see, e.g., [30]), which may lead to undesired leakage between the corresponding parameter updates, reducing the reliability and interpretability of the inversion results. In this context, mode-decomposition-based strategies have been proposed to precondition the

adjoint-state gradient, with the aim of reducing $V_P - V_S$ cross-talk (see, e.g., [41]).

These considerations motivate the development of accurate, physically consistent and computationally efficient P–S separation procedures. This is the general framework of the present thesis, whose specific focus is on Poisson-based separation strategies in bounded computational domains.

1.2. Objectives and contributions of this work

Poisson-based separation in bounded domains

Among the different approaches proposed for elastic wave-field separation, this thesis focuses on Poisson-based formulations arising from Helmholtz-type decompositions of the elastic wave-field. In these methods, the compressional component of the wave-field is recovered as the gradient of a scalar potential, which is in turn obtained as the solution of an auxiliary scalar Poisson equation, while the shear component is obtained either through an additional potential problem or by subtraction from the total field. This class of methods is particularly appealing because, in practical applications, Poisson-based separations have been shown to preserve the amplitudes, phases and spatial structures of both direct and converted P and S events with good accuracy. Moreover, in rectangular computational domains, which are particularly relevant in numerical seismology, the auxiliary Poisson problems can be solved efficiently by means of fast trigonometric transforms, making these methods suitable for large-scale seismic simulations. A first Poisson-based strategy was proposed in [48], where the P and S components are computed by solving, respectively, a scalar Poisson problem for the compressional potential and a vector Poisson problem for the shear potential. A later formulation in [47] simplified this construction by recovering the S component as the residual between the total wave-field and the reconstructed P component. In this way, the separation is reduced to the solution of a single scalar Poisson equation, leading to a substantial decrease in computational cost.

However, the same computational point of view that makes these methods attractive also tends to conceal a delicate mathematical ambiguity. In bounded computational domains, the auxiliary Poisson equation does not define a separation procedure by itself: in order to obtain a meaningful and well-posed elliptic problem, it must be completed with boundary conditions. In several transform-based implementations, these boundary conditions are not explicitly stated at the level of a continuous elliptic boundary-value problem. Rather, they are implicitly encoded in the choice of the transform basis used to solve the discrete equations. For instance, implementations based on sine transforms, such as the one proposed in [48], correspond to homogeneous Dirichlet boundary conditions,

whereas FFT-based solvers, such as the one proposed in [47], implicitly impose periodic boundary conditions. The practical relevance of this boundary issue is already visible in the behavior of the corresponding separation procedures. In the sine-transform-based formulation of [48], boundary artifacts were reported and explicitly related to the Dirichlet boundary conditions used in the fast Poisson solver. In the FFT-based formulation of [47], artificial-boundary artifacts were addressed through a mitigation strategy based on reducing the interaction between the wave-field and the boundaries of the separation domain. However, residual artifacts were still observed at the fluid free surface, where the boundary is physical and cannot be moved away by the same extension mechanism. These observations suggest that boundary effects in Poisson-based separation are not merely incidental numerical artifacts, but reflect the boundary conditions through which the auxiliary Poisson problem is closed.

Objectives and contributions

The first objective of this thesis is therefore to clarify the role of boundary conditions in Poisson-based P–S separation in bounded domains, by interpreting the problem within the functional framework of the *Helmholtz–Weyl decomposition theorem*. In this setting, the scalar Poisson equation is not regarded as an isolated numerical tool, but as part of an elliptic boundary-value problem whose boundary conditions contribute to the mathematical definition of the separated fields. This viewpoint makes it possible to analyze the Poisson–Neumann and Poisson–Dirichlet formulations as two distinct realizations of the irrotational/solenoidal decomposition of the elastic wave-field in a bounded computational domain.

A second objective is to use this interpretation to clarify the origin of boundary-induced leakage mechanisms. Since different boundary closures impose different constraints on the separated wave-fields, they may generate different spurious modal conversions when the total wave-field reaches the boundary with non-negligible amplitude. This provides a mathematical explanation for the boundary artifacts observed in Poisson-based separation methods and motivates a domain-extension mitigation strategy, inspired by the absorbing-layer treatment proposed in [47].

On the numerical side, the thesis develops fast transform-based solvers for the auxiliary Poisson problems, designed to be consistent with both the boundary conditions of the corresponding formulation and the staggered-grid arrangement inherited from the elastic wave solver. For the Poisson–Neumann formulation, a second-order finite-difference solver is adopted, since it allows the non-homogeneous Neumann datum to be incorporated in a simple and consistent way. For the Poisson–Dirichlet formulation, the explicit spec-

tral structure of the continuous Dirichlet Laplacian motivates a continuous-like spectral approach, whose behavior is discussed in relation to both theoretical considerations and numerical experiments.

The distinction between artificial and physical boundaries becomes essential in the presence of a free surface. In this case, the boundary cannot be moved away by absorbing layers, and the boundary condition imposed on the auxiliary Poisson problem directly affects the separated fields near the physical boundary. This issue is especially relevant in fluid free surface configurations. In this setting, the thesis shows that the non-homogeneous Neumann formulation is more consistent with the absence of shear waves in the fluid, whereas the homogeneous Dirichlet formulation may induce spurious P-to-S leakage close to the free surface.

These considerations motivate the development of a Poisson–mixed formulation. The idea is to impose non-homogeneous Neumann boundary conditions on the physical free surface, while retaining homogeneous Dirichlet boundary conditions on the artificial boundaries surrounded by absorbing layers. In this way, the mixed formulation inherits the physical consistency of the Neumann condition at the fluid free surface, and, at the same time, the structure of the mixed boundary-value problem allows one to construct an efficient solver based on a spectral approach analogous to the one adopted for the Poisson–Dirichlet formulation.

The final objective of this thesis is to investigate the use of P–S separation in the context of Elastic Full Waveform Inversion, with the aim of reducing the coupling between V_P and V_S . In this setting, the separation is used to modify the modal structure of the adjoint-state gradients. The purpose of the construction is not to fully decouple the multiparameter elastic inverse problem; rather, it is to reduce a specific volumetric structural pathway of $V_P \rightarrow V_S$ cross-talk. This point is developed through a formal, yet structurally and physically motivated, analysis of the modified adjoint-state gradients. The resulting separated-gradient formulation is therefore understood as a targeted cross-talk mitigation strategy, whose effect is assessed through synthetic inversion tests.

1.3. Structure of the thesis

The thesis is organized so as to move progressively from the physical and mathematical foundations of P–S separation, through its numerical realization, and finally to its application to Elastic Full Waveform Inversion. More precisely:

- **Chapter 2 – *Basics of elastic wave propagation in linear elastic and isotropic media.***

This chapter introduces the physical and mathematical background of elastic wave propagation used throughout the thesis. The elastic wave equation is briefly derived in both *displacement-only* and *velocity-stress formulations*. The chapter then presents the classical time-harmonic plane-wave analysis in homogeneous and unbounded isotropic media, leading to the *acoustic tensor* and to its diagonalization into P and S eigenmodes. This provides the local characterization of P- and S-waves as irrotational and solenoidal components of the displacement field. Finally, the chapter discusses the restriction to the two-dimensional P–SV setting and the interpretation of this modal picture in heterogeneous media, in domains that are not unbounded in every direction, and in the presence of fluid regions.

- **Chapter 3 – *Numerical modeling of elastic wave propagation.***

This chapter describes the numerical solver used to approximate the elastic wave equation and to generate the elastic wave-fields analyzed throughout the thesis. It introduces the staggered-grid discretization of the *velocity-stress formulation*, which also defines the discrete setup used later by the Poisson solvers. The adopted finite-difference scheme, based on a second-order approximation in time and a fourth-order approximation in space, is then presented. Finally, the chapter discusses the stability and numerical dispersion properties of the scheme, sponge absorbing layers, and the treatment of heterogeneous elastic parameters.

- **Chapter 4 – *Mathematical foundations of the P–S elastic wave-field separation.***

This chapter places the P–S separation problem within a rigorous functional-analytic framework. It recalls a well-posedness result for abstract second-order linear evolutionary equations and applies it to the *displacement-only formulation* of the elastic wave equation. The chapter then introduces the *Helmholtz–Weyl decomposition theorem* and interprets it in the context of elastic wave-field separation, identifying the irrotational and solenoidal components with the P and S fields, respectively, and highlighting the role of the *harmonic-gradient* contribution.

- **Chapter 5 – *P–S separation with non-homogeneous Neumann boundary conditions.***

This chapter develops the Poisson–Neumann formulation of the P–S separation. Starting from the *Helmholtz–Weyl decomposition theorem*, the P scalar potential is characterized as the solution of an auxiliary Poisson problem with non-homogeneous Neumann boundary conditions, whose well-posedness, mathematical meaning and

physical interpretation are discussed. The chapter then presents the second-order finite-difference approximation of the problem on the staggered grid and the diagonalization of the resulting discrete problem by means of fast trigonometric transforms. Finally, a domain-extension mitigation strategy is introduced to reduce boundary-induced artifacts in the separated fields.

- **Chapter 6 – *P–S separation with homogeneous Dirichlet boundary conditions.***

This chapter develops the Poisson–Dirichlet formulation of the P–S separation, discussing the mathematical meaning and physical interpretation of homogeneous Dirichlet conditions on the P scalar potential in comparison with the Poisson–Neumann case. It then introduces an alternative continuous-like spectral solver, based on the approximation of the analytical spectral representation of the continuous Poisson–Dirichlet solution using the information available on the staggered grid, rather than on an explicit discretization of the differential operators. The chapter concludes by assessing the accuracy of the scheme and the effectiveness of the domain-extension mitigation strategy also in this setting.

- **Chapter 7 – *Comparison of the P–SV separation strategies in unbounded media.***

This chapter compares the Poisson–Neumann and Poisson–Dirichlet formulations in effectively unbounded configurations, where all boundaries are equipped with absorbing layers and the domain-extension mitigation strategy is employed. The comparison is carried out on synthetic test cases of increasing complexity. The chapter also analyzes the spectral content of the simulated wave-fields through quantitative indicators, in order to interpret the observed behavior of the separation algorithms and assess the practical relevance of the band-limitedness assumption underlying the exactness of the Poisson–Dirichlet solver.

- **Chapter 8 – *Influence of the free surface boundary condition.***

This chapter studies the effect of physical free surfaces on Poisson-based P–SV separation. It analyzes the interaction between the free surface condition and the mathematical boundary conditions imposed on the auxiliary Poisson problems. The Poisson–Neumann and Poisson–Dirichlet formulations are compared in both solid and fluid free surface configurations, where the fluid case reveals the most relevant differences and motivates the mixed formulation presented in the following chapter.

- **Chapter 9 – *P–S separation with mixed boundary conditions.***

This chapter introduces the Poisson–mixed formulation of the P–S separation, in

which non-homogeneous Neumann boundary conditions are imposed at the physical free surface and homogeneous Dirichlet boundary conditions are enforced on the remaining artificial boundaries. This choice combines the physical consistency of the Neumann closure at a fluid free surface with the spectral structure induced by the Dirichlet closure on the artificial boundaries. The well-posedness of the resulting formulation is discussed, and a fast trigonometric-transform-based solver is developed through a spectral approach analogous to the one adopted for the Poisson–Dirichlet formulation. The mixed strategy is then tested in fluid free surface configurations and compared with the Poisson–Neumann and Poisson–Dirichlet formulations.

- **Chapter 10 – *Application to the Elastic Full Waveform Inversion.***

This chapter investigates the use of P–S separation in Elastic Full Waveform Inversion. After recalling the adjoint-state formulation of the isotropic multiparameter E–FWI problem, it introduces a separated-gradient formulation in which the P and S components of the *forward* and *adjoint wave-fields* are used to select the modal interactions entering the gradient computation. The modified gradients are then analyzed from a structural and physical viewpoint, using the linearized forward and adjoint problems together with elastic Born scattering *radiation patterns* to interpret their effect on the $V_P - V_S$ cross-talk. Finally, the approach is tested on synthetic inversion examples.

- **Chapter 11 – *Conclusions and future developments.***

This chapter summarizes the main contributions of the thesis and discusses the limitations of the proposed framework, which provide the basis for outlining possible directions for future research.

The thesis is completed by two appendices. Appendix A collects the definition of the source wavelet and the detailed description of the models used in the separation and inversion tests, providing a self-contained reference for the simulation setups employed throughout the numerical experiments. Appendix B recalls the main auxiliary results of linear algebra and functional analysis used throughout the thesis.

2 | Basics of elastic wave propagation in linear elastic and isotropic media

This chapter briefly recalls the fundamental equations governing the propagation of elastic waves in linear isotropic media. A comprehensive treatment of linear elasticity can be found in classical references such as chapter 6.1 in [17]. The aim of this chapter is mainly to establish the notation and recall some results that are important for the subsequent analysis.

Starting from the balance of linear momentum and the constitutive law of linear isotropic elasticity, we first derive the elastic wave equation and present both its *displacement-only formulation* and its *velocity–stress formulation*. We then analyze the structure of elastic waves in an unbounded, homogeneous and isotropic medium through a time-harmonic plane-wave analysis, which leads to the diagonalization of the *acoustic tensor* and reveals the existence of two fundamental propagation modes, commonly referred to as P- and S-waves. The associated irrotational and solenoidal properties of these modes provide the physical motivation for the wave-field separation strategies investigated in the following chapters.

2.1. The elastic wave equation in linear elastic and isotropic media

Let us consider a linear elastic and isotropic medium, occupying a domain $\Omega \subset \mathbb{R}^n$, with $n = 2, 3$, over the time interval $I = (0, T) \subset \mathbb{R}_+$. We denote by

$$\underline{u} : I \times \Omega \rightarrow \mathbb{R}^n, \quad \underline{u} = \underline{u}(t, \underline{x}), \quad [u_i] = m$$

the displacement field, describing the deviation of a material particle located at position $\underline{x} \in \Omega$ from its equilibrium configuration at time $t \in I$.

Let us denote by

$$\underline{f} : I \times \Omega \rightarrow \mathbb{R}^n, \quad \underline{f} = \underline{f}(t, \underline{x}), \quad [f_i] = \text{N m}^{-3}$$

a generic body force term. Then, the motion of the elastic medium is governed by the balance of linear momentum, which reads

$$\rho \frac{\partial^2 \underline{u}}{\partial t^2} - \text{div}(\bar{\bar{\sigma}}) = \underline{f} \quad (2.1)$$

where

$$\rho : \Omega \rightarrow \mathbb{R}, \quad \rho = \rho(\underline{x}) > 0, \quad [\rho] = \text{kg m}^{-3}$$

represents the mass density of the medium, and

$$\bar{\bar{\sigma}} : I \times \Omega \rightarrow \mathbb{R}^{n \times n}, \quad \bar{\bar{\sigma}} = \bar{\bar{\sigma}}(t, \underline{x}), \quad [\sigma_{ij}] = \text{Pa}$$

is the *Cauchy stress tensor*.

In the framework of linear elasticity, that is, under the assumption of infinitesimal deformations, the constitutive law relating the *Cauchy stress tensor* to the strain tensor associated with displacement field is linear, namely,

$$\bar{\bar{\sigma}} = \mathbf{C} : \bar{\bar{\varepsilon}}(\underline{u}), \quad \sigma_{ij} = \sum_{h,k=1}^n \mathbf{C}_{ijhk} \varepsilon_{hk}(\underline{u})$$

where

$$\mathbf{C} : \Omega \rightarrow \mathbb{R}^{n \times n \times n \times n}, \quad \mathbf{C} = \mathbf{C}(\underline{x}), \quad [\mathbf{C}_{ijhk}] = \text{Pa}$$

denotes the fourth-order *elasticity tensor* characterizing the mechanical properties of the medium, and

$$\bar{\bar{\varepsilon}}(\underline{u}) = \text{Sym}(\nabla \underline{u}) = \frac{1}{2}(\nabla \underline{u} + \nabla \underline{u}^\top), \quad \varepsilon_{ij}(\underline{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

defines the so-called *infinitesimal strain tensor*.

In the case of isotropic linear elasticity, the fourth-order *elasticity tensor* $\mathbf{C}$ is completely characterized by two scalar parameters, called *Lamé moduli*

$$\begin{aligned} \mu : \Omega \rightarrow \mathbb{R}, \quad \mu = \mu(\underline{x}) > 0, \quad [\mu] &= \text{Pa} \\ \lambda : \Omega \rightarrow \mathbb{R}, \quad \lambda = \lambda(\underline{x}) > -\frac{2}{n}\mu, \quad [\lambda] &= \text{Pa} \end{aligned}$$

and the constitutive relation takes the well-known form

$$\bar{\sigma} = 2\mu \bar{\varepsilon}(\underline{u}) + \lambda \text{Tr}(\bar{\varepsilon}(\underline{u}))\bar{\mathbb{I}} = 2\mu \bar{\varepsilon}(\underline{u}) + \lambda \text{div}(\underline{u})\bar{\mathbb{I}} \quad (2.2)$$

where $\bar{\mathbb{I}} \in \mathbb{R}^{n \times n}$ denotes the identity tensor.

Substituting the constitutive law (2.2) into the balance of linear momentum (2.1), we get the elastic wave equation for linear elastic and isotropic media in its *displacement-only formulation*

$$\rho \frac{\partial^2 \underline{u}}{\partial t^2} - \text{div} \left(2\mu \bar{\varepsilon}(\underline{u}) + \lambda \text{div}(\underline{u})\bar{\mathbb{I}} \right) = \underline{f} \quad \text{in } I \times \Omega \quad (2.3)$$

An equivalent first-order formulation of the elastic wave equation is obtained by introducing the velocity field

$$\underline{v} : I \times \Omega \rightarrow \mathbb{R}^n, \quad \underline{v} = \underline{v}(t, \underline{x}) = \frac{\partial \underline{u}}{\partial t}(t, \underline{x}), \quad [v_i] = \text{m s}^{-1}$$

In terms of the velocity field, the balance of linear momentum (2.1) becomes

$$\rho \frac{\partial \underline{v}}{\partial t} - \text{div}(\bar{\sigma}) = \underline{f} \quad (2.4)$$

Moreover, formally differentiating with respect to time the constitutive law (2.2), we obtain

$$\frac{\partial \bar{\sigma}}{\partial t} = 2\mu \bar{\varepsilon}(\underline{v}) + \lambda \text{div}(\underline{v})\bar{\mathbb{I}} \quad (2.5)$$

Therefore, coupling equations (2.4) and (2.5), the elastic wave equation in linear elastic and isotropic media can be equivalently written in the so-called *velocity-stress formulation*:

$$\begin{cases} \rho \frac{\partial \underline{v}}{\partial t} - \text{div}(\bar{\sigma}) = \underline{f} & \text{in } I \times \Omega \\ \frac{\partial \bar{\sigma}}{\partial t} = 2\mu \bar{\varepsilon}(\underline{v}) + \lambda \text{div}(\underline{v})\bar{\mathbb{I}} & \text{in } I \times \Omega \end{cases} \quad (2.6)$$

2.2. P–S diagonalization of the acoustic tensor in an unbounded and homogeneous medium

In order to analyze the fundamental propagation modes of elastic waves, let us consider the particular case of an unbounded homogeneous medium, with vanishing forcing term,

that is

$$\Omega = \mathbb{R}^n, \quad \underline{f} \equiv \underline{0}, \quad \rho \equiv \rho_0 > 0, \quad \mu \equiv \mu_0 > 0, \quad \lambda \equiv \lambda_0 > -\frac{2}{n}\mu_0$$

Under these assumptions, the elastic wave equation in *displacement-only formulation*, as given by equation (2.3), can be formally rewritten in the form of the homogeneous *Navier equation*

$$\rho_0 \frac{\partial^2 \underline{u}}{\partial t^2} - \mu_0 \Delta \underline{u} - (\mu_0 + \lambda_0) \nabla \operatorname{div}(\underline{u}) = \underline{0} \quad \text{in } I \times \mathbb{R}^n \quad (2.7)$$

To study the propagation properties of elastic waves in this setting, we look for time-harmonic plane-wave solutions of the form

$$\underline{u}(t, \underline{x}) = \Re \left(\underline{a} e^{-i(\omega t - \underline{k} \cdot \underline{x})} \right) \quad (2.8)$$

where $\underline{a} \in \mathbb{C}^n$, $[a_i] = \text{m}$, is the so-called *polarization vector*, which determines the amplitude and direction of oscillation of the wave; $\underline{k} \in \mathbb{R}^n$, $[k_i] = \text{m}^{-1}$, is the *wave vector*, which determines the wavelength and direction of propagation; and $\omega \in \mathbb{R}$, $[\omega] = \text{s}^{-1}$ denotes the angular frequency.

Since equation (2.7) is linear with real coefficients and the real part operator is itself linear, the present analysis can be equivalently carried out using the complex field

$$\tilde{\underline{u}} = \underline{a} e^{-i(\omega t - \underline{k} \cdot \underline{x})} \quad (2.9)$$

and the corresponding physical displacement field is obtained by taking its real part.

Substituting the expression (2.9) into the differential operators appearing in equation (2.7), we obtain

$$\begin{aligned} \frac{\partial^2 \tilde{\underline{u}}}{\partial t^2} &= -\omega^2 \tilde{\underline{u}} = -\omega^2 \underline{a} e^{-i(\omega t - \underline{k} \cdot \underline{x})} \\ \Delta \tilde{\underline{u}} &= -\|\underline{k}\|_{\mathbb{R}^n}^2 \tilde{\underline{u}} = -\|\underline{k}\|_{\mathbb{R}^n}^2 \underline{a} e^{-i(\omega t - \underline{k} \cdot \underline{x})} \\ \nabla \operatorname{div}(\tilde{\underline{u}}) &= -(\underline{k} \otimes \underline{k}) \tilde{\underline{u}} = -(\underline{k} \otimes \underline{k}) \underline{a} e^{-i(\omega t - \underline{k} \cdot \underline{x})} \end{aligned}$$

Thus, reassembling equation (2.7) yields

$$\left(-\rho_0 \omega^2 \underline{a} + \mu_0 \|\underline{k}\|_{\mathbb{R}^n}^2 \underline{a} + (\mu_0 + \lambda_0)(\underline{k} \otimes \underline{k}) \underline{a} \right) e^{-i(\omega t - \underline{k} \cdot \underline{x})} = \underline{0} \quad \text{in } I \times \mathbb{R}^n \quad (2.10)$$

Since the exponential factor never vanishes, (2.10) reduces to the following algebraic equation

$$\mu_0 \|\underline{k}\|_{\mathbb{R}^n}^2 \underline{a} + (\mu_0 + \lambda_0)(\underline{k} \otimes \underline{k}) \underline{a} = \rho_0 \omega^2 \underline{a} \quad (2.11)$$

Let us introduce the wavenumber k , the unit propagation vector $\hat{e}$ and the wave velocity c , respectively defined by

$$k = \|\underline{k}\|_{\mathbb{R}^n}, \quad \hat{e} = \frac{\underline{k}}{k}, \quad c = \frac{\omega}{k}$$

Substituting these expressions into equation (2.11) leads to

$$\mu_0 \underline{a} + (\mu_0 + \lambda_0)(\hat{e} \otimes \hat{e}) \underline{a} = \rho_0 c^2 \underline{a} \quad (2.12)$$

The *acoustic tensor*, function of the unit propagation vector, is then defined as

$$\bar{\bar{A}} \in \mathbb{R}^{n \times n}, \quad \bar{\bar{A}} = \bar{\bar{A}}(\hat{e}) = \mu_0 \bar{\bar{I}} + (\mu_0 + \lambda_0)(\hat{e} \otimes \hat{e}) \quad (2.13)$$

In this way, equation (2.12) takes the form of the following algebraic eigenvalue problem

$$\bar{\bar{A}}(\hat{e}) \underline{a} = \rho_0 c^2 \underline{a} \quad (2.14)$$

which expresses the necessary and sufficient condition for a time-harmonic plane-wave to propagate in an infinite, homogeneous, linear elastic and isotropic medium, namely: the *polarization vector* must be an eigenvector of the *acoustic tensor* with associated eigenvalue equal to $\rho_0 c^2$.

Moreover, notice that, since the *acoustic tensor* $\bar{\bar{A}}(\hat{e})$ is real and symmetric, then, it follows from the *spectral theorem for symmetric matrices* (see appendix B, theorem B.1) that its eigenvalues are real and it admits an orthonormal basis of real eigenvectors. Therefore, the *polarization vectors* associated with propagating time-harmonic plane-waves can be chosen as

$$\underline{a} \in \mathbb{R}^n$$

without loss of generality. This is also consistent with the fact that the physical displacement field is obtained by taking the real part of the complex-valued ansatz (2.9).

Orthogonal decomposition and spectral structure of the *acoustic tensor*

Let us consider the one-dimensional vector subspace associated with the propagation direction

$$V_{\parallel} \subset \mathbb{R}^n, \quad V_{\parallel} = \text{span}(\hat{e}), \quad \dim(V_{\parallel}) = 1$$

and its $(n - 1)$ -dimensional orthogonal complement

$$V_{\perp} \subset \mathbb{R}^n, \quad V_{\perp} = (V_{\parallel})^{\perp} = \{\underline{v} \in \mathbb{R}^n \mid \underline{v} \cdot \hat{e} = 0\}, \quad \dim(V_{\perp}) = n - 1$$

Since $\mathbb{R}^n$ is a Hilbert space, endowed with the standard Euclidean scalar product, and $V_{\parallel}$ is a finite-dimensional subspace, hence closed, thanks to the *orthogonal decomposition theorem* (see appendix B, theorem B.2), the following orthogonal decomposition holds

$$\mathbb{R}^n = V_{\parallel} \oplus V_{\perp} \quad (2.15)$$

which implies that

$$\forall \underline{v} \in \mathbb{R}^n, \exists! \underline{v}_{\parallel} \in V_{\parallel}, \underline{v}_{\perp} \in V_{\perp} \mid \underline{v} = \underline{v}_{\parallel} + \underline{v}_{\perp}$$

where $\underline{v}_{\parallel}$ and $\underline{v}_{\perp}$ are the orthogonal projections of $\underline{v}$ onto $V_{\parallel}$ and $V_{\perp}$, respectively. That is,

$$\underline{v}_{\parallel} = \bar{\bar{\Pi}}_{\parallel} \underline{v}, \quad \underline{v}_{\perp} = \bar{\bar{\Pi}}_{\perp} \underline{v}$$

where the projection operators are defined by

$$\bar{\bar{\Pi}}_{\parallel} \in \mathbb{R}^{n \times n}, \quad \bar{\bar{\Pi}}_{\parallel} \underline{v} = (\hat{e} \otimes \hat{e}) \underline{v} \in V_{\parallel} \quad (2.16)$$

$$\bar{\bar{\Pi}}_{\perp} \in \mathbb{R}^{n \times n}, \quad \bar{\bar{\Pi}}_{\perp} = \bar{\bar{\mathbf{I}}} - \bar{\bar{\Pi}}_{\parallel}, \quad \bar{\bar{\Pi}}_{\perp} \underline{v} = (\bar{\bar{\mathbf{I}}} - (\hat{e} \otimes \hat{e})) \underline{v} \in V_{\perp} \quad (2.17)$$

and they satisfy, by construction

$$\bar{\bar{\Pi}}_{\parallel} \underline{v} = \underline{v}, \quad \bar{\bar{\Pi}}_{\perp} \underline{v} = \underline{0}, \quad \forall \underline{v} \in V_{\parallel} \quad (2.18)$$

$$\bar{\bar{\Pi}}_{\perp} \underline{v} = \underline{v}, \quad \bar{\bar{\Pi}}_{\parallel} \underline{v} = \underline{0}, \quad \forall \underline{v} \in V_{\perp} \quad (2.19)$$

Using this orthogonal decomposition, the action of the *acoustic tensor* can be readily characterized. Indeed, we can rewrite its expression, as given by (2.13) as follows:

$$\bar{\bar{A}}(\hat{e}) = \mu_0 (\bar{\bar{\mathbf{I}}} - (\hat{e} \otimes \hat{e})) + (\lambda_0 + 2\mu_0)(\hat{e} \otimes \hat{e})$$

which corresponds, in view of (2.16) and (2.17), to

$$\bar{\bar{A}}(\hat{e}) = \mu_0 \bar{\bar{\Pi}}_{\perp} + (\lambda_0 + 2\mu_0) \bar{\bar{\Pi}}_{\parallel}$$

This representation shows that the acoustic tensor acts diagonally with respect to the orthogonal decomposition (2.15). Indeed, let $\underline{a} \in \mathbb{R}^n$:

- If $\underline{a} \in V_{\parallel}$, then, thanks to (2.18),

$$\bar{\bar{A}}(\hat{e}) \underline{a} = \mu_0 \cancel{\bar{\Pi}_{\perp}} \underline{a} + (\lambda_0 + 2\mu_0) \bar{\Pi}_{\parallel} \underline{a} = (\lambda_0 + 2\mu_0) \underline{a} \quad (2.20)$$

Therefore, $\underline{a} \in V_{\parallel}$ is an eigenvector of the *acoustic tensor* $\bar{\bar{A}}(\hat{e})$, with associated eigenvalue $\lambda_0 + 2\mu_0$, with multiplicity one.

- If $\underline{a} \in V_{\perp}$, then, thanks to (2.19),

$$\bar{\bar{A}}(\hat{e}) \underline{a} = \mu_0 \bar{\Pi}_{\perp} \underline{a} + (\lambda_0 + 2\mu_0) \cancel{\bar{\Pi}_{\parallel}} \underline{a} = \mu_0 \underline{a} \quad (2.21)$$

Therefore, $\underline{a} \in V_{\perp}$ is an eigenvector of the *acoustic tensor* $\bar{\bar{A}}(\hat{e})$, with associated eigenvalue μ_0 , with multiplicity $n - 1$.

Combining equations (2.20) and (2.21) with the original form of the eigenvalue problem (2.14), we get

$$\begin{aligned} \underline{a} \in V_{\parallel} &\Rightarrow \lambda_0 + 2\mu_0 = \rho_0 c^2 \Rightarrow c = V_P = \sqrt{\frac{\lambda_0 + 2\mu_0}{\rho_0}} \\ \underline{a} \in V_{\perp} &\Rightarrow \mu_0 = \rho_0 c^2 \Rightarrow c = V_S = \sqrt{\frac{\mu_0}{\rho_0}} \end{aligned}$$

Physical interpretation of P- and S-waves

The spectral characterization of the acoustic tensor provides a clear physical interpretation of the fundamental propagation modes of elastic waves in unbounded, homogeneous, linear elastic and isotropic media.

The previous analysis shows that, in such a medium, there exist three admissible linearly independent *polarization vectors* $\underline{a}$ for a time-harmonic plane-wave of the form (2.8), which necessarily coincide with the eigenvectors of the *acoustic tensor* $\bar{\bar{A}}(\hat{e})$. Therefore, one belongs to the subspace $V_{\parallel}$, while the other two belong to its orthogonal complement $V_{\perp}$.

If $\underline{a} \in V_{\parallel}$, then the displacement $\underline{u}$ is polarized along the wave propagation direction. In this case, the oscillations of the medium occur in the same direction as the wave propagation, and the corresponding mode is therefore longitudinal. The associated propagation velocity is

$$V_P = \sqrt{\frac{\lambda_0 + 2\mu_0}{\rho_0}}, \quad [V_P] = \text{m s}^{-1} \quad (2.22)$$

and the corresponding wave is called a compressional or P-wave.

On the other hand, if $\underline{a} \in V_\perp$, then the displacement is orthogonal to the propagation direction. In this case, the oscillations of the medium occur in directions perpendicular to the wave propagation, and the corresponding mode is therefore transverse. The associated propagation velocity is

$$V_S = \sqrt{\frac{\mu_0}{\rho_0}}, \quad [V_S] = \text{m s}^{-1} \quad (2.23)$$

and the corresponding wave is called shear or S-wave.

We emphasize that these two modes exhaust all possible time-harmonic plane-wave solutions of the elastic wave equation in unbounded, homogeneous, linear elastic and isotropic media, as shown by the previous spectral analysis of the *acoustic tensor*.

Moreover, from equations (2.22) and (2.23), it follows that

$$V_P > V_S$$

since $\lambda_0 + 2\mu_0 > \mu_0$ for any physically admissible values of the *Lamé moduli*. Therefore, compressional waves always propagate faster than shear waves.

A further fundamental characterization of these two propagation modes can be obtained in terms of the divergence and curl of the corresponding displacement field. Indeed, considering a time-harmonic plane wave of the form (2.9), a direct computation yields

$$\text{div}(\tilde{\underline{u}}) = \text{i} (\underline{k} \cdot \underline{a}) e^{-\text{i}(\omega t - \underline{k} \cdot \underline{x})}, \quad \text{curl}(\tilde{\underline{u}}) = \begin{cases} \text{i} (k_1 a_2 - k_2 a_1) e^{-\text{i}(\omega t - \underline{k} \cdot \underline{x})} & \text{if } n = 2 \\ \text{i} (\underline{k} \times \underline{a}) e^{-\text{i}(\omega t - \underline{k} \cdot \underline{x})} & \text{if } n = 3 \end{cases} \quad (2.24)$$

If $\underline{a} \in V_\parallel$, that is, $\underline{a} = \alpha \hat{e}$, $\alpha \in \mathbb{R}$, then one gets, if $n = 2$

$$k_1 a_2 - k_2 a_1 = \alpha k (e_1 e_2 - e_2 e_1) = 0$$

and, analogously, if $n = 3$

$$\underline{k} \times \underline{a} = \alpha k (\hat{e} \times \hat{e}) = \underline{0}$$

Therefore, in both cases, according to (2.24), we conclude

$$\underline{a} \in V_\parallel \Rightarrow \text{curl}(\tilde{\underline{u}}) = \underline{0}$$

Hence, the displacement field of a time-harmonic plane P-wave is irrotational, which is consistent with the fact that compressional waves are associated with purely volumetric

deformations.

Conversely, if $\underline{a} \in V_\perp$, then, by definition, $\underline{a} \cdot \hat{e} = 0$, so that

$$\underline{k} \cdot \underline{a} = k (\hat{e} \cdot \underline{a}) = 0$$

Thus, according to (2.24), we obtain

$$\underline{a} \in V_\perp \Rightarrow \operatorname{div}(\tilde{\underline{u}}) = 0$$

Hence, the displacement field of a time-harmonic plane S-wave is solenoidal, which is consistent with the fact that shear waves are associated with purely distortional deformations.

Therefore, in unbounded, homogeneous, linear elastic and isotropic media, compressional time-harmonic plane-waves are characterized by irrotational displacement fields, whereas shear time-harmonic plane-waves correspond to solenoidal displacement fields.

Restriction to the two-dimensional P–SV setting

In the following chapters, we will restrict attention to a two-dimensional (i.e., $n = 2$) configuration, namely we consider domains $\Omega \subset \mathbb{R}^2$. Accordingly, we consider displacement fields of the form

$$\underline{u} : I \times \Omega \rightarrow \mathbb{R}^2, \quad \underline{u}(t, x, z) = (u_x(t, x, z), u_z(t, x, z))$$

and propagation directions confined in the same plane, namely

$$\hat{e} = (e_x, e_z)$$

In this setting, the transverse subspace $V_\perp$ is one dimensional, more precisely

$$V_\perp = \operatorname{span}(\hat{s}), \quad \hat{s} = (-e_z, e_x)$$

Thus, in two space dimensions, there exist two admissible linearly independent *polarization vectors* for a time-harmonic plane-wave of the form (2.8): one longitudinal, aligned with $\hat{e}$, and one transverse, aligned with $\hat{s}$. In the seismological terminology adopted in this work, this in-plane shear mode will be referred to as SV (with “V” standing for vertical, since z denotes the depth).

Degenerate fluid case and extension beyond the unbounded, homogeneous, time-harmonic plane-wave setting

A fluid medium can be interpreted as a degenerate case of linear elasticity, characterized by the absence of resistance to shear deformations, namely

$$\mu_0 = 0$$

From a physical viewpoint, this reflects the fact that a fluid cannot sustain shear stresses and only supports isotropic (pressure) stresses. In terms of elastic parameters, this corresponds to the case in which the Poisson ratio approaches the limit $\nu = 1/2$ with a fixed finite value of λ :

$$\nu = \frac{\lambda}{2(\lambda + \mu)} \rightarrow \frac{1}{2}, \quad \mu \rightarrow 0$$

This limiting fluid regime should not be confused with the incompressible solid limit, which is obtained for $\lambda \rightarrow +\infty$ with μ fixed, positive and finite, despite yielding the same limiting value of the Poisson ratio.

As a consequence, the *acoustic tensor* reduces to

$$\bar{\bar{A}}(\hat{e}) = \lambda_0 (\hat{e} \otimes \hat{e})$$

and the eigenspace $V_\perp$ is associated with a vanishing eigenvalue, so that

$$V_S = \sqrt{\frac{\mu_0}{\rho_0}} = 0$$

Therefore, shear waves cannot propagate in a fluid, and the wave-field is purely compressional.

In more realistic settings, involving heterogeneous media and bounded domains, the propagation of elastic waves is considerably more complex. The presence of material discontinuities or boundaries (such as free surfaces or interfaces) gives rise to reflection, refraction and diffraction phenomena, which are generally accompanied by mode conversions between compressional and shear waves. These effects are classically described, for instance, by the Zoeppritz equations at interfaces (see, e.g., chapter 5.2 in [1]), and by amplitude-versus-offset (AVO) analysis, which describes the variation of reflection amplitudes with the angle of incidence (see, e.g., chapter 3.5 in [26]). Moreover, boundaries and interfaces may support intrinsically coupled wave modes, such as Rayleigh and Love waves at solid free surfaces (see, e.g., chapters 7.3 and 7.5 in [1]; [31]), Stoneley waves at solid-solid interfaces (see, e.g., [33]), or Scholte waves at fluid-solid interfaces (see, e.g., [2]).

In such configurations, the wave-field is no longer composed of independent propagation modes, but rather of a superposition of P- and S-wave components that continuously interact, convert and interfere with each other. Nevertheless, the characterization in terms of divergence and curl retains a clear physical meaning. Even in heterogeneous media and for general wave-fields, the irrotational content of the displacement field can still be associated with compressional motion, whereas the solenoidal content is related to shear motion. This is consistent, in a local sense, with the classical characterization of P- and S-waves based on their polarization with respect to the propagation direction, with P-waves oscillating parallel to the local direction of propagation, and S-waves orthogonally to it. Therefore, although this identification is no longer exact in a strict mathematical sense, it provides a physically meaningful and practically useful framework to interpret and separate the different wave modes, including both direct and converted waves.

In the following, this interpretation will be adopted as a physically motivated basis for wave-field separation. More precisely, the compressional P wave-field will be identified with the irrotational component of the displacement field, whereas the shear S wave-field will be identified with its solenoidal component. Accordingly, we consider the decomposition:

$$\underline{u} = \underline{u}_P + \underline{u}_S \quad (2.25)$$

$$\text{curl}(\underline{u}_P) = \underline{0}, \quad \text{div}(\underline{u}_S) = 0 \quad (2.26)$$

where $\underline{u}_P$ and $\underline{u}_S$ denote, respectively, the irrotational and solenoidal components of the wave-field.

3 | Numerical modeling of elastic wave propagation

In order to numerically simulate elastic wave propagation in heterogeneous media, finite-difference methods represent a widely adopted approach in computational seismology, due to their computational efficiency and their effectiveness in modeling wave propagation in complex media on structured grids.

In this work, we adopt an explicit second-order accurate scheme in time and fourth-order accurate scheme in space, following the formulation proposed by Levander [23]. The method is based on the first-order *velocity–stress formulation* of the elastic wave equation (2.6), discretized on a staggered grid. This class of methods, originally introduced by Madariaga [25] and later developed by Virieux [38] and subsequent authors, is particularly well suited for wave propagation problems.

In particular, the staggered grid arrangement allows for a consistent discretization of the governing equations, leading to reduced numerical dispersion. Moreover, in combination with the *velocity–stress formulation*, it enables an effective treatment of heterogeneous media, including strong parameter contrasts and fluid-solid interfaces.

The aim of this chapter is to provide a self-contained description of the numerical scheme adopted in this work. We first introduce the staggered grid discretization of the velocity–stress system and the associated finite-difference operators. We then briefly discuss the main stability and dispersion properties of the scheme. Finally, we describe the treatment of artificial boundaries and the implementation of heterogeneous elastic parameters on the staggered grid.

3.1. Staggered grid finite-difference discretization of the elastic wave equation in *velocity–stress formulation*

In this section, we describe both the staggered grid arrangement and the finite-difference scheme adopted to discretize the velocity–stress system (2.6) on such a grid.

3.1.1. Staggered grid setup

Let $L_x, L_z, T > 0$. We consider the space-time computational domain

$$I \times \Omega = (0, T) \times (0, L_x) \times (0, L_z) \subset \mathbb{R}_+ \times \mathbb{R}^2$$

Over this domain, we introduce a staggered grid characterized by the following parameters:

- $N_x \geq 1$: number of cells along the x -direction;
- $N_z \geq 1$: number of cells along the z -direction;
- $N_t \geq 1$: number of time-steps;
- $h_x = \frac{L_x}{N_x} > 0$: grid spacing along the x -direction;
- $h_z = \frac{L_z}{N_z} > 0$: grid spacing along the z -direction;
- $\Delta t = \frac{T}{N_t} > 0$: time-step size.

In practice, we will restrict ourselves to uniform grids, such that $h_x = h_z = h$. However, for the sake of generality, most derivations will be carried out keeping h_x and h_z distinct.

We introduce the following index sets associated with the collocation points of the staggered grid:

- Indices for the cell centers:

$$\Sigma_i^{(c)} = \{0, \dots, N_x - 1\}, \quad \Sigma_j^{(c)} = \{0, \dots, N_z - 1\}, \quad \Sigma^{(c)} = \Sigma_i^{(c)} \times \Sigma_j^{(c)}$$

- Indices for the centers of the vertical cell edges:

$$\Sigma_i^{(v)} = \{0, \dots, N_x\}, \quad \Sigma_j^{(v)} = \{0, \dots, N_z - 1\}, \quad \Sigma^{(v)} = \Sigma_i^{(v)} \times \Sigma_j^{(v)}$$

- Indices for the centers of the horizontal cell edges:

$$\Sigma_i^{(h)} = \{0, \dots, N_x - 1\}, \quad \Sigma_j^{(h)} = \{0, \dots, N_z\}, \quad \Sigma^{(h)} = \Sigma_i^{(h)} \times \Sigma_j^{(h)}$$

- Indices for the cell vertices:

$$\Sigma_i^{(n)} = \{0, \dots, N_x\}, \quad \Sigma_j^{(n)} = \{0, \dots, N_z\}, \quad \Sigma^{(n)} = \Sigma_i^{(n)} \times \Sigma_j^{(n)}$$

- Indices for the integer time levels:

$$\Theta^{(i)} = \{0, \dots, N_t\}$$

- Indices for the half time levels:

$$\Theta^{(h)} = \{0, \dots, N_t - 1\}$$

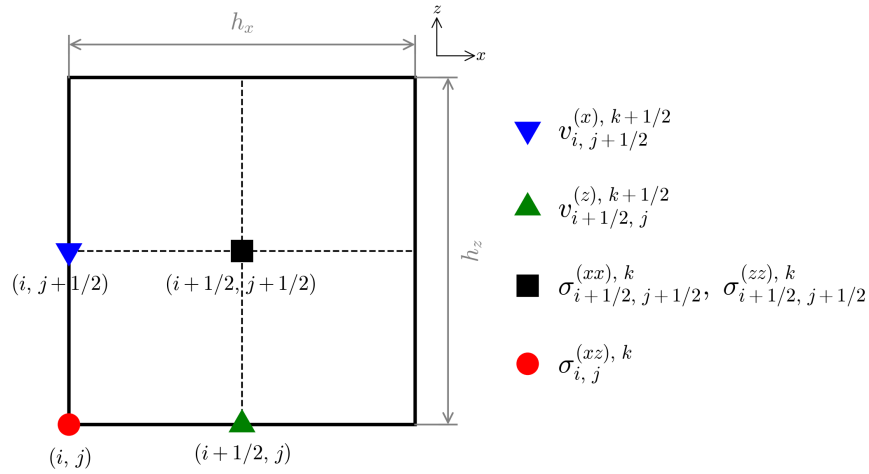


Figure 3.1: Staggered grid arrangement for the velocity-stress formulation.

We discretize the first-order velocity-stress system (2.6) on the staggered grid defined above. The unknown fields are represented in discrete form by degrees of freedom associated with the collocation points of the staggered grid. In particular, as illustrated in figure 3.1:

- The degrees of freedom of the horizontal component of the velocity are collocated at the centers of the vertical cell edges, in the nodes

$$(x_i, z_{j+1/2}) = (ih_x, (j + 1/2)h_z), \quad (i, j) \in \Sigma^{(v)}$$

In time, they are defined at half time levels

$$t^{k+1/2} = (k + 1/2)\Delta t, \quad k \in \Theta^{(h)}$$

Therefore, they are denoted by $v_{i,j+1/2}^{(x),k+1/2}$.

- The degrees of freedom of the vertical component of the velocity are collocated at the centers of the horizontal cell edges, in the nodes

$$(x_{i+1/2}, z_j) = ((i + 1/2)h_x, jh_z), \quad (i, j) \in \Sigma^{(h)}$$

In time, they are defined at half time levels and are therefore denoted by $v_{i+1/2,j}^{(z),k+1/2}$.

- The degrees of freedom of the diagonal components of the stress tensor are collocated at the cell centers, in the nodes

$$(x_{i+1/2}, z_{j+1/2}) = ((i + 1/2)h_x, (j + 1/2)h_z), \quad (i, j) \in \Sigma^{(c)}$$

In time, they are defined at integer time levels

$$t^k = k\Delta t, \quad k \in \Theta^{(i)}$$

Therefore, they are denoted by $\sigma_{i+1/2,j+1/2}^{(xx),k}$ and $\sigma_{i+1/2,j+1/2}^{(zz),k}$.

- The degrees of freedom of the off-diagonal components of the stress tensor are collocated at the cell vertices, in the nodes

$$(x_i, z_j) = (ih_x, jh_z), \quad (i, j) \in \Sigma^{(n)}$$

In time, they are defined at integer time levels and are therefore denoted by $\sigma_{i,j}^{(xz),k}$.

3.1.2. Second-order in time, fourth-order in space finite-difference scheme

We now describe the explicit finite-difference scheme adopted to discretize the velocity–stress system (2.6) on the staggered grid introduced in the previous section.

The time discretization is performed using a centered second-order accurate scheme, while spatial derivatives are approximated by centered fourth-order accurate finite-difference operators, as described by Levander in [23].

More precisely, let f be a sufficiently smooth function of time. Using the staggered-in-time discretization introduced in section 3.1.1, its time derivative at the time level t^k can be approximated by the second-order centered finite-difference formula

$$\frac{df}{dt}(t^k) = \frac{f(t^{k+1/2}) - f(t^{k-1/2})}{\Delta t} + \mathcal{O}(\Delta t^2) \approx \frac{f^{k+1/2} - f^{k-1/2}}{\Delta t} \quad (3.1)$$

Let g be a sufficiently smooth function of space. Using the staggered-in-space discretization introduced in section 3.1.1, its spatial derivative at the node x_i can be approximated by the fourth-order centered finite-difference formula

$$\begin{aligned} \frac{dg}{dx}(x_i) &= \frac{9}{8h} \left(g(x_{i+1/2}) - g(x_{i-1/2}) \right) - \frac{1}{24h} \left(g(x_{i+3/2}) - g(x_{i-3/2}) \right) + \mathcal{O}(h^4) \approx \\ &\approx \frac{9}{8h} (g_{i+1/2} - g_{i-1/2}) - \frac{1}{24h} (g_{i+3/2} - g_{i-3/2}) \end{aligned} \quad (3.2)$$

A general framework for the construction of finite-difference operators based on polynomial interpolation is presented in [16].

The numerical scheme is obtained by replacing the time and space derivatives in the velocity–stress system (2.6) with the finite-difference approximations (3.1) and (3.2), and enforcing the resulting equations at the corresponding staggered grid points. For brevity, the index ranges are not explicitly reported in the equations below. Each equation is understood to hold at the appropriate staggered grid locations, namely:

- The equation for $v^{(x)}$ is defined for all $(i, j, k) \in \Sigma^{(v)} \times \Theta^{(h)}$;
- The equation for $v^{(z)}$ is defined for all $(i, j, k) \in \Sigma^{(h)} \times \Theta^{(h)}$;
- The equations for $\sigma^{(xx)}$ and $\sigma^{(zz)}$ are defined for all $(i, j, k) \in \Sigma^{(c)} \times \Theta^{(i)}$;
- The equation for $\sigma^{(xz)}$ is defined for all $(i, j, k) \in \Sigma^{(n)} \times \Theta^{(i)}$.

The resulting time-advancing scheme reads as follows:

$$\left\{ \begin{array}{l} R_{i,j+1/2} \frac{v_{i,j+1/2}^{(x),k+1/2} - v_{i,j+1/2}^{(x),k-1/2}}{\Delta t} = D_x^{(4)} \sigma_{i,j+1/2}^{(xx),k} + D_z^{(4)} \sigma_{i,j+1/2}^{(xz),k} + f_x(t^k, x_i, z_{j+1/2}) \\ R_{i+1/2,j} \frac{v_{i+1/2,j}^{(z),k+1/2} - v_{i+1/2,j}^{(z),k-1/2}}{\Delta t} = D_x^{(4)} \sigma_{i+1/2,j}^{(xz),k} + D_z^{(4)} \sigma_{i+1/2,j}^{(zz),k} + f_z(t^k, x_{i+1/2}, z_j) \\ \frac{\sigma_{i+1/2,j+1/2}^{(xx),k+1} - \sigma_{i+1/2,j+1/2}^{(xx),k}}{\Delta t} = (L_{i+1/2,j+1/2} + 2M_{i+1/2,j+1/2}) D_x^{(4)} v_{i+1/2,j+1/2}^{(x),k+1/2} \\ \quad + M_{i+1/2,j+1/2} D_z^{(4)} v_{i+1/2,j+1/2}^{(z),k+1/2} \\ \frac{\sigma_{i+1/2,j+1/2}^{(zz),k+1} - \sigma_{i+1/2,j+1/2}^{(zz),k}}{\Delta t} = (L_{i+1/2,j+1/2} + 2M_{i+1/2,j+1/2}) D_z^{(4)} v_{i+1/2,j+1/2}^{(z),k+1/2} \\ \quad + M_{i+1/2,j+1/2} D_x^{(4)} v_{i+1/2,j+1/2}^{(x),k+1/2} \\ \frac{\sigma_{i,j}^{(xz),k+1} - \sigma_{i,j}^{(xz),k}}{\Delta t} = M_{i,j} \left(D_z^{(4)} v_{i,j}^{(x),k+1/2} + D_x^{(4)} v_{i,j}^{(z),k+1/2} \right) \end{array} \right. \quad (3.3)$$

where, to lighten the notation, we use the symbols $D_x^{(4)}$, $D_z^{(4)}$ to denote the fourth-order centered finite-difference operators defined by (3.2). For instance

$$D_z^{(4)} \sigma_{i,j+1/2}^{(xz),k} = \frac{9}{8h_z} \left(\sigma_{i,j+1}^{(xz),k} - \sigma_{i,j}^{(xz),k} \right) - \frac{1}{24h_z} \left(\sigma_{i,j+2}^{(xz),k} - \sigma_{i,j-1}^{(xz),k} \right)$$

Moreover, the symbols R , M and L denote the material parameters ρ , μ and λ , respectively, suitably interpolated at the staggered grid collocation nodes according to the procedure described in section 3.3.2.

Finally, we specify the initialization of the scheme and the treatment of the boundary nodes. To model homogeneous initial conditions, the degrees of freedom are initialized to zero at $k = -1/2$ for the velocity components, and at $k = 0$ for the stress tensor components, at all their collocation nodes.

Moreover, in order to preserve the centered fourth-order finite-difference stencils up to the boundaries of the computational domain, ghost nodes are introduced outside the physical domain, at collocation points corresponding to indices such as $i = -1/2, -3/2$ and/or $j = -1/2, -3/2$. The values at the ghost nodes are assigned consistently with the considered boundary conditions. In the case of absorbing boundaries, the ghost-node values are set to zero. In combination with the absorbing layers described in section 3.3.1, this choice has a negligible impact on the solution, since the wave-field is strongly attenuated before reaching the outer boundary. The numerical treatment of the free surface boundary

condition is discussed in section 8.1.

3.2. Stability and dispersion properties of the numerical scheme

To assess the stability and dispersion properties of the proposed scheme, we resort to the classical von Neumann analysis, based on the Fourier analysis of discrete plane waves, originally introduced in early works by Crank & Nicolson [9] and Charney et al. [6].

The analysis is carried out under the usual assumptions of a homogeneous and unbounded medium, by considering time-harmonic plane-wave solutions, as in (2.9), for all field variables (velocity and stress components), sampled on the staggered grid described in section 3.1.1.

In what follows, we adopt the standard framework described by Virieux in [38]. Rather than presenting the full algebraic derivation, we only outline the main steps and directly state the resulting *dispersion relations*.

Substituting the time-harmonic plane-wave ansatz into the discrete velocity-stress system (3.3) and eliminating the stress amplitudes by direct substitution, the problem can be reduced to a linear algebraic system for the two Fourier coefficients associated with the velocity components, namely

$$\bar{\bar{M}} \underline{a} = \underline{0} \quad (3.4)$$

where the matrix $\bar{\bar{M}} \in \mathbb{R}^{2 \times 2}$ is given by

$$\bar{\bar{M}} = \begin{bmatrix} \xi_t^2 - \frac{1}{R}[(L + 2M)\xi_x^2 + M\xi_z^2] & -\frac{1}{R}(L + M)\xi_x\xi_z \\ -\frac{1}{R}(L + M)\xi_x\xi_z & \xi_t^2 - \frac{1}{R}[M\xi_x^2 + (L + 2M)\xi_z^2] \end{bmatrix}$$

Here, $R = \rho$, $M = \mu$ and $L = \lambda$, since the medium is assumed homogeneous, and the quantities ξ_t , ξ_x and ξ_z are defined as

$$\xi_t = \xi_t(\omega) = \frac{1}{\Delta t} \sin\left(\frac{\omega}{2}\Delta t\right) \quad (3.5)$$

$$\xi_x = \xi_x(k_x) = \frac{1}{h_x} \left[\frac{9}{8} \sin\left(\frac{k_x}{2}h_x\right) - \frac{1}{24} \sin\left(\frac{3k_x}{2}h_x\right) \right] \quad (3.6)$$

$$\xi_z = \xi_z(k_z) = \frac{1}{h_z} \left[\frac{9}{8} \sin\left(\frac{k_z}{2}h_z\right) - \frac{1}{24} \sin\left(\frac{3k_z}{2}h_z\right) \right] \quad (3.7)$$

The linear system (3.4) admits a non-trivial solution $\underline{a} \neq \underline{0}$ if and only if the determinant of $\bar{M}$ is equal to zero. Imposing this requirement yields the following conditions, called *dispersion relations*:

$$\xi_t^2 = V_P^2(\xi_x^2 + \xi_z^2), \quad \xi_t^2 = V_S^2(\xi_x^2 + \xi_z^2) \quad (3.8)$$

where we denoted, according to (2.22) and (2.23),

$$V_P = \sqrt{\frac{L + 2M}{R}}, \quad V_S = \sqrt{\frac{M}{R}}$$

These relations correspond to the discrete counterparts of the P- and S-wave modes and define the conditions governing their numerical propagation.

3.2.1. Stability properties

To derive a stability condition for the numerical scheme (3.3), we analyze the *dispersion relations* (3.8). According to (3.5), for each wave mode, they can be written in the form

$$\sin^2\left(\frac{\omega}{2}\Delta t\right) = \Delta t^2 V^2(\xi_x^2 + \xi_z^2) \quad (3.9)$$

where V denotes either the P-wave velocity V_P or the S-wave velocity V_S .

Within the von Neumann framework, a necessary condition for stability is that the angular frequency ω is real for every wave vector $\underline{k} = (k_x, k_z) \in \mathbb{R}^2$. Since, for real arguments, the left-hand side of equation (3.9) is bounded from above by unity, the existence of real solutions requires

$$\max_{k_x, k_z \in \mathbb{R}} (\xi_x^2(k_x) + \xi_z^2(k_z)) \leq \frac{1}{\Delta t^2 V^2} \quad (3.10)$$

The maximum is attained for $k_x h_x = k_z h_z = \pi$, up to periodicity, yielding

$$\max_{k_x, k_z \in \mathbb{R}} (\xi_x^2(k_x) + \xi_z^2(k_z)) = \frac{49}{36} \left(\frac{1}{h_x^2} + \frac{1}{h_z^2} \right) \quad (3.11)$$

Stability requires the angular frequency to be real for all admissible modes. Therefore, the stability condition must be satisfied for both branches of the *dispersion relations* (3.8). Since $V_P > V_S$, the most restrictive condition is obtained by considering the P-wave velocity. Hence, combining equations (3.10) and (3.11), one obtains the following stability criterion:

$$\Delta t \leq \frac{6}{7 V_P \sqrt{\frac{1}{h_x^2} + \frac{1}{h_z^2}}}$$

which simplifies, in case of uniform grid, i.e., $h_x = h_z = h$, to

$$\Delta t \leq \frac{6}{7\sqrt{2}} \frac{h}{V_P} \approx 0.606 \frac{h}{V_P}$$

It is worth pointing out that this stability condition is more restrictive, by about 17%, than that associated with the second-order finite-difference scheme on the same staggered grid (see [38]).

As a final remark, we briefly justify why requiring a real angular frequency ω is necessary for stability. If the right-hand side of (3.9) exceeds unity, the equation admits no real solutions. Allowing for a complex angular frequency $\omega \in \mathbb{C}$, one obtains complex conjugate roots

$$\omega = \omega_r \pm i\omega_i, \quad \omega_i > 0$$

one of which, when substituted into the time-harmonic plane-wave ansatz, yields exponential growth in time, thus leading to instability.

3.2.2. Dispersion properties

Numerical dispersion refers to the phenomenon whereby the numerical propagation velocity of discrete waves differs from the physical one, exhibiting a dependence on the wavenumber and on the direction of propagation. In particular, the dependence on the wavenumber implies that different Fourier components propagate at different speeds, leading to phase errors, while the dependence on the direction of propagation gives rise to the so-called numerical anisotropy.

Let us consider a uniform grid, i.e., $h_x = h_z = h$. We introduce the following parameters:

- $\gamma = \frac{7\sqrt{2}}{6} \frac{V_P}{h} \Delta t$, *Courant number* normalized with respect to the stability limit, so that $\gamma = 1$ corresponds to the stability threshold of the scheme;
- $\theta \in [0, 2\pi)$, angle between the propagation direction and the x -axis, defined through

$$\underline{k} = (k_x, k_z) = (k \cos \theta, k \sin \theta)$$

- $H = \frac{k h}{2\pi} = \frac{h}{\lambda}$, inverse of the number of grid points per wavelength.

From the *dispersion relations* (3.8) one obtains the expressions of the normalized numerical

P- and S-wave velocities, which, respectively, read as follows:

$$Q_P(H, \theta, \gamma) = \frac{7\sqrt{2}}{6\pi\gamma H} \arcsin \left[\frac{6\gamma}{7\sqrt{2}} \sqrt{\left(\frac{9}{8}B_1 - \frac{1}{24}B_2\right)^2 + \left(\frac{9}{8}C_1 - \frac{1}{24}C_2\right)^2} \right] \quad (3.12)$$

$$Q_S(H, \theta, \gamma, \nu) = \frac{1}{A} \frac{7\sqrt{2}}{6\pi\gamma H} \arcsin \left[A \frac{6\gamma}{7\sqrt{2}} \sqrt{\left(\frac{9}{8}B_1 - \frac{1}{24}B_2\right)^2 + \left(\frac{9}{8}C_1 - \frac{1}{24}C_2\right)^2} \right] \quad (3.13)$$

where we denoted

$$B_1 = B_1(H, \theta) = \sin(\pi H \cos \theta), \quad B_2 = B_2(H, \theta) = \sin(3\pi H \cos \theta)$$

$$C_1 = C_1(H, \theta) = \sin(\pi H \sin \theta), \quad C_2 = C_2(H, \theta) = \sin(3\pi H \sin \theta)$$

$$A = A(\nu) = \frac{V_S}{V_P} = \sqrt{\frac{1-2\nu}{2(1-\nu)}}$$

with $\nu \in (-1, 0.5)$ representing the Poisson ratio. The quantities Q_P and Q_S are the ratios between the numerical and the physical propagation velocities of P- and S-waves, respectively. Since the propagation velocity is defined as the ratio between the angular frequency and the wavenumber, it follows that

$$Q_P = \frac{\omega}{k V_P}, \quad Q_S = \frac{\omega}{k V_S},$$

where, for each mode, ω is obtained from the corresponding branch of the *dispersion relations*. Therefore, deviations of Q_P and Q_S from unity directly quantify the numerical dispersion error.

The dispersion properties of the scheme are illustrated through a set of representative plots of the normalized numerical velocities Q_P and Q_S as functions of H , for varying propagation directions, normalized *Courant numbers*, and, for S-waves, Poisson ratios.

From figures 3.2, 3.3 and 3.4, the following observations can be drawn:

- For both P- and S-waves, all plots show that the deviation from unity increases with H . This indicates that, for a fixed grid spacing h , higher-wavenumber Fourier components exhibit the largest deviation between numerical and physical propagation velocities, and are therefore the most affected by numerical dispersion.

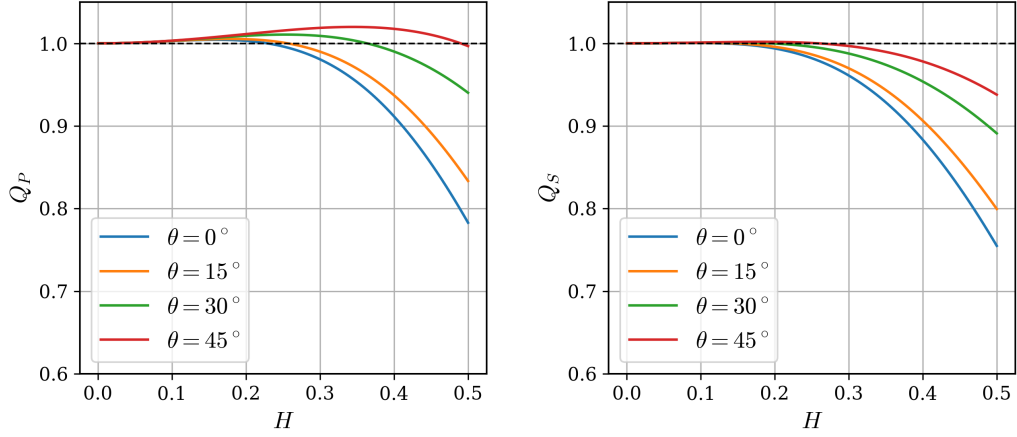


Figure 3.2: Normalized numerical velocities Q_P (left) and Q_S (right) as functions of H , for different propagation directions, parametrized by the angle θ , with $\gamma = 0.75$ and $\nu = 0.25$, highlighting the effect of numerical anisotropy.

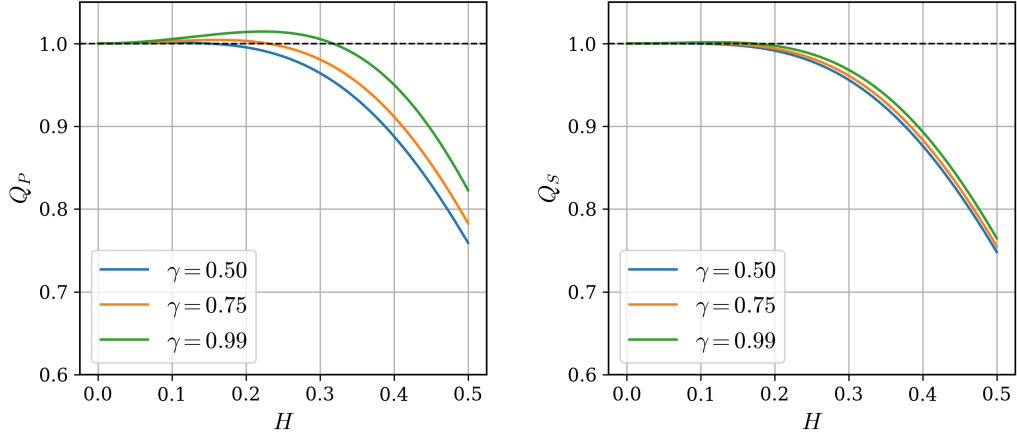


Figure 3.3: Normalized numerical velocities Q_P (left) and Q_S (right) as functions of H , for different values of the normalized *Courant number* γ , with $\theta = 0^\circ$ and $\nu = 0.25$, highlighting the effect of approaching the stability limit ($\gamma \rightarrow 1$).

- The plots suggest that a value $H \approx 0.2$, corresponding to approximately five grid points per minimum wavelength, is sufficient to keep numerical dispersion effects negligible for both Q_P and Q_S . Since $V_S < V_P$, the condition associated with Q_S is more restrictive and therefore governs the resolution requirement. This represents a significant improvement over the second-order in space finite-difference scheme on the same staggered grid, which typically requires $H \approx 0.1$, i.e., about ten grid points per minimum S wavelength. In the presence of fluid regions, where $V_S = 0$, this criterion should instead be interpreted in terms of the minimum non-zero

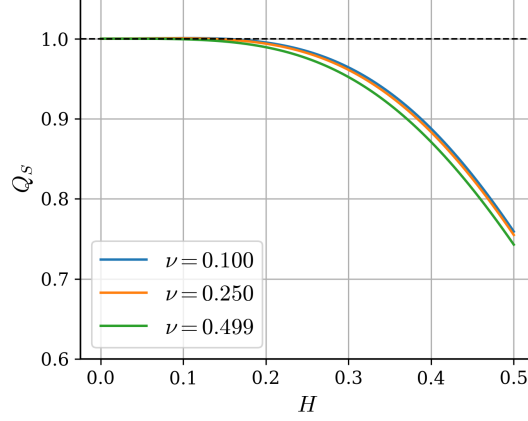


Figure 3.4: Normalized numerical velocity Q_S as function of H , for different values of the Poisson ratio ν , with $\theta = 0^\circ$ and $\gamma = 0.75$, showing the weak dependence of Q_S on the Poisson ratio as the fluid limit $\nu \rightarrow 0.5$ is approached.

propagation velocity in the domain.

- Figure 3.2 shows that the numerical dispersion depends on the propagation direction, with larger deviations observed for smaller values of θ . This indicates that numerical anisotropy is maximal along the coordinate axes ($\theta = 0^\circ$) and minimal for $\theta = 45^\circ$.
- Figure 3.3 suggests that the scheme can be operated at relatively large fractions of the stability limit, i.e., $\gamma \leq 0.75$, while still maintaining negligible dispersion errors for $H \approx 0.2$.
- Finally, unlike in standard finite-difference schemes on collocated grids (see, e.g., chapter 2 in [3]), equation (3.12) shows that Q_P is independent of the Poisson ratio ν , while figure 3.4 indicates that Q_S exhibits only a weak dependence on ν and remains below unity. Moreover, no degeneracy is observed as $\nu \rightarrow 0.5$, indicating that the scheme remains well behaved in presence of fluid regions and fluid-solid interfaces.

In agreement with the above analysis, in order to ensure both numerical stability and negligible dispersion, the parameters γ and H are chosen so that

$$\gamma \leq \gamma_{\max} = 0.75, \quad H \leq H_{\max} = 0.2 \quad (3.14)$$

Once admissible values of H and γ have been selected, the grid spacing is defined as

$$h = H \lambda_{\min} = H \frac{V_{\min}}{f_{\max}} \quad (3.15)$$

where $f_{\max}$ denotes the maximum frequency significantly excited by the source, and $V_{\min}$ is the minimum non-zero propagation velocity in the computational domain. The time step is then defined according to

$$\Delta t = \gamma \frac{6}{7\sqrt{2}} \frac{h}{V_{P,\max}} \quad (3.16)$$

where $V_{P,\max}$ denotes the maximum P-wave velocity in the computational domain. These relations provide a practical guideline for selecting the discretization parameters in the numerical simulations.

3.3. Absorbing boundaries and treatment of heterogeneous elastic parameters

In this section, we discuss two additional aspects of the numerical scheme that are essential in practical simulations. First, we describe the treatment of the artificial boundaries of the computational domain through absorbing layers. We then present the interpolation strategy adopted for the elastic parameters on the staggered grid in heterogeneous media.

3.3.1. Sponge layer absorbing boundaries

In practice, the numerical simulation of wave propagation in an infinite medium is not feasible, and the computational domain Ω must necessarily be bounded. As a consequence, the so-called artificial boundaries of the domain may, if not properly treated, generate spurious reflections that contaminate the numerical solution. In order to mimic wave propagation in an unbounded medium and suppress such non-physical reflections, it is common practice to introduce absorbing layers surrounding the artificial boundaries of the computational domain. Among the various techniques proposed in the literature, we adopt in this work the so-called sponge layer (or Gaussian taper) approach, originally introduced by Cerjan et al. [5], as it provides a good compromise between implementation simplicity and effectiveness in attenuating spurious reflections.

The sponge-layer technique consists in introducing a multiplicative damping profile that smoothly attenuates the wave-field as it approaches the artificial boundaries of the computational domain.

Let $L > 0$ and let $x \in (0, L)$. In one dimension, we denote by d the distance from the nearest absorbing boundary. For instance, if absorbing layers are introduced at both ends

of the interval, one has

$$d : [0, L] \rightarrow [0, L/2], \quad d(x) = \min(x, L - x)$$

Let $\ell > 0$, with $\ell \ll L$, denote the thickness of the absorbing layer. We define the normalized distance

$$s : [0, \ell] \rightarrow [0, 1], \quad s(d) = \frac{\ell - d}{\ell}$$

so that $s = 0$ at the interface between the physical domain and the absorbing layer, and $s = 1$ at the computational boundary.

The damping profile is then defined as

$$\alpha : [0, L] \rightarrow (0, 1], \quad \alpha(d) = \begin{cases} e^{-\alpha_0^2 s(d)^2} & d \leq \ell \\ 1 & d > \ell \end{cases}$$

where $\alpha_0 > 0$ controls the strength of the damping.

Finally, the sponge profile in the physical space is obtained by composition as

$$G : [0, L] \rightarrow (0, 1], \quad G(x) = \alpha(d(x))$$

In two dimensions, for a rectangular domain $\Omega = (0, L_x) \times (0, L_z)$, the damping is applied independently along each coordinate direction. Denoting by $d_x(x)$ and $d_z(z)$ the distances from the absorbing boundaries along the x - and z -directions, respectively, the two-dimensional sponge mask is constructed as

$$G : \Omega \rightarrow (0, 1], \quad G(x, z) = \alpha(d_x(x)) \alpha(d_z(z))$$

This approach naturally handles the damping at the corners of the domain, where the attenuation contributions from each coordinate direction overlap.

At each time step, all field variables are multiplied by the sponge mask at their respective collocation points. In particular, the velocity components are first damped and then used to update the stress components. This ordering ensures that the damping consistently affects both velocity and stress fields, leading to an effective attenuation of outgoing waves before they reach the artificial boundaries. The parameters ℓ and α_0 are problem-dependent and must be chosen empirically in order to balance reflection suppression and computational cost.

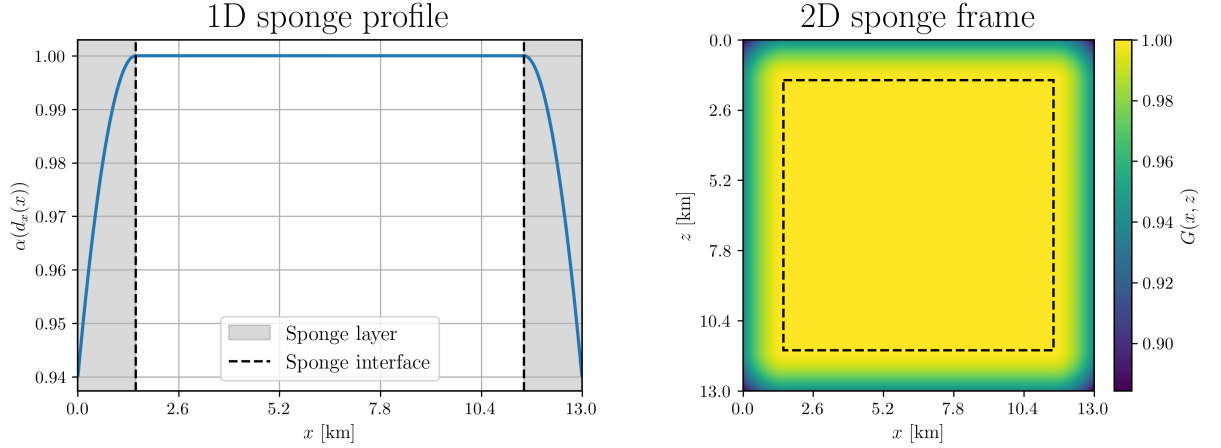


Figure 3.5: Illustration of the sponge-layer damping strategy. Left: one-dimensional sponge profile along the x -direction, $\alpha(d_x(x))$, with the shaded regions denoting the absorbing layers. Right: corresponding two-dimensional absorbing frame $G(x, z)$, obtained as the product of the damping profiles along the two coordinate directions. The dashed square delimits the inner physical domain.

3.3.2. Treatment of heterogeneous elastic parameters on a staggered grid

In heterogeneous media, the material parameters must be consistently defined at the staggered grid locations where the field variables are evaluated. Following the approach proposed by Moczo et al. [29], the values of the material parameters are obtained by considering local volume averages of the governing equations, leading to an equivalent medium representation at the staggered grid scale.

Within this framework, the density ρ is averaged arithmetically over the cell volume, while the second Lamé modulus μ and the two-dimensional bulk modulus $\kappa = \lambda + \mu$ are averaged harmonically, namely

$$R(x, z) = \frac{1}{h_x h_z} \int_{x-h_x/2}^{x+h_x/2} \int_{z-h_z/2}^{z+h_z/2} \rho(\xi, \eta) d\eta d\xi$$

$$M(x, z) = \left(\frac{1}{h_x h_z} \int_{x-h_x/2}^{x+h_x/2} \int_{z-h_z/2}^{z+h_z/2} \frac{1}{\mu(\xi, \eta)} d\eta d\xi \right)^{-1}$$

$$K(x, z) = \left(\frac{1}{h_x h_z} \int_{x-h_x/2}^{x+h_x/2} \int_{z-h_z/2}^{z+h_z/2} \frac{1}{\kappa(\xi, \eta)} d\eta d\xi \right)^{-1}$$

and the first Lamé modulus λ can be reconstructed as

$$L(x, z) = K(x, z) - M(x, z)$$

This choice is consistent with the continuity of displacement and traction across material interfaces.

In the present work, the material parameters are assumed to be stored at the cell centers, and the integrals above are accordingly approximated by suitable averages of their values at the neighboring cell centers.

Therefore, the values of the density at the vertical edge centers, collocation points of the degrees of freedom of the horizontal component of the velocity, are assigned through the arithmetic average of its values at the centers of the left and right neighboring cells

$$R(x_i, z_{j+1/2}) = \frac{1}{2} \left(\rho(x_{i+1/2}, z_{j+1/2}) + \rho(x_{i-1/2}, z_{j+1/2}) \right), \quad \forall (i, j) \in \Sigma^{(v)}$$

and are denoted by $R_{i,j+1/2}$.

Similarly, the values of the density at the horizontal edge centers, collocation points of the degrees of freedom of the vertical component of the velocity, are assigned through the arithmetic average of its values at the centers of the upper and lower neighboring cells

$$R(x_{i+1/2}, z_j) = \frac{1}{2} \left(\rho(x_{i+1/2}, z_{j+1/2}) + \rho(x_{i+1/2}, z_{j-1/2}) \right), \quad \forall (i, j) \in \Sigma^{(h)}$$

and are denoted by $R_{i+1/2,j}$.

Analogously, the values of the second Lamé modulus at the cell vertices, collocation points of the degrees of freedom of the off-diagonal components of the stress tensor, are assigned through the harmonic average of its value at the centers of the four neighboring cells

$$M(x_i, z_j) = \frac{4}{\frac{1}{\mu(x_{i+1/2}, z_{j+1/2})} + \frac{1}{\mu(x_{i+1/2}, z_{j-1/2})} + \frac{1}{\mu(x_{i-1/2}, z_{j+1/2})} + \frac{1}{\mu(x_{i-1/2}, z_{j-1/2})}}, \quad \forall (i, j) \in \Sigma^{(n)}$$

and are denoted by $M_{i,j}$.

Finally, since the cell centers coincide with the collocation points of the diagonal components of the stress tensor, the values of the Lamé moduli there require no averaging and coincide with the stored parameter values, namely

$$M(x_{i+1/2}, z_{j+1/2}) = \mu(x_{i+1/2}, z_{j+1/2}), \quad \forall (i, j) \in \Sigma^{(c)}$$

$$L(x_{i+1/2}, z_{j+1/2}) = \kappa(x_{i+1/2}, z_{j+1/2}) - \mu(x_{i+1/2}, z_{j+1/2}) = \lambda(x_{i+1/2}, z_{j+1/2}), \quad \forall (i, j) \in \Sigma^{(c)}$$

and are denoted by $M_{i+1/2,j+1/2}$ and $L_{i+1/2,j+1/2}$, respectively.

4 | Mathematical foundations of the P–S elastic wave-field separation

The purpose of this chapter is to establish the mathematical framework underlying the P–S decomposition of the elastic wave-field, which constitutes the core tool employed in the subsequent analysis and numerical developments.

We begin by addressing the well-posedness of the elastic wave equation within an abstract functional setting. In particular, we recall a general existence and uniqueness result for second-order linear evolutionary equations and discuss its applicability to the elastodynamic system in its *displacement-only formulation*, under suitable assumptions on the material parameters. This justifies interpreting the wave-field as a well-defined element of an appropriate function space, and for interpreting it consistently within a variational framework.

The second part of the chapter is devoted to the *Helmholtz–Weyl decomposition theorem*. We present this result as an orthogonal decomposition of vector fields into irrotational and solenoidal components, in a form suitable for the analysis of elastic wave-fields. This decomposition provides a natural framework for defining the P–S separation as a projection of the elastic wave-field onto the corresponding subspaces. In particular, compressional P-waves are associated with the irrotational component of the field, while shear S-waves correspond to its solenoidal part, consistently with the physical interpretation discussed in chapter 2.2.

It will also be emphasized that, while the decomposition itself is well defined once the functional setting is fixed, its interpretation in terms of P and S components is not uniquely determined without additional modeling choices, a fact that plays a crucial role in practical implementations of wave-field separation. This aspect will be discussed in more detail in the following chapters, where the decomposition will be connected to the solution of auxiliary Poisson problems.

The numerical approximation introduced in chapter 3 leverages the first-order *velocity–stress formulation*, which is particularly well suited for staggered-grid finite-difference discretizations in heterogeneous media. However, in this chapter, we discuss theoretical results relying on the *displacement-only formulation* because it provides a more natural framework for the variational analysis of the elastic wave equation and for the functional characterization of the Helmholtz–Weyl decomposition. The two formulations represent equivalent descriptions of the same physical model and can be formally related by introducing the velocity as an auxiliary variable and rewriting the second-order system as a first-order evolutionary problem (see section 2.1). Their connection at the discrete level will be made explicit in section 5.2.1, where the numerical implementation of the first wave-field separation strategy is introduced.

4.1. Well-posedness of the elastic wave equation

In this section, we first recall a general existence and uniqueness result for abstract second-order linear evolutionary equations, and then specialize it to the elastic wave equation.

4.1.1. Existence and uniqueness theorem for abstract second order linear evolutionary PDEs

We start by stating a classical well-posedness result for abstract second-order linear evolutionary equations in Hilbert spaces. We refer to chapter 8 in [24] and chapter 7.2 in [10] for detailed treatments, and to chapter 10.3 in [4] for a concise formulation; see also chapter 7.3 in [12].

Let $(V, (\cdot, \cdot)_V)$ and $(H, (\cdot, \cdot)_H)$ be separable Hilbert spaces, $V \subset H$, such that V is dense in H and the embedding $V \hookrightarrow H$ is continuous. Identifying H with its dual H^* by means of the *Riesz representation theorem for Hilbert spaces* (see appendix B, theorem B.3), we obtain the so-called Hilbert triplet

$$V \hookrightarrow H \cong H^* \hookrightarrow V^* \quad (4.1)$$

where V^* denotes the dual space of V .

Let now $T > 0$ and set $I = (0, T) \subset \mathbb{R}_+$. For each $t \in \bar{I}$, let

$$a(t) : V \times V \rightarrow \mathbb{R} \quad (4.2)$$

be a bilinear form such that

- For every $u, v \in V$, the map $a(\cdot; u, v)$ is continuously differentiable, that is

$$a(\cdot; u, v) \in C^1(\bar{I}), \quad \forall u, v \in V$$

- For every $t \in \bar{I}$, the form $a(t; \cdot, \cdot)$ is symmetric, i.e.

$$a(t; u, v) = a(t; v, u), \quad \forall u, v \in V$$

- The form $a(t; \cdot, \cdot)$ is uniformly continuous (i.e., bounded), namely there exists $M > 0$ such that

$$|a(t; u, v)| \leq M \|u\|_V \|v\|_V, \quad \forall u, v \in V, \quad \forall t \in \bar{I}$$

- The form $a(t; \cdot, \cdot)$ is uniformly weakly coercive, i.e., there exist $\lambda, \alpha > 0$ such that

$$a(t; u, u) + \lambda \|u\|_H^2 \geq \alpha \|u\|_V^2, \quad \forall u \in V, \quad \forall t \in \bar{I}$$

We can now state the classical existence and uniqueness result for abstract second-order linear evolutionary equations, in the formulation proposed by Brezis (see chapter 10 in [4], theorem 10.14).

Theorem 4.1 (Well-posedness of abstract second-order linear evolutionary equations). *Let us consider the Hilbert triplet (4.1) and the bilinear form (4.2), satisfying all the assumptions stated above. Moreover, let*

$$f \in L^2(I; H), \quad u_0 \in V, \quad v_0 \in H$$

Then, there exists a unique function u such that

$$u \in C(\bar{I}; V), \quad \frac{\partial u}{\partial t} \in C(\bar{I}; H), \quad \frac{\partial^2 u}{\partial t^2} \in L^2(I; V^*)$$

which is a weak solution of the problem

$$\begin{cases} \left\langle \frac{\partial^2 u}{\partial t^2}(t), v \right\rangle_{V^*, V} + a(t; u(t), v) = (f(t), v)_H & \text{for a.e. } t \in I, \quad \forall v \in V \\ u(0) = u_0 & \text{in } V \\ \frac{\partial u}{\partial t}(0) = v_0 & \text{in } H \end{cases}$$

where $\langle \cdot, \cdot \rangle_{V^*, V}$ denotes the duality pairing between V^* and V .

Remark 4.1. We use standard notation for Bochner spaces and time-dependent function spaces. In particular, for a Banach space X , the space $L^2(I; X)$ denotes the set of square-integrable functions from $I = (0, T)$ into X in the Bochner sense, while $C(\bar{I}; X)$ denotes the space of functions that are continuous from $\bar{I} = [0, T]$ into X with respect to the norm of X .

4.1.2. Application to the elastic wave equation

We now specialize theorem 4.1 to the elastic wave equation in linear elastic and isotropic media, written in its *displacement-only formulation* introduced in (2.3), under homogeneous Dirichlet boundary conditions and zero initial data.

Let $\Omega \subset \mathbb{R}^n$, with $n = 2, 3$, be a bounded domain, such that $\partial\Omega \in \text{Lip}$; let $T > 0$ and set $I = (0, T)$. We consider the following problem:

$$\begin{cases} \rho \frac{\partial^2 \underline{u}}{\partial t^2} - \operatorname{div} \left(2\mu \bar{\varepsilon}(\underline{u}) + \lambda \operatorname{div}(\underline{u}) \bar{\mathbf{I}} \right) = \underline{f} & \text{in } I \times \Omega \\ \underline{u} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{u} = \frac{\partial \underline{u}}{\partial t} = \underline{0} & \text{in } \{0\} \times \bar{\Omega} \end{cases} \quad (4.3)$$

In order to recast problem (4.3) into the abstract framework of theorem 4.1, we introduce the Hilbert spaces

$$V = [H_0^1(\Omega)]^n, \quad H = [L^2(\Omega)]^n$$

endowed with the standard $[H^1(\Omega)]^n$ and $[L^2(\Omega)]^n$ scalar products, respectively.

We assume that the material parameters satisfy the following boundedness and positivity conditions:

$$\begin{aligned} \rho &\in L^\infty(\Omega), \quad \exists \rho_0 > 0 \text{ such that } \rho(\underline{x}) \geq \rho_0 \text{ a.e. in } \Omega \\ \mu &\in L^\infty(\Omega), \quad \exists \mu_0 > 0 \text{ such that } \mu(\underline{x}) \geq \mu_0 \text{ a.e. in } \Omega \\ \lambda &\in L^\infty(\Omega), \quad \exists \kappa_0 > 0 \text{ such that } \lambda(\underline{x}) + \frac{2}{n}\mu(\underline{x}) \geq \kappa_0 \text{ a.e. in } \Omega \end{aligned}$$

As for the forcing term, we assume

$$\underline{f} \in L^2(I; H)$$

Since $\rho(\underline{x}) \geq \rho_0 > 0$ a.e. in Ω , equation (4.3) can be equivalently rewritten by dividing both sides by ρ , yielding a form consistent with the abstract framework. The resulting weak formulation reads

$$\begin{cases} \left\langle \frac{\partial^2 \underline{u}}{\partial t^2}(t), \underline{v} \right\rangle_{V^*, V} + a(\underline{u}(t), \underline{v}) = \left(\frac{1}{\rho} \underline{f}(t), \underline{v} \right)_H & \text{for a.e. } t \in I, \forall \underline{v} \in V \\ \underline{u}(0) = \underline{0} & \text{in } V \\ \frac{\partial \underline{u}}{\partial t}(0) = \underline{0} & \text{in } H \end{cases} \quad (4.4)$$

where the form $a : V \times V \rightarrow \mathbb{R}$ is defined by

$$a(\underline{u}, \underline{v}) = \int_{\Omega} \left(\frac{2\mu}{\rho} \bar{\bar{\varepsilon}}(\underline{u}) : \bar{\bar{\varepsilon}}(\underline{v}) + \frac{\lambda}{\rho} \operatorname{div}(\underline{u}) \operatorname{div}(\underline{v}) \right) d\Omega \quad (4.5)$$

It remains to verify that a satisfies the assumptions of theorem 4.1. From (4.5), it follows that a is bilinear, symmetric, and time-independent. Therefore, it suffices to establish its (uniform) continuity and weak coercivity.

We start by proving the (uniform) continuity of the bilinear form a . Let $\underline{u}, \underline{v} \in V$, then, thanks to the boundedness and positivity assumptions on the material parameters, and by applying the *Cauchy–Schwarz inequality*, we obtain

$$|a(\underline{u}, \underline{v})| \leq \frac{2 \|\mu\|_{L^\infty(\Omega)}}{\rho_0} \|\bar{\bar{\varepsilon}}(\underline{u})\|_{L^2(\Omega)} \|\bar{\bar{\varepsilon}}(\underline{v})\|_{L^2(\Omega)} + \frac{\|\lambda\|_{L^\infty(\Omega)}}{\rho_0} \|\operatorname{div}(\underline{u})\|_{L^2(\Omega)} \|\operatorname{div}(\underline{v})\|_{L^2(\Omega)}$$

For notational simplicity, we denote by $\|\cdot\|_{L^p(\Omega)}$, $p \in [1, +\infty]$, the L^p norm of scalar, vector, and tensor fields, the meaning being clear from the context. Using standard inequalities following directly from the definitions of the symmetric gradient and the divergence, we have for all $\underline{v} \in V$:

$$\|\bar{\bar{\varepsilon}}(\underline{v})\|_{L^2(\Omega)} \leq \|\nabla \underline{v}\|_{L^2(\Omega)}, \quad \|\operatorname{div}(\underline{v})\|_{L^2(\Omega)} \leq \sqrt{n} \|\nabla \underline{v}\|_{L^2(\Omega)}$$

Hence, by definition of the norm in V , we obtain

$$|a(\underline{u}, \underline{v})| \leq \frac{1}{\rho_0} \left(2 \|\mu\|_{L^\infty(\Omega)} + n \|\lambda\|_{L^\infty(\Omega)} \right) \|\underline{u}\|_V \|\underline{v}\|_V$$

which proves the (uniform) continuity of the bilinear form a .

We now prove the (uniform) coercivity of the bilinear form a . Let $\underline{u} \in V$, then

$$a(\underline{u}, \underline{u}) = \int_{\Omega} \left(\frac{2\mu}{\rho} |\bar{\bar{\varepsilon}}(\underline{u})|^2 + \frac{\lambda}{\rho} \operatorname{div}(\underline{u})^2 \right) d\Omega \quad (4.6)$$

Exploiting the isotropic-deviatoric decomposition of the strain tensor

$$\bar{\bar{\varepsilon}}(\underline{u}) = \operatorname{iso}(\bar{\bar{\varepsilon}}(\underline{u})) + \operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u})) = \frac{1}{n} \operatorname{div}(\underline{u}) \bar{\mathbf{I}} + \operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u}))$$

and, since the isotropic and deviatoric components are orthogonal with respect to the $[L^2(\Omega)]^{n \times n}$ scalar product, we get

$$|\bar{\bar{\varepsilon}}(\underline{u})|^2 = |\operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u}))|^2 + \frac{1}{n} \operatorname{div}(\underline{u})^2 \quad (4.7)$$

Substituting this identity into equation (4.6), we find

$$a(\underline{u}, \underline{u}) = \int_{\Omega} \left(\frac{2\mu}{\rho} |\operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u}))|^2 + \frac{1}{\rho} \left[\lambda + \frac{2}{n} \mu \right] \operatorname{div}(\underline{u})^2 \right) d\Omega$$

Thanks to the boundedness and positivity assumptions on the material parameters, we obtain

$$a(\underline{u}, \underline{u}) \geq \frac{\min\{2\mu_0, \kappa_0\}}{\|\rho\|_{L^\infty(\Omega)}} \int_{\Omega} \left(|\operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u}))|^2 + \operatorname{div}(\underline{u})^2 \right) d\Omega$$

On the other hand, from (4.7), it follows that

$$|\operatorname{dev}(\bar{\bar{\varepsilon}}(\underline{u}))|^2 + \operatorname{div}(\underline{u})^2 \geq |\bar{\bar{\varepsilon}}(\underline{u})|^2$$

Hence, we infer

$$a(\underline{u}, \underline{u}) \geq \frac{\min\{2\mu_0, \kappa_0\}}{\|\rho\|_{L^\infty(\Omega)}} \|\bar{\bar{\varepsilon}}(\underline{u})\|_{L^2(\Omega)}^2$$

Finally, thanks to *Korn's inequality* (see appendix B, theorem B.4), we conclude

$$a(\underline{u}, \underline{u}) \geq C_K \frac{\min\{2\mu_0, \kappa_0\}}{\|\rho\|_{L^\infty(\Omega)}} \|\underline{u}\|_V^2$$

which proves that a is (uniformly) coercive, and, therefore, also (uniformly) weakly coercive.

Thus, all the assumptions of theorem 4.1 are satisfied. Hence, problem (4.4) admits a

unique weak solution $\underline{u}$ such that

$$\underline{u} \in C(\bar{I}; V), \quad \frac{\partial \underline{u}}{\partial t} \in C(\bar{I}; H), \quad \frac{\partial^2 \underline{u}}{\partial t^2} \in L^2(I; V^*) \quad (4.8)$$

Remark 4.2 (Interpretation of the well-posedness result).

The previous result provides a rigorous well-posedness framework for the elastic wave equation in the displacement-only formulation under homogeneous Dirichlet boundary conditions and almost everywhere strictly positive shear modulus μ .

In the remainder of this work, however, we consider more general configurations arising in numerical simulations — such as free surface boundary conditions, absorbing layers, and heterogeneous media possibly containing fluid regions where $\mu = 0$ — in which the displacement field is instead obtained from the first-order velocity–stress formulation.

In this broader setting, the resulting wave-field may fall outside the functional framework of theorem 4.1. Nevertheless, the above result serves as a rigorous reference model, ensuring that, under standard physical assumptions, the displacement field can be interpreted as a well-defined and sufficiently regular object.

This justifies, at a formal level, the use of variational arguments and differential operators in the subsequent analysis, where analogous regularity properties are assumed for the displacement field reconstructed from the numerical solution.

4.2. Helmholtz–Weyl decomposition theorem and its application to P–S elastic wave-field separation

We begin by recalling the *Helmholtz–Weyl decomposition theorem*, which characterizes the orthogonal splitting of vector fields into irrotational and solenoidal components. This decomposition will play a central role in the formulation of the P–S separation of the elastic wave-field.

4.2.1. Helmholtz–Weyl decomposition theorem

We now state the *Helmholtz–Weyl decomposition theorem* for vector fields. We adopt the formulation of theorem 7.1.16 in [12], which is based on the classical result in chapter 1 of [37].

Theorem 4.2 (Helmholtz–Weyl decomposition).

Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$ be open, bounded and connected, such that $\partial\Omega \in \text{Lip}$. Then

$$[L^2(\Omega)]^n = G_1(\Omega) \oplus G_2(\Omega) \oplus G_3(\Omega)$$

Equivalently,

$$\forall \underline{u} \in [L^2(\Omega)]^n, \exists! (\underline{u}_1, \underline{u}_2, \underline{u}_3) \in G_1(\Omega) \times G_2(\Omega) \times G_3(\Omega) \mid \underline{u} = \underline{u}_1 + \underline{u}_2 + \underline{u}_3$$

Moreover,

$$G_i(\Omega) \perp G_j(\Omega), \text{ in } [L^2(\Omega)]^n, \quad \forall i \neq j, \quad i, j \in \{1, 2, 3\}$$

where

$$G_1(\Omega) = \{ \underline{v} \in [L^2(\Omega)]^n \mid \operatorname{div}(\underline{v}) = 0, \gamma_\nu(\underline{v}) = 0 \}$$

$$G_2(\Omega) = \{ \underline{v} \in [L^2(\Omega)]^n \mid \operatorname{div}(\underline{v}) = 0, \exists h \in H^1(\Omega) \text{ s.t. } \underline{v} = \nabla h \}$$

$$G_3(\Omega) = \{ \underline{v} \in [L^2(\Omega)]^n \mid \exists g \in H_0^1(\Omega) \text{ s.t. } \underline{v} = \nabla g \}$$

and $\gamma_\nu : H_{\operatorname{div}}(\Omega) \rightarrow H^{-1/2}(\partial\Omega)$ denotes the normal trace operator.

The *Helmholtz–Weyl decomposition theorem* states that every vector field $\underline{u} \in [L^2(\Omega)]^n$ can be uniquely decomposed as the sum of three mutually orthogonal components, each with a clear mathematical characterization. More precisely:

- $\underline{u}_1 \in G_1(\Omega)$ is solenoidal, indeed $\operatorname{div}(\underline{u}_1) = 0$, with vanishing normal trace on $\partial\Omega$;
- $\underline{u}_3 \in G_3(\Omega)$ is irrotational, since $\underline{u}_3 = \nabla g$ for some $g \in H_0^1(\Omega)$, and therefore $\operatorname{curl}(\underline{u}_3) = \underline{0}$;
- $\underline{u}_2 \in G_2(\Omega)$ is both solenoidal, indeed $\operatorname{div}(\underline{u}_2) = 0$, and irrotational, since $\underline{u}_2 = \nabla h$ for some $h \in H^1(\Omega)$, and therefore $\operatorname{curl}(\underline{u}_2) = \underline{0}$.

In particular, $\Delta h = \operatorname{div}(\nabla h) = \operatorname{div}(\underline{u}_2) = 0$, so this component is referred to as the *harmonic-gradient* contribution.

4.2.2. Application to the elastic P–S wave-field separation

We now describe how the Helmholtz–Weyl decomposition can be employed for the P–S separation of an elastic wave-field.

First, we fix a time $t \in I$ and extract a snapshot of the wave-field, that is, we consider the vector field $\underline{u} = \underline{u}(t)$. Owing to the regularity properties established in section 4.1.2,

and consistently with remark 4.2, the pointwise evaluation in time is well-defined and the field $\underline{u}(t)$ can be regarded as belonging to a suitable space $V \subset [H^1(\Omega)]^n$, namely

$$\underline{u}(t) \in V \subset [H^1(\Omega)]^n \quad (4.9)$$

and hence, in particular, $\underline{u}(t) \in [L^2(\Omega)]^n$.

Under these assumptions, the *Helmholtz–Weyl decomposition theorem* (4.2) applies and yields

$$\underline{u} = \underline{u}_1 + \underline{u}_2 + \underline{u}_3, \quad \underline{u}_i \in G_i(\Omega), \quad i = 1, 2, 3 \quad (4.10)$$

Following the physical interpretation introduced in section 2.2, we identify the P-wave component with the irrotational part of the displacement field, $\underline{u}_P$, and the S-wave component with the solenoidal part, $\underline{u}_S$. Let us denote by $\mathcal{U}_P$ and $\mathcal{U}_S$ the corresponding subspaces, i.e.,

$$\mathcal{U}_P, \mathcal{U}_S \subset [L^2(\Omega)]^n, \quad \underline{u}_P \in \mathcal{U}_P, \quad \underline{u}_S \in \mathcal{U}_S$$

Therefore, consistently with the mathematical characterization discussed at the end of section 4.2.1, we consider

$$G_3(\Omega) \subset \mathcal{U}_P, \quad G_1(\Omega) \subset \mathcal{U}_S$$

However, the component $\underline{u}_2 \in G_2(\Omega)$ is both irrotational and solenoidal. This gives rise to an intrinsic ambiguity in the definition of the P and S subspaces. Two natural choices are possible. Either

$$\mathcal{U}_P = G_2(\Omega) \oplus G_3(\Omega), \quad \mathcal{U}_S = G_1(\Omega) \quad (4.11)$$

meaning that

$$\underline{u}_P = \underline{u}_2 + \underline{u}_3, \quad \underline{u}_S = \underline{u}_1$$

or

$$\mathcal{U}_P = G_3(\Omega), \quad \mathcal{U}_S = G_1(\Omega) \oplus G_2(\Omega) \quad (4.12)$$

that is

$$\underline{u}_P = \underline{u}_3, \quad \underline{u}_S = \underline{u}_1 + \underline{u}_2$$

both of which are consistent with the above physical interpretation and mathematical characterization.

For the moment, we keep the discussion at a general level. Independently of the specific

choice, the mutual orthogonality of $G_1(\Omega)$, $G_2(\Omega)$ and $G_3(\Omega)$ ensures that

$$[L^2(\Omega)]^n = \mathcal{U}_P \oplus \mathcal{U}_S, \quad \mathcal{U}_P = \mathcal{U}_S^\perp$$

Therefore, by the *orthogonal decomposition theorem* (see appendix B, theorem B.2), the following projection operators are well defined

$$\Pi_P : [L^2(\Omega)]^n \rightarrow \mathcal{U}_P, \quad \underline{u}_P = \Pi_P(\underline{u}) \quad (4.13)$$

$$\Pi_S : [L^2(\Omega)]^n \rightarrow \mathcal{U}_S, \quad \underline{u}_S = \Pi_S(\underline{u}) \quad (4.14)$$

with $\Pi_P + \Pi_S = \text{Id}$, which allow us to extract the P and S components of the displacement field, thus performing the P–S separation of the wave-field $\underline{u} = \underline{u}(t)$.

The role of the *harmonic-gradient* contribution and its impact on the definition of the projectors will be analyzed in the following chapters. In particular, we discuss how the projectors (4.13) and (4.14) can be constructed via auxiliary Poisson problems, and how the assignment of the *harmonic-gradient* contribution to either the P or the S component naturally depends on the boundary conditions of the associated Poisson problems, leading to the two choices (4.11) and (4.12).

5 | P–S separation with non-homogeneous Neumann boundary conditions

In the previous chapter, the P–S wave-field separation has been introduced within a rigorous functional framework, based on the *Helmholtz–Weyl decomposition theorem* 4.2. In particular, the separation has been interpreted as an orthogonal decomposition of the displacement field into irrotational and solenoidal components.

The objective of this chapter is to provide an explicit construction of the corresponding projection operators. In particular, we focus on the case in which the *harmonic-gradient* contribution is included in the P-wave component, corresponding to choice (4.11). In this setting, the construction of the P projector leads to the solution of an auxiliary Poisson problem equipped with non-homogeneous Neumann boundary conditions. This formulation naturally arises from the structure of the *Helmholtz–Weyl decomposition theorem*.

We begin by introducing the Poisson–Neumann problem, discussing its well-posedness and clarifying the physical meaning of the associated non-homogeneous Neumann boundary conditions in the context of P–S wave-field separation. We then address its numerical approximation, focusing on a second-order finite-difference discretization and on the spectral properties of the corresponding discrete operator, which enable an efficient solution strategy based on its diagonalization. Finally, we describe the resulting P–SV separation algorithm and examine the boundary effects induced by the formulation, together with a strategy to mitigate the corresponding artifacts.

5.1. The Poisson–Neumann problem

Let $\underline{u} = \underline{u}(t) \in V \subset [H^1(\Omega)]^n$ be a snapshot of the wave-field, as introduced in (4.9). According to the *Helmholtz–Weyl decomposition theorem* 4.2, the vector field $\underline{u}$ admits

the unique decomposition (4.10), namely

$$\underline{u} = \underline{u}_1 + \underline{u}_2 + \underline{u}_3, \quad \underline{u}_i \in G_i(\Omega), \quad i = 1, 2, 3$$

By definition of the subspaces $G_2(\Omega)$ and $G_3(\Omega)$, the components $\underline{u}_2$ and $\underline{u}_3$ can be written as gradients of scalar potentials, namely

$$\underline{u}_2 = \nabla h, \quad h \in H^1(\Omega), \quad \Delta h = 0$$

$$\underline{u}_3 = \nabla g, \quad g \in H_0^1(\Omega)$$

Therefore, the displacement field can be rewritten as

$$\underline{u} = \underline{u}_1 + \nabla f \tag{5.1}$$

where we introduced the scalar potential

$$f = h + g \in H^1(\Omega)$$

Taking the divergence on both sides of equation (5.1), and recalling that $\underline{u}_1 \in G_1(\Omega)$ is solenoidal, we obtain

$$\operatorname{div}(\underline{u}) = \cancel{\operatorname{div}(\underline{u}_1)} + \operatorname{div}(\nabla f) = \Delta f$$

Hence, the scalar potential f satisfies the following Poisson equation:

$$-\Delta f = -\operatorname{div}(\underline{u}) \quad \text{in } \Omega \tag{5.2}$$

where the equality is understood in the weak sense. Since, by assumption, $\underline{u} \in V \subset [H^1(\Omega)]^n$, it follows that $\operatorname{div}(\underline{u}) \in L^2(\Omega)$, and therefore the distribution $-\Delta f$ is represented by an $L^2(\Omega)$ function.

In order to identify the boundary conditions to be coupled with equation (5.2), let us reconsider decomposition (5.1). First, we observe that, since $\underline{u} \in V \subset [H^1(\Omega)]^n$, it follows that

$$\underline{u} \in H_{\operatorname{div}}(\Omega)$$

Moreover, since $f \in H^1(\Omega)$ and $\Delta f \in L^2(\Omega)$, we also have

$$\nabla f \in H_{\operatorname{div}}(\Omega)$$

Therefore, the normal trace operator is well defined on both $\underline{u}$ and ∇f . Applying the

normal trace operator to both sides of (5.1), and recalling that $\underline{u}_1 \in G_1(\Omega)$ has vanishing normal trace on $\partial\Omega$, we obtain

$$\gamma_\nu(\underline{u}) = \cancel{\gamma_\nu(\underline{u}_1)} + \gamma_\nu(\nabla f) = \gamma_\nu(\nabla f) \quad \text{in } H^{-1/2}(\partial\Omega)$$

At the formal level, this corresponds to the non-homogeneous Neumann boundary condition

$$\nabla f \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} \quad \text{on } \partial\Omega \quad (5.3)$$

where $\hat{\nu}$ denotes the outward normal unit vector to $\partial\Omega$.

Hence, coupling equation (5.2) with boundary condition (5.3), we are naturally led to the following Poisson–Neumann problem

$$\begin{cases} -\Delta f = -\operatorname{div}(\underline{u}) & \text{in } \Omega \\ \nabla f \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} & \text{on } \partial\Omega \end{cases} \quad (5.4)$$

The solution of the Poisson–Neumann problem (5.4) allows us to explicitly construct the P and S components of the wave-field. Indeed, once the scalar potential $f \in H^1(\Omega)$ is determined, we define

$$\underline{u}_P = \nabla f, \quad \underline{u}_S = \underline{u} - \underline{u}_P \quad (5.5)$$

In particular, the mapping $\underline{u} \mapsto \nabla f$ realizes the projection operator Π_P , while the S projector is obtained as $\Pi_S = \operatorname{Id} - \Pi_P$.

We now inspect how the *harmonic-gradient* contribution enters the construction. Recalling that $f = h + g$, with h harmonic, we observe that

$$\Delta f = \Delta g + \cancel{\Delta h} = \Delta g \quad \text{in } \Omega$$

Therefore, the Poisson equation (5.2) only determines g , while the harmonic contribution h is not fixed by the equation itself. On the other hand, the non-homogeneous Neumann boundary conditions (5.3) enforce

$$\nabla f \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} \quad \text{on } \partial\Omega$$

involving the full scalar potential $f = h + g$. As a consequence, the harmonic component h is implicitly determined by the boundary conditions.

Hence, this construction yields

$$\underline{u}_P = \nabla f = \nabla h + \nabla g = \underline{u}_2 + \underline{u}_3$$

$$\underline{u}_S = \underline{u} - \underline{u}_P = (\underline{u}_1 + \underline{u}_2 + \underline{u}_3) - \underline{u}_P = \underline{u}_1$$

so that the *harmonic-gradient* contribution $\underline{u}_2$ is included in the P-wave component, effectively realizing choice (4.11):

$$\underline{u}_P \in \mathcal{U}_P = G_2(\Omega) \oplus G_3(\Omega), \quad \underline{u}_S \in \mathcal{U}_S = G_1(\Omega)$$

This reasoning shows that the assignment of the harmonic component is entirely dictated by the boundary conditions of the auxiliary Poisson problem. This aspect will be crucial in the comparison with the alternative formulation based on homogeneous Dirichlet boundary conditions, where the harmonic component is instead excluded from the P-wave contribution, as we will discuss in chapter 6.

5.1.1. Well-posedness of the Poisson–Neumann problem

In this section, we address the well-posedness of the Poisson–Neumann problem (5.4). In particular, we discuss how the lack of uniqueness can be resolved by a suitable restriction of the space of admissible solutions, leading to a well-posed variational formulation of the problem.

The well-posedness of the Poisson–Neumann problem is classical; see, e.g., theorem 4.10 in [27] for a fully general treatment, and chapter 7.1.3 in [12] for a formulation closer to the present setting.

Theorem 5.1 (Well-posedness of the Poisson–Neumann problem).

Let $\Omega \subset \mathbb{R}^n$, open and bounded, such that $\partial\Omega \in Lip$. Moreover, let

$$b \in L^2(\Omega), \quad g \in H^{-1/2}(\partial\Omega)$$

Then, the problem

$$\begin{cases} -\Delta f = b & \text{in } \Omega \\ \nabla f \cdot \hat{\nu} = g & \text{on } \partial\Omega \end{cases}$$

admits a weak solution $f \in H^1(\Omega)$ if and only if the following compatibility condition is satisfied:

$$\int_{\Omega} b \, d\Omega + \langle g, 1 \rangle = 0$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$.

Moreover, in this case, the weak solution is not unique: if $f \in H^1(\Omega)$ is a weak solution, then the set of weak solutions can be written as

$$\{f + c \mid c \in \mathbb{R}\}$$

In the present framework, the data of the problem (5.4) are

$$b = -\operatorname{div}(\underline{u}) \in L^2(\Omega), \quad g = \gamma_\nu(\underline{u}) \in H^{-1/2}(\partial\Omega)$$

Moreover, the compatibility condition is trivially verified by the *generalized Gauss–Green formula* (see appendix B, theorem B.5), indeed

$$-\int_{\Omega} \operatorname{div}(\underline{u}) \, d\Omega = \langle \gamma_\nu(\underline{u}), 1 \rangle \implies \int_{\Omega} b \, d\Omega + \langle g, 1 \rangle = 0$$

Therefore, the Poisson–Neumann problem (5.4) admits infinitely many weak solutions $f \in H^1(\Omega)$, defined up to an additive constant $c \in \mathbb{R}$.

This indeterminacy can be easily removed by imposing a normalization condition, which implicitly fixes the additive constant c , that is, by restricting the space of admissible weak solutions. The choice of a specific c among the infinitely many admissible ones does not affect the decomposition, since the P-component is defined as $\underline{u}_P = \nabla f$, and is therefore invariant under the addition of a constant to f . A common approach is to seek solutions with zero average, leading to the following space of admissible weak solutions:

$$H_*^1(\Omega) = \left\{ f \in H^1(\Omega) \mid \int_{\Omega} f \, d\Omega = 0 \right\}$$

In this setting, the Poisson–Neumann problem becomes well-posed. Indeed, by restricting the solution space to $H_*^1(\Omega)$, existence and uniqueness follow directly from the *Lax–Milgram lemma* (see appendix B, theorem B.6). More precisely, the weak formulation of problem (5.4) reads as follows:

Find $f \in H_*^1(\Omega)$ such that

$$\int_{\Omega} \nabla f \cdot \nabla v \, d\Omega = \int_{\Omega} \underline{u} \cdot \nabla v \, d\Omega, \quad \forall v \in H_*^1(\Omega)$$

where the right-hand side is obtained by combining the divergence and boundary terms through the *generalized Gauss–Green formula*.

First, we observe that $H_*^1(\Omega)$ is a Hilbert space. Indeed, consider the functional

$$L : H^1(\Omega) \rightarrow \mathbb{R}, \quad L(v) = \int_{\Omega} v \, d\Omega$$

Since L is linear and continuous, its kernel

$$\ker(L) = \left\{ v \in H^1(\Omega) \mid \int_{\Omega} v \, d\Omega = 0 \right\} = H_*^1(\Omega)$$

is a closed subspace of $H^1(\Omega)$. Therefore, $H_*^1(\Omega)$ is complete with respect to the norm induced by the H^1 inner product, and hence it is a Hilbert space.

Then, we need to show the continuity and coercivity of the bilinear form

$$a : H_*^1(\Omega) \times H_*^1(\Omega) \rightarrow \mathbb{R}, \quad a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega$$

The continuity is immediate from the *Cauchy–Schwarz inequality*. Let $u, v \in H_*^1(\Omega)$, then

$$|a(u, v)| \leq \|\nabla u\|_{L^2(\Omega)} \|\nabla v\|_{L^2(\Omega)} \leq \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)}$$

The coercivity, instead, follows from the *Poincaré–Wirtinger inequality* (see appendix B, theorem B.7), which, on $H_*^1(\Omega)$, reduces to the standard *Poincaré inequality*. Let $u \in H_*^1(\Omega)$, then

$$a(u, u) = \|\nabla u\|_{L^2(\Omega)}^2 \geq \frac{1}{C_P^2 + 1} \|u\|_{H^1(\Omega)}^2$$

Finally, we show the continuity of the linear functional

$$F : H_*^1(\Omega) \rightarrow \mathbb{R}, \quad \langle F, v \rangle = \int_{\Omega} \underline{u} \cdot \nabla v \, d\Omega$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $(H_*^1(\Omega))^*$ and $H_*^1(\Omega)$. This follows again from the *Cauchy–Schwarz inequality*. Indeed, for all $v \in H_*^1(\Omega)$,

$$|\langle F, v \rangle| \leq \|\underline{u}\|_{L^2(\Omega)} \|\nabla v\|_{L^2(\Omega)} \leq \|\underline{u}\|_{L^2(\Omega)} \|v\|_{H^1(\Omega)}$$

Hence, by the *Lax–Milgram lemma*, there exists a unique weak solution $f \in H_*^1(\Omega)$, i.e., with zero mean, to the Poisson–Neumann problem (5.4).

5.1.2. Physical interpretation of non-homogeneous Neumann boundary conditions

The physical interpretation of the non-homogeneous Neumann boundary conditions (5.3) is particularly transparent in the context of the P–S wave-field separation.

Recalling that, according to (5.5), the P component of the displacement field is given by $\underline{u}_P = \nabla f$, the non-homogeneous Neumann boundary conditions (5.3) can be equivalently written as

$$\underline{u}_P \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} \quad \text{on } \partial\Omega$$

As a consequence, the S component, defined as $\underline{u}_S = \underline{u} - \underline{u}_P$, satisfies

$$\underline{u}_S \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} - \underline{u}_P \cdot \hat{\nu} = 0 \quad \text{on } \partial\Omega$$

This shows that enforcing the non-homogeneous Neumann boundary conditions (5.3) corresponds to forcing the S-wave component to have a zero normal component at the boundary. As a result, it is purely tangential to $\partial\Omega$. This reflects the defining property of the solenoidal subspace $G_1(\Omega)$, to which $\underline{u}_S$ belongs, whose elements have vanishing normal trace on $\partial\Omega$.

This constraint, which arises from the mathematical formulation, is not physically representative in general, since the S-wave component of the displacement field may exhibit a non-vanishing normal trace at the boundary, as illustrated in figure 5.1. This leads to the following behavior. Consider a displacement field that is purely S, i.e.,

$$\underline{u} = \underline{u}_S, \quad \underline{u}_P = \underline{0}$$

When such an S-wave reaches the boundary of the domain, it generally exhibits a non-vanishing normal component, that is,

$$\underline{u} \cdot \hat{\nu} = \underline{u}_S \cdot \hat{\nu} \neq 0 \quad \text{on } \partial\Omega$$

Although, as discussed in section 2.2, in the ideal case of a purely S-wave, the physical bulk field is approximately solenoidal, i.e., $\text{div}(\underline{u}) = \text{div}(\underline{u}_S) \approx 0$, this non-zero normal component triggers the Poisson–Neumann problem (5.4) through the boundary conditions

$$\nabla f \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} \quad \text{on } \partial\Omega$$

As a consequence, the solution of the Poisson–Neumann problem generates a non-trivial

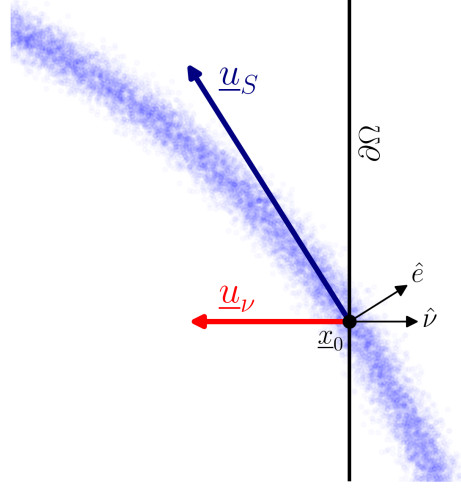


Figure 5.1: Schematic representation of an S-wave impinging on the boundary $\partial\Omega$. The blue cloud represents the local wavefront, whose propagation direction is indicated by the unit propagation vector $\hat{e}$. The associated displacement field $\underline{u}_S$, shown in dark blue, is orthogonal to $\hat{e}$, consistently with the transverse polarization of S-waves. At the point of incidence $\underline{x}_0 \in \partial\Omega$, the displacement generally exhibits a non-vanishing normal component, highlighted in red and given by $\underline{u}_\nu = (\underline{u}_S \cdot \hat{\nu}) \hat{\nu}$, where $\hat{\nu}$ denotes the outward unit normal to the boundary.

scalar potential f , leading to a non-zero P-wave component $\underline{u}_P = \nabla f$, even though the physical field is purely S. This contribution is therefore entirely spurious and is expected to remain localized near the portions of the boundary where the S-wave impinges. Hence, when a purely S-wave interacts with the boundary, one expects the generation of numerical artifacts in the reconstructed P-wave component through this mechanism.

5.2. Numerical solution of the Poisson–Neumann problem

In this section, we address the numerical solution of the Poisson–Neumann problem for the P–S wave-field separation. Restricting the analysis to the two-dimensional setting, the solenoidal component $\underline{u}_S$ coincides with the SV wave-field, and the decomposition takes the form of a P–SV separation.

We first introduce a second-order finite-difference discretization and then exploit the spectral properties of the discrete Neumann Laplacian to construct an efficient solver. The resulting formulation is used to define the complete P–SV separation algorithm, whose computational cost is briefly analyzed.

Finally, we examine the boundary effects induced by the separation approach, together with a strategy to mitigate the corresponding artifacts.

5.2.1. Second-order finite-difference approximation of the Poisson–Neumann problem

We first describe the staggered grid setup for the Poisson problem, and then present a second-order finite-difference discretization under the non-homogeneous Neumann boundary conditions (5.3).

Staggered grid setup for the Poisson problem

The discretization of the Poisson–Neumann problem (5.4) is carried out on the same staggered grid introduced in section 3.1.1, defined over the rectangular computational domain $\Omega = (0, L_x) \times (0, L_z)$.

The numerical scheme introduced in section 3.1.2 discretizes the *velocity–stress formulation* of the elastic wave equation and is therefore formulated in terms of velocity and stress variables. In contrast, the P–S separation described in the previous sections is expressed in terms of the displacement field at a given time instant.

For this reason, the degrees of freedom of the displacement components are reconstructed from those of the corresponding velocity components. This is achieved through a numerical time integration based on the second-order trapezoidal rule. This choice preserves the second-order accuracy in time of the numerical scheme (3.3).

As a consequence, the displacement components are naturally located at the same grid nodes and time levels as the corresponding velocity components. More precisely, they are computed as

$$\begin{aligned} u_{i,j+1/2}^{(x),k+1/2} &= u_{i,j+1/2}^{(x),k-1/2} + \frac{\Delta t}{2} \left(v_{i,j+1/2}^{(x),k+1/2} + v_{i,j+1/2}^{(x),k-1/2} \right), \quad \forall (i, j, k) \in \Sigma^{(v)} \times \Theta^{(h)} \\ u_{i+1/2,j}^{(z),k+1/2} &= u_{i+1/2,j}^{(z),k-1/2} + \frac{\Delta t}{2} \left(v_{i+1/2,j}^{(z),k+1/2} + v_{i+1/2,j}^{(z),k-1/2} \right), \quad \forall (i, j, k) \in \Sigma^{(h)} \times \Theta^{(h)} \end{aligned}$$

To complete the definition, the displacement field is initialized at time level $k = -1/2$ by setting all components to zero. In what follows, we fix a time level $k \in \Theta^{(h)}$ and consider the reconstructed displacement components at that time level, dropping the time superscript for notational convenience.

We now describe the collocation of the degrees of freedom of all the fields involved in the P–SV decomposition.

- The degrees of freedom of the horizontal component of the displacement and of its P and SV contributions are collocated at the centers of the vertical cell edges and are denoted by $u_{i,j+1/2}^{(x)}$, $u_{P,i,j+1/2}^{(x)}$ and $u_{S,i,j+1/2}^{(x)}$, for all $(i, j) \in \Sigma^{(v)}$.
- The degrees of freedom of the vertical component of the displacement and of its P and SV contributions are collocated at the centers of the horizontal edges, and are denoted by $u_{i+1/2,j}^{(z)}$, $u_{P,i+1/2,j}^{(z)}$ and $u_{S,i+1/2,j}^{(z)}$, for all $(i, j) \in \Sigma^{(h)}$.
- The degrees of freedom of the scalar potential are collocated at the cell centers, and are denoted by $f_{i+1/2,j+1/2}$, for all $(i, j) \in \Sigma^{(c)}$.

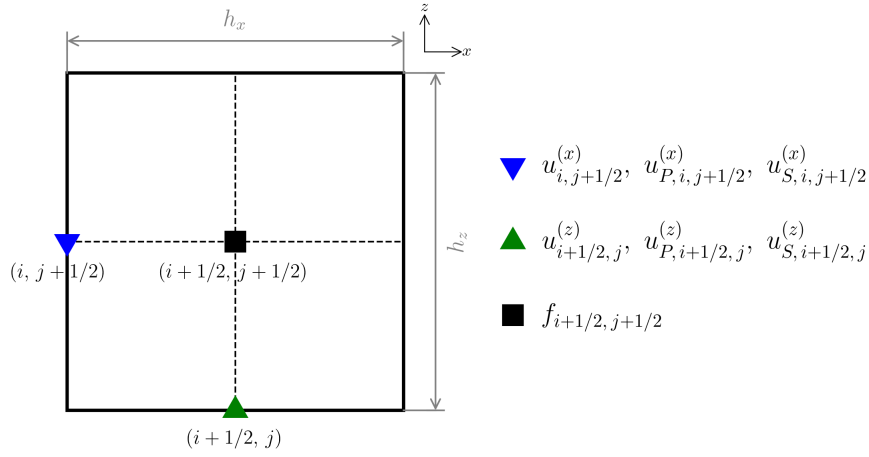


Figure 5.2: Staggered grid arrangement for the auxiliary Poisson problems.

This staggered grid arrangement, illustrated in figure 5.2, will be employed for the numerical solution of all the auxiliary Poisson problems associated with the different separation strategies considered in this work.

Discrete formulation of the Poisson–Neumann problem

The spatial derivatives are approximated by means of a second-order centered finite-difference scheme, obtained by applying in space the same discrete approximation introduced in (3.1). Accordingly, the divergence of the displacement field at the cell centers is approximated by

$$\operatorname{div}_h(\underline{u})_{i+1/2,j+1/2} = \frac{u_{i+1,j+1/2}^{(x)} - u_{i,j+1/2}^{(x)}}{h_x} + \frac{u_{i+1/2,j+1}^{(z)} - u_{i+1/2,j}^{(z)}}{h_z}, \quad \forall (i, j) \in \Sigma^{(c)} \quad (5.6)$$

and the gradient of the scalar potential at the centers of the cell edges by

$$\begin{aligned} (\nabla_h f)_{i,j+1/2}^{(x)} &= \frac{f_{i+1/2,j+1/2} - f_{i-1/2,j+1/2}}{h_x}, \quad \forall (i, j) \in \Sigma^{(v)} \\ (\nabla_h f)_{i+1/2,j}^{(z)} &= \frac{f_{i+1/2,j+1/2} - f_{i+1/2,j-1/2}}{h_z}, \quad \forall (i, j) \in \Sigma^{(h)} \end{aligned} \quad (5.7)$$

Consistently, the Laplacian of the scalar potential at the cell centers is discretized as $\Delta_h = \text{div}_h(\nabla_h)$, explicitly

$$\begin{aligned} (\Delta_h f)_{i+1/2,j+1/2} &= \frac{f_{i+3/2,j+1/2} - 2f_{i+1/2,j+1/2} + f_{i-1/2,j+1/2}}{h_x^2} + \\ &+ \frac{f_{i+1/2,j+3/2} - 2f_{i+1/2,j+1/2} + f_{i+1/2,j-1/2}}{h_z^2}, \quad \forall (i, j) \in \Sigma^{(c)} \end{aligned} \quad (5.8)$$

Thus, the discretization of the Poisson equation (5.2) reads

$$-\Delta_h f_{i+1/2,j+1/2} = -\text{div}_h(\underline{u})_{i+1/2,j+1/2}, \quad \forall (i, j) \in \Sigma^{(c)} \quad (5.9)$$

We now have to impose the non-homogeneous Neumann boundary conditions (5.3). In order to explicitly enforce them, keeping the same centered stencil also at the boundary nodes, we employ the ghost-nodes elimination technique, which reduces to a modification of the discrete equation (5.9) at the boundary nodes.

For illustration, we report the explicit form of the discrete equations at the bottom boundary internal nodes and at the bottom-left corner node. The remaining boundary nodes can be treated analogously.

We first consider the bottom boundary internal nodes, identified by $i = 1, \dots, N_x - 2$, $j = 0$. The ghost values $f_{i+1/2,-1/2}$ appearing in the discrete Laplacian are eliminated by enforcing the Neumann boundary condition through the centered finite-difference approximation introduced above, namely

$$(\nabla_h f)_{i+1/2,0}^{(z)} = u_{i+1/2,0}^{(z)}$$

which yields

$$f_{i+1/2,-1/2} = f_{i+1/2,1/2} - h_z u_{i+1/2,0}^{(z)}$$

Substituting into (5.9), we obtain

$$-\frac{f_{i+3/2,1/2} - 2f_{i+1/2,1/2} + f_{i-1/2,1/2}}{h_x^2} - \frac{f_{i+1/2,3/2} - f_{i+1/2,1/2}}{h_z^2} = -\operatorname{div}_h(\underline{u})_{i+1/2,1/2} - \frac{u_{i+1/2,0}^{(z)}}{h_z}$$

The bottom-left corner node is identified by $i = 0, j = 0$. This node lies at the intersection of the bottom and left boundaries. The ghost values $f_{1/2,-1/2}$ and $f_{-1/2,1/2}$ appearing in the discrete Laplacian are eliminated by enforcing the Neumann boundary conditions associated with the bottom and left boundaries through the centered finite-difference approximation introduced above, namely

$$(\nabla_h f)_{1/2,0}^{(z)} = u_{1/2,0}^{(z)}, \quad (\nabla_h f)_{0,1/2}^{(x)} = u_{0,1/2}^{(x)}$$

which yield

$$f_{1/2,-1/2} = f_{1/2,1/2} - h_z u_{1/2,0}^{(z)}, \quad f_{-1/2,1/2} = f_{1/2,1/2} - h_x u_{0,1/2}^{(x)}$$

Substituting into (5.9), we obtain

$$-\frac{f_{3/2,1/2} - f_{1/2,1/2}}{h_x^2} - \frac{f_{1/2,3/2} - f_{1/2,1/2}}{h_z^2} = -\operatorname{div}_h(\underline{u})_{1/2,1/2} - \left(\frac{u_{0,1/2}^{(x)}}{h_x} + \frac{u_{1/2,0}^{(z)}}{h_z} \right)$$

The previous derivations show that, after elimination of the ghost values, the second-order finite-difference approximation of the Poisson–Neumann problem can be equivalently recast, up to a modification of the right-hand side accounting for the boundary contributions, as a discrete Poisson equation equipped with homogeneous discrete Neumann boundary conditions, namely

$$\begin{cases} -\Delta_h f_{i+1/2,j+1/2} = b_{h,i+1/2,j+1/2} & \forall (i,j) \in \Sigma^{(c)} \\ f_{-1/2,j+1/2} = f_{1/2,j+1/2} & \forall j \in \Sigma_j^{(c)} \\ f_{N_x+1/2,j+1/2} = f_{N_x-1/2,j+1/2} & \forall j \in \Sigma_j^{(c)} \\ f_{i+1/2,-1/2} = f_{i+1/2,1/2} & \forall i \in \Sigma_i^{(c)} \\ f_{i+1/2,N_z+1/2} = f_{i+1/2,N_z-1/2} & \forall i \in \Sigma_i^{(c)} \end{cases} \quad (5.10)$$

This observation is crucial, as it allows one to exploit the spectral diagonalization of the discrete Neumann Laplacian for the numerical solution of the problem, as discussed in the following subsection.

Finally, we observe that, in general, the discrete problem (5.10) admits a solution if and only if the following compatibility condition is satisfied:

$$\sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} b_{h,i+1/2,j+1/2} = 0 \quad (5.11)$$

This condition represents the discrete counterpart of the continuous compatibility condition stated in theorem 5.1 for the Poisson–Neumann problem. In the present setting, it is automatically verified, up to machine precision, as a consequence of the discrete divergence theorem. Indeed, the right-hand side b_h is constructed from the discrete divergence of the displacement field, with boundary fluxes consistently incorporated through the ghost-node elimination procedure, so that its global sum vanishes.

5.2.2. Application of the basic spectral properties of the discrete Neumann Laplacian to the numerical solution of the Poisson–Neumann problem

We exploit the spectral properties of the discrete Neumann Laplacian to construct an efficient numerical solution of the Poisson–Neumann problem. In particular, owing to the diagonalization of the discrete operator in a cosine basis, the resulting linear system can be decoupled into a set of independent scalar equations. This approach naturally leads to a fast Poisson–Neumann solver based on the Discrete Cosine Transform (DCT).

To this end, we recall the basic spectral properties of the discrete Neumann Laplacian, which play a central role in the construction of such efficient solvers. These properties are classical and follow from the diagonalization of second-order centered finite-difference operators by cosine modes associated with the DCT (see, e.g., [34]).

Theorem 5.2 (Basic spectral properties of the discrete Neumann Laplacian).

Consider the discrete eigenvalue problem

$$\left\{ \begin{array}{ll} -\Delta_h \phi_{i+1/2,j+1/2} = \lambda \phi_{i+1/2,j+1/2} & \forall (i, j) \in \Sigma^{(c)} \\ \phi_{-1/2,j+1/2} = \phi_{1/2,j+1/2} & \forall j \in \Sigma_j^{(c)} \\ \phi_{N_x+1/2,j+1/2} = \phi_{N_x-1/2,j+1/2} & \forall j \in \Sigma_j^{(c)} \\ \phi_{i+1/2,-1/2} = \phi_{i+1/2,1/2} & \forall i \in \Sigma_i^{(c)} \\ \phi_{i+1/2,N_z+1/2} = \phi_{i+1/2,N_z-1/2} & \forall i \in \Sigma_i^{(c)} \end{array} \right.$$

Then, for all $(n, m) \in \Sigma^{(c)}$, the eigenpairs are given by

$$\begin{aligned}\phi_{i+1/2, j+1/2}^{(n, m)} &= \alpha^{(n, m)} \cos\left(\frac{\pi n}{N_x}(i + 1/2)\right) \cos\left(\frac{\pi m}{N_z}(j + 1/2)\right), \quad \forall (i, j) \in \Sigma^{(c)} \\ \lambda^{(n, m)} &= \frac{4}{h_x^2} \sin^2\left(\frac{\pi n}{2N_x}\right) + \frac{4}{h_z^2} \sin^2\left(\frac{\pi m}{2N_z}\right)\end{aligned}$$

with $\lambda^{(n, m)} \geq 0$.

Moreover, the eigenfunctions $\{\phi^{(n, m)}\}_{(n, m) \in \Sigma^{(c)}} \subset \mathbb{R}^{N_x \times N_z}$ form a basis of $\mathbb{R}^{N_x \times N_z}$, namely

$$\mathbb{R}^{N_x \times N_z} = \text{span}\left(\{\phi^{(n, m)}\}_{(n, m) \in \Sigma^{(c)}}\right)$$

Furthermore, the normalization coefficients $\{\alpha^{(n, m)}\}_{(n, m) \in \Sigma^{(c)}} \subset \mathbb{R}$ can be chosen so that the eigenfunctions are orthonormal with respect to the standard Euclidean scalar product, that is

$$(\phi^{(n, m)}, \phi^{(p, q)})_h = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} \phi_{i+1/2, j+1/2}^{(n, m)} \phi_{i+1/2, j+1/2}^{(p, q)} = \delta_{n, p} \delta_{m, q}$$

for all $(n, m), (p, q) \in \Sigma^{(c)}$.

In the discrete Poisson–Neumann problem (5.10), both the degrees of freedom of the scalar potential, collected in the values $\{f_{i+1/2, j+1/2}\}_{(i, j) \in \Sigma^{(c)}}$, and those of the discrete right-hand side, collected in $\{b_{h, i+1/2, j+1/2}\}_{(i, j) \in \Sigma^{(c)}}$, can be identified with elements of $\mathbb{R}^{N_x \times N_z}$. Therefore, by theorem 5.2, both quantities can be expanded in the orthonormal basis of eigenfunctions of the discrete Neumann Laplacian:

$$\begin{aligned}f_{i+1/2, j+1/2} &= \sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \hat{f}^{(n, m)} \phi_{i+1/2, j+1/2}^{(n, m)}, \quad \forall (i, j) \in \Sigma^{(c)} \\ b_{h, i+1/2, j+1/2} &= \sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \hat{b}_h^{(n, m)} \phi_{i+1/2, j+1/2}^{(n, m)}, \quad \forall (i, j) \in \Sigma^{(c)}\end{aligned}$$

where the coefficients $\{\hat{f}^{(n, m)}\}_{(n, m) \in \Sigma^{(c)}}$, $\{\hat{b}_h^{(n, m)}\}_{(n, m) \in \Sigma^{(c)}} \subset \mathbb{R}$ can be explicitly computed as

$$\hat{f}^{(n, m)} = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} f_{i+1/2, j+1/2} \phi_{i+1/2, j+1/2}^{(n, m)}, \quad \forall (n, m) \in \Sigma^{(c)} \quad (5.12)$$

$$\hat{b}_h^{(n, m)} = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} b_{h, i+1/2, j+1/2} \phi_{i+1/2, j+1/2}^{(n, m)}, \quad \forall (n, m) \in \Sigma^{(c)} \quad (5.13)$$

Substituting the expansions into the equation of the discrete Poisson–Neumann problem (5.10), we obtain

$$\sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \hat{f}^{(n,m)} \left(-\Delta_h \phi_{i+1/2, j+1/2}^{(n,m)} \right) = \sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \hat{b}_h^{(n,m)} \phi_{i+1/2, j+1/2}^{(n,m)}, \quad \forall (i, j) \in \Sigma^{(c)}$$

Since $\{\phi_{i+1/2, j+1/2}^{(n,m)}\}_{(n,m) \in \Sigma^{(c)}}$ are eigenfunctions of the discrete Neumann Laplacian, the previous equation can be written as

$$\sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \left(\lambda^{(n,m)} \hat{f}^{(n,m)} - \hat{b}_h^{(n,m)} \right) \phi_{i+1/2, j+1/2}^{(n,m)} = 0, \quad \forall (i, j) \in \Sigma^{(c)}$$

Let us now take any $(p, q) \in \Sigma^{(c)}$, multiply both sides by $\phi^{(p,q)}$ and sum over i and j . By rearranging the terms, we obtain

$$\sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \left[\left(\lambda^{(n,m)} \hat{f}^{(n,m)} - \hat{b}_h^{(n,m)} \right) \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} \phi_{i+1/2, j+1/2}^{(n,m)} \phi_{i+1/2, j+1/2}^{(p,q)} \right] = 0$$

By the discrete orthonormality of the eigenfunctions, it follows that

$$\sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \left(\lambda^{(n,m)} \hat{f}^{(n,m)} - \hat{b}_h^{(n,m)} \right) \delta_{n,p} \delta_{m,q} = \lambda^{(p,q)} \hat{f}^{(p,q)} - \hat{b}_h^{(p,q)} = 0$$

Thus, by the arbitrariness of $(p, q) \in \Sigma^{(c)}$, we get

$$\lambda^{(n,m)} \hat{f}^{(n,m)} - \hat{b}_h^{(n,m)} = 0, \quad \forall (n, m) \in \Sigma^{(c)}$$

Let us now analyze the equation corresponding to the first mode $(n, m) = (0, 0)$. From theorem 5.2, we have that the first eigenvalue of the discrete Neumann Laplacian is null:

$$\lambda^{(0,0)} = 0$$

and its associated eigenfunction is constant over the grid:

$$\phi_{i+1/2, j+1/2}^{(0,0)} = \alpha^{(0,0)} \in \mathbb{R}, \quad \forall (i, j) \in \Sigma^{(c)}$$

Moreover, due to the discrete compatibility condition (5.11), we have that

$$\hat{b}_h^{(0,0)} = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} \phi_{i+1/2, j+1/2}^{(0,0)} b_{h, i+1/2, j+1/2} = \alpha^{(0,0)} \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} b_{h, i+1/2, j+1/2} = 0$$

Therefore, the first modal equation reduces to

$$\lambda^{(0,0)} \hat{f}^{(0,0)} = \hat{b}_h^{(0,0)} \implies 0 \cdot \hat{f}^{(0,0)} = 0$$

which is satisfied $\forall f^{(0,0)} \in \mathbb{R}$. This reflects the fact that the discrete Neumann Laplacian has a non-trivial kernel consisting of constant functions. As a consequence, exactly as in the continuous case, the solution of the discrete Poisson–Neumann problem is defined up to an additive constant.

To remove this indeterminacy, we impose the normalization condition

$$\hat{f}^{(0,0)} = 0$$

which is equivalent to prescribing zero discrete average, namely

$$\sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} f_{i+1/2, j+1/2} = \frac{\hat{f}^{(0,0)}}{\alpha^{(0,0)}} = 0$$

This choice is the discrete counterpart of restricting the solution space, in the continuous setting, to the subspace

$$H_*^1(\Omega) = \left\{ f \in H^1(\Omega) \mid \int_{\Omega} f \, d\Omega = 0 \right\}$$

which ensures uniqueness of the weak solution to the Poisson–Neumann problem (5.4).

With this normalization, the solution is uniquely determined, and its expansion coefficients are given by

$$\hat{f}^{(n,m)} = \begin{cases} 0 & (n, m) = (0, 0) \\ \frac{\hat{b}_h^{(n,m)}}{\lambda^{(n,m)}} & (n, m) \neq (0, 0) \end{cases} \quad (5.14)$$

Finally, the degrees of freedom of the scalar potential at the cell centers are reconstructed as

$$f_{i+1/2, j+1/2} = \sum_{n=0}^{N_x-1} \sum_{m=0}^{N_z-1} \hat{f}^{(n,m)} \phi_{i+1/2, j+1/2}^{(n,m)}, \quad \forall (i, j) \in \Sigma^{(c)} \quad (5.15)$$

5.2.3. Description of the P–SV separation algorithm and computational cost analysis

We now describe the algorithm implementing the P–SV separation strategy based on the Poisson–Neumann problem, and provide an estimate of its computational cost. The analysis focuses on the asymptotic complexity of the main operations.

The computation of the expansion coefficients of the discrete right-hand side b_h in (5.13), as well as the reconstruction of the degrees of freedom of the scalar potential f from (5.15), can be efficiently carried out via Discrete Cosine Transforms (DCT). These transforms are implemented through standard FFT-based fast trigonometric algorithms. Accordingly, all double summations appearing in the algorithmic description are to be understood as FFT-based DCT operations, rather than as direct matrix-vector products.

The Poisson–Neumann P–SV separation algorithm can be described through the following sequence of steps:

1. Compute the degrees of freedom of the discrete right-hand side $b_{h,i+1/2,j+1/2}$ for all $(i, j) \in \Sigma^{(c)}$ by evaluating the discrete divergence of the displacement field according to (5.6) and incorporating the boundary contributions arising from the ghost-node elimination procedure. The computational cost of this step amounts to that of a single sweep over the computational grid:

$$\mathcal{O}(N_x N_z)$$

2. Compute the expansion coefficients of the discrete right-hand side $\hat{b}_h^{(n,m)}$ for all $(n, m) \in \Sigma^{(c)}$ according to (5.13). The computational cost of this step corresponds to that of a separable two-dimensional DCT-II, implemented via two successive one-dimensional transforms along the coordinate directions:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

3. Compute the expansion coefficients of the scalar potential $\hat{f}^{(n,m)}$ for all $(n, m) \in \Sigma^{(c)}$ according to (5.14). The computational cost of this step amounts to that of a single sweep over the modes:

$$\mathcal{O}(N_x N_z)$$

4. Reconstruct the degrees of freedom of the scalar potential $f_{i+1/2,j+1/2}$ for all $(i, j) \in \Sigma^{(c)}$ according to (5.15). The computational cost of this step corresponds to that

of a separable two-dimensional DCT-III (inverse of DCT-II, up to normalization), implemented via two successive one-dimensional transforms along the coordinate directions:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

5. Compute the degrees of freedom of the P component of the displacement field by evaluating the discrete gradient of the scalar potential according to (5.7) and obtain those of the SV component by subtraction:

$$\begin{aligned} u_{P,i,j+1/2}^{(x)} &= (\nabla_h f)_{i,j+1/2}^{(x)}, & u_{S,i,j+1/2}^{(x)} &= u_{i,j+1/2}^{(x)} - u_{P,i,j+1/2}^{(x)}, & \forall (i, j) \in \Sigma^{(v)} \\ u_{P,i+1/2,j}^{(z)} &= (\nabla_h f)_{i+1/2,j}^{(z)}, & u_{S,i+1/2,j}^{(z)} &= u_{i+1/2,j}^{(z)} - u_{P,i+1/2,j}^{(z)}, & \forall (i, j) \in \Sigma^{(h)} \end{aligned}$$

The computational cost of this step amounts to a single sweep over the computational grid.

Hence, the overall asymptotic complexity of the proposed Poisson–Neumann P–SV separation algorithm is

$$\mathcal{O}(N_x N_z \log(N_x N_z))$$

with the dominant contribution arising from the DCT-based steps two and four.

5.2.4. Boundary effects and mitigation strategy

In this subsection, we investigate the boundary effects induced by the Poisson–Neumann formulation of the P–SV wave-field separation, and illustrate a strategy to mitigate the resulting artifacts. As discussed in Section 5.1.2, the enforcement of non-homogeneous Neumann boundary conditions introduces a constraint on the normal component of the reconstructed fields, which may lead to the generation of spurious contributions in the vicinity of the boundary. In particular, when a purely SV-wave impinges on $\partial\Omega$, the boundary condition may trigger the Poisson problem and produce a non-physical P component, localized near the boundary.

To illustrate this effect, we consider the homogeneous solid model introduced in appendix A.2.1. The source term is defined as a vertical force with a Ricker wavelet temporal profile (see appendix A.1), with central frequency $f_0 = 10$ Hz, injected at $(x_s, z_s) = (5.0 \text{ km}, 5.0 \text{ km})$.

We consider a representative snapshot of the wave-field, extracted at $t \approx 2.00$ s and shown in figure 5.3. It captures the SV-wave impinging on $\partial\Omega$, while the faster P-wave

has already exited the computational domain. This configuration allows us to clearly isolate and analyze the behavior of the separation procedure in the critical case of an SV-wave interacting with the boundary.

SV-wave at the boundary – full wave-field ($t \approx 2.00$ s)

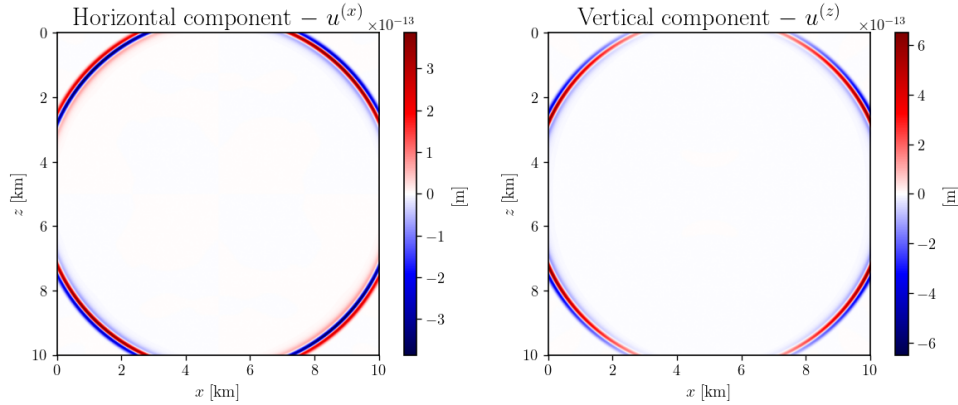


Figure 5.3: Snapshot of the full wave-field when the SV-wave impinges on $\partial\Omega$ ($t \approx 2.00$ s). The horizontal (left) and vertical (right) components of the displacement field are shown.

The decomposition is initially performed on the computational domain $\Omega = \Omega_{\text{int}}$, where $\Omega_{\text{int}} \subset \mathbb{R}^2$ denotes the original physical domain of interest introduced in appendix A.2.1, excluding the outer absorbing layers. The resulting P and SV components are shown in figures 5.4 and 5.5, respectively.

As shown in the left panels of figure 5.4, the decomposition produces a non-vanishing P component, despite the fact that the underlying physical wave-field is predominantly solenoidal. This spurious contribution is non-negligible, being of the same order of magnitude as the physical SV-wave, and is localized in the vicinity of the boundary. Coherently, the left panels of figure 5.5 exhibit a distortion of the SV component in the regions where the wave impinges on $\partial\Omega$. This behavior is consistent with the discussion in section 5.1.2. In particular, the non-homogeneous Neumann boundary conditions activate the Poisson problem through the normal component of the displacement field at $\partial\Omega$, thereby generating a spurious irrotational contribution. As a result, a non-physical P-wave component appears near the boundary, even though the underlying displacement field is of SV type. At the same time, the SV-wave appears distorted, since its normal component is forced to vanish at the boundary. On the other hand, the structure of the wave-field in the interior of the domain is correctly captured, with the spurious effects remaining confined near $\partial\Omega$.

We now assess the effectiveness of a mitigation strategy based on extending the computational domain, following an approach similar to the one proposed in [47]. In practice,

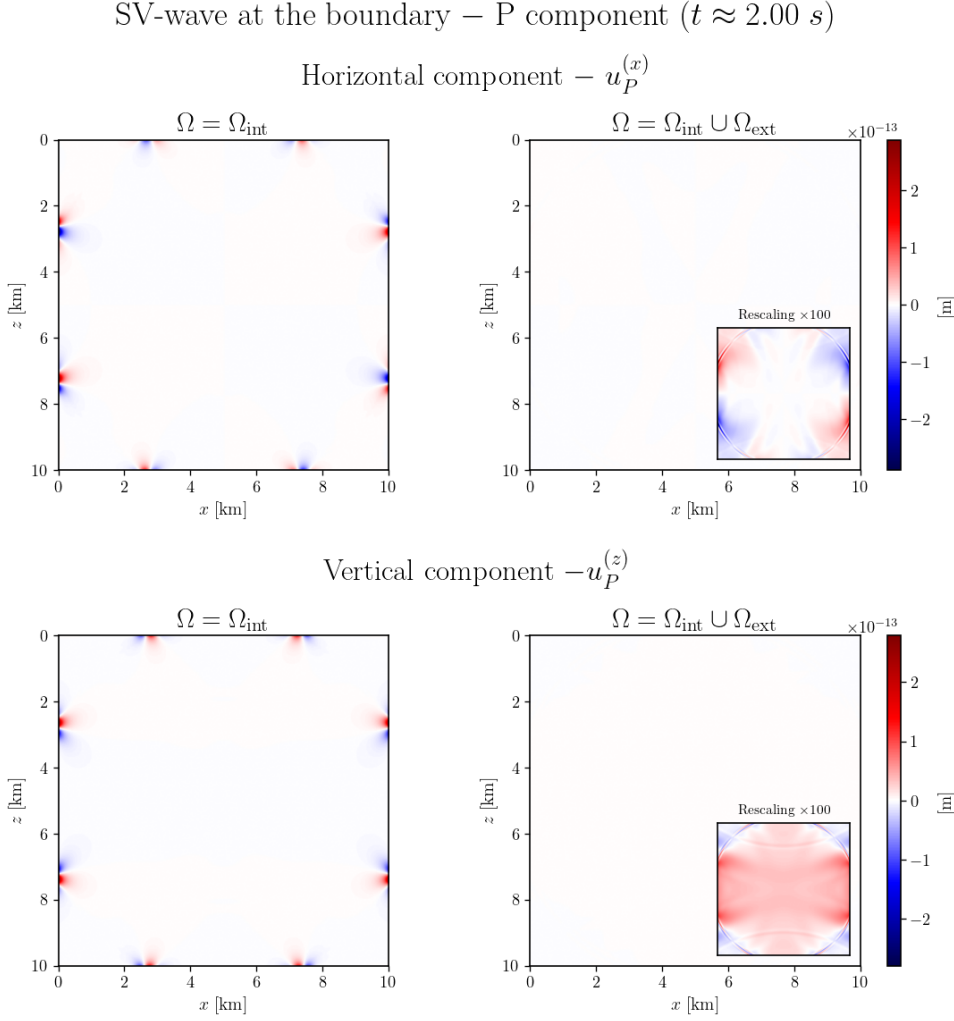


Figure 5.4: P component of the wave-field, when the SV-wave impinges on $\partial\Omega$ ($t \approx 2.00$ s). Left: absorbing layers excluded ($\Omega = \Omega_{\text{int}}$). Right: absorbing layers included ($\Omega = \Omega_{\text{int}} \cup \Omega_{\text{ext}}$). The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

the Poisson–Neumann problem is solved on an enlarged computational domain

$$\Omega = \Omega_{\text{int}} \cup \Omega_{\text{ext}}$$

where Ω_{ext} represents the external region of space occupied by the absorbing layers, introduced to create a buffer region between the artificial boundary and the domain of interest. The decomposition is computed on the extended domain and then restricted to the internal domain Ω_{int} . More precisely, once the scalar potential f is computed on the extended domain, the P and SV components are evaluated by restricting the reconstruction to Ω_{int} ,

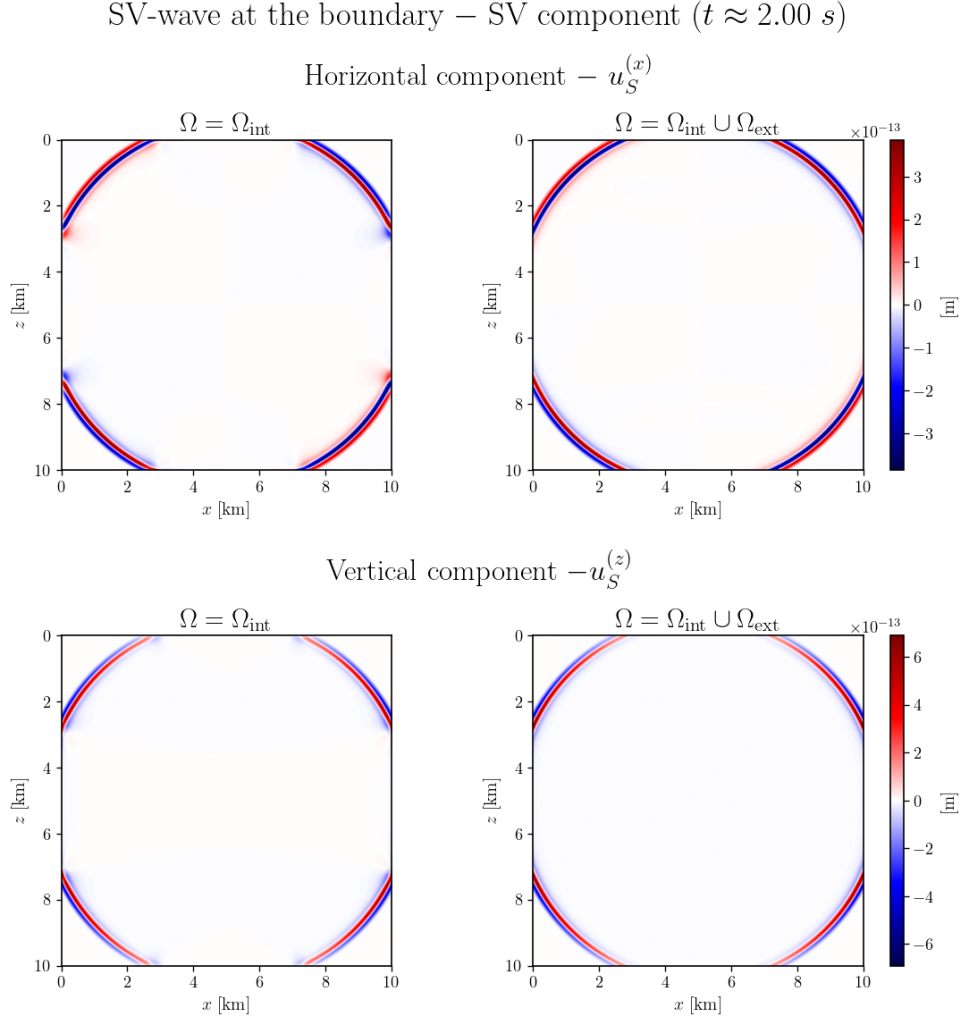


Figure 5.5: SV component of the wave-field, when the SV-wave impinges on $\partial\Omega$ ($t \approx 2.00$ s). Left: absorbing layers excluded ($\Omega = \Omega_{\text{int}}$). Right: absorbing layers included ($\Omega = \Omega_{\text{int}} \cup \Omega_{\text{ext}}$). The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

namely

$$\underline{u}_P = \nabla f|_{\Omega_{\text{int}}}, \quad \underline{u}_S = \underline{u}|_{\Omega_{\text{int}}} - \underline{u}_P$$

As shown in the right panels of figure 5.4, the spurious P component generated in the case of an SV-wave impinging on $\partial\Omega$ is strongly reduced when the extended domain is employed, to the point of not being visible on the common color scale. In particular, the non-physical contribution is mainly confined within Ω_{ext} , while the decomposition inside Ω_{int} is substantially unaffected. The rescaled insets reveal a residual leakage in the reconstructed P component, whose amplitude is roughly two orders of magnitude smaller than that of the physical wave-field. It is comparable to the spurious reflections arising

from the absorbing boundaries Ω_{ext} and is therefore negligible in practice. This weak contribution exhibits a structure aligned with the P-wavefront and is accompanied by faint boundary-induced halos penetrating into Ω_{int} . These halos originate from the distortion of the wave-field within Ω_{ext} , where the absorbing layers alter the local structure of the displacement field, causing the SV-wave to acquire a non-negligible divergence. Since the Poisson problem is non-local, this spurious divergence generates a residual irrotational component that propagates weakly back into Ω_{int} . Nevertheless, these effects remain of practically negligible amplitude, so that the decomposition within the region of interest is effectively preserved.

The complementary configuration, namely a P-wave interacting with the boundary, does not exhibit significant additional boundary-induced artifacts and is therefore not reported.

In light of these results, the Poisson–Neumann P–SV separation will be employed throughout the remainder of this work in combination with the domain extension strategy described above, in order to mitigate the boundary-induced artifacts associated with the incidence of SV-waves.

6 | P–S separation with homogeneous Dirichlet boundary conditions

In the previous chapter, the P–S wave-field separation has been constructed by explicitly defining the associated projection operators through the solution of a Poisson problem equipped with non-homogeneous Neumann boundary conditions. This formulation corresponds to assigning the *harmonic-gradient* contribution to the P-wave component, in accordance with choice (4.11).

In this chapter, we investigate an alternative construction of the P–S separation, namely the case in which the scalar potential is defined as the solution of a Poisson problem equipped with homogeneous Dirichlet boundary conditions. This choice is motivated by the approach proposed by H. Zhu in [48], in which the Poisson equation is solved through the diagonalization of the discrete Laplacian (5.8) via Discrete Sine Transforms (DST), implicitly enforcing homogeneous Dirichlet boundary conditions at the discrete level.

The objective of this chapter is to provide a rigorous mathematical interpretation of this choice within the framework of the Helmholtz–Weyl decomposition. In particular, we show that this formulation corresponds to a different realization of the decomposition, in which the *harmonic-gradient* contribution is not included in the irrotational field, and is therefore implicitly contained in the S-wave component, thus realizing choice (4.12).

The chapter is organized as follows. We first introduce the Poisson–Dirichlet problem and briefly discuss its well-posedness, together with a physical interpretation of the associated homogeneous Dirichlet boundary conditions in the context of P–S wave-field separation. We then address its numerical solution, showing how, in rectangular domains, the spectral properties of the continuous Dirichlet Laplacian enable an explicit analytical representation of the solution, which leads to the construction of the corresponding discrete algorithm. Finally, we analyze the boundary artifacts induced by the formulation and investigate the accuracy of the proposed approach.

6.1. The Poisson–Dirichlet problem

Let $\underline{u} = \underline{u}(t) \in V \subset [H^1(\Omega)]^n$ be a snapshot of the wave-field, as introduced in (4.9). In this chapter, we define the scalar potential f as the solution of the following Poisson–Dirichlet problem:

$$\begin{cases} -\Delta f = -\operatorname{div}(\underline{u}) & \text{in } \Omega \\ f = 0 & \text{on } \partial\Omega \end{cases} \quad (6.1)$$

Once problem (6.1) is solved, in analogy with the previous chapter, we define the P and S components of the wave-field according to (5.5), thus realizing the projection operators Π_P and $\Pi_S = \operatorname{Id} - \Pi_P$.

We now inspect how the *harmonic-gradient* contribution enters the construction. We recall that, as already observed in section 5.1, since $f = g + h \in H^1(\Omega)$, with $h \in H^1(\Omega)$ harmonic, we have

$$\Delta f = \Delta g + \Delta h = \Delta g \quad \text{in } \Omega$$

Therefore, the Poisson equation determines g , while the harmonic contribution h is not fixed by the equation itself. On the other hand, the homogeneous Dirichlet boundary conditions enforce

$$\gamma_0(f) = 0 \quad \text{in } H^{1/2}(\partial\Omega)$$

which implies

$$\gamma_0(h) = -\gamma_0(g) \quad \text{in } H^{1/2}(\partial\Omega)$$

Since, according to theorem 4.2, $g \in H_0^1(\Omega)$, it follows that $\gamma_0(g) = 0$ on $\partial\Omega$, and therefore

$$\gamma_0(h) = 0 \quad \text{in } H^{1/2}(\partial\Omega)$$

At the formal level, this corresponds to the homogeneous Dirichlet boundary condition

$$h = 0 \quad \text{on } \partial\Omega$$

Hence, the harmonic component is required to satisfy the following Poisson–Dirichlet problem:

$$\begin{cases} -\Delta h = 0 & \text{in } \Omega \\ h = 0 & \text{on } \partial\Omega \end{cases} \quad (6.2)$$

We now show that the only solution of problem (6.2) is the trivial one. To this end, we consider its weak formulation, which reads:

Find $h \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \nabla h \cdot \nabla v \, d\Omega = 0, \quad \forall v \in H_0^1(\Omega)$$

Taking $v = h \in H_0^1(\Omega)$, we obtain

$$\|\nabla h\|_{L^2(\Omega)}^2 = 0$$

Therefore, thanks to *Poincaré inequality*, we can conclude

$$0 \leq \|h\|_{L^2(\Omega)} \leq C_P \|\nabla h\|_{L^2(\Omega)} \implies \|h\|_{L^2(\Omega)} = 0$$

which is equivalent to

$$h = 0 \quad \text{in } \Omega$$

Hence, when homogeneous Dirichlet boundary conditions are coupled with the Poisson equation for the scalar potential $f = g + h$, the harmonic component h is forced to vanish. As a consequence, the scalar potential coincides with the component $g \in H_0^1(\Omega)$, and problem (6.1) is equivalent to the following Poisson–Dirichlet problem:

$$\begin{cases} -\Delta g = -\operatorname{div}(\underline{u}) & \text{in } \Omega \\ g = 0 & \text{on } \partial\Omega \end{cases}$$

Accordingly, this construction yields

$$\underline{u}_P = \nabla f = \nabla g = \underline{u}_3$$

$$\underline{u}_S = \underline{u} - \underline{u}_P = (\underline{u}_1 + \underline{u}_2 + \underline{u}_3) - \underline{u}_P = \underline{u}_1 + \underline{u}_2$$

so that the *harmonic-gradient* contribution $\underline{u}_2$ is included in the S-wave component, effectively realizing choice (4.12):

$$\underline{u}_P \in \mathcal{U}_P = G_3(\Omega), \quad \underline{u}_S \in \mathcal{U}_S = G_1(\Omega) \oplus G_2(\Omega)$$

This shows that, as in the non-homogeneous Neumann formulation, the assignment of the harmonic component is entirely dictated by the boundary conditions of the auxiliary Poisson problem. In contrast with the non-homogeneous Neumann case, the homogeneous Dirichlet boundary conditions force it to vanish, leading to its exclusion from the P-wave component, and it is therefore included in the S-wave component.

Finally, we briefly address the well-posedness of the Poisson–Dirichlet problems introduced in this section. To this end, we consider their weak formulation in $H_0^1(\Omega)$, endowed with the scalar product

$$(u, v)_{H_0^1(\Omega)} = \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega$$

which is equivalent to the standard $(\cdot, \cdot)_{H^1(\Omega)}$ thanks to *Poincaré inequality*.

By the *Riesz representation theorem for Hilbert spaces* (see appendix B, theorem B.3), for any continuous linear functional $L \in H^{-1}(\Omega)$, there exists a unique $f \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \nabla f \cdot \nabla v \, d\Omega = \langle L, v \rangle, \quad \forall v \in H_0^1(\Omega)$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$.

In the Poisson–Dirichlet problem (6.1) we consider the functional

$$\langle L, v \rangle = - \int_{\Omega} \operatorname{div}(\underline{u}) v \, d\Omega$$

while in problem (6.2) we have $L \equiv 0$. In both cases, the functional L is linear and continuous on $H_0^1(\Omega)$, since $\operatorname{div}(\underline{u}) \in L^2(\Omega)$.

Therefore, all the Poisson–Dirichlet problems introduced in this section admit a unique solution in $H_0^1(\Omega)$.

6.1.1. Physical interpretation of homogeneous Dirichlet boundary conditions

The physical interpretation of homogeneous Dirichlet boundary conditions in the context of the P–S wave-field separation is not as straightforward as the one for the non-homogeneous Neumann boundary conditions presented in section 5.1.2.

To gain geometric insight, we temporarily assume that

$$\partial\Omega \in C^1, \quad f \in C^1(\bar{\Omega}), \quad \nabla f(\underline{x}) \neq \underline{0}, \quad \forall \underline{x} \in \partial\Omega$$

In this idealized setting, since $f = 0$ on $\partial\Omega$, the boundary $\partial\Omega$ is a regular isoline of f at level 0. As the gradient is orthogonal to the level sets of f , and recalling that, according to (5.5), the P component of the displacement field is given by $\underline{u}_P = \nabla f$, we infer

$$\nabla f \cdot \hat{\tau} = \underline{u}_P \cdot \hat{\tau} = 0 \quad \text{on } \partial\Omega$$

where $\hat{\tau}$ denotes the tangent unit vector to $\partial\Omega$.

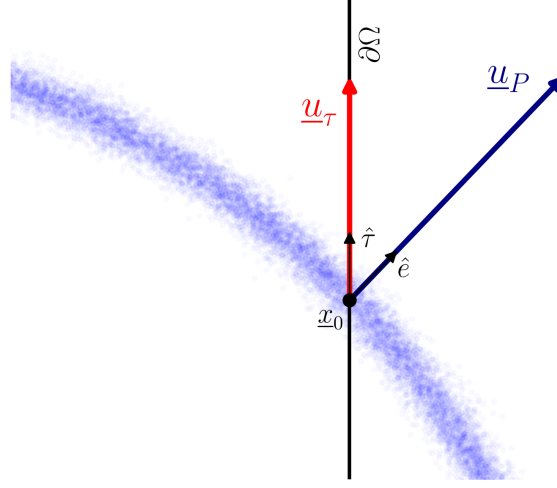


Figure 6.1: Schematic representation of a P-wave impinging on the boundary $\partial\Omega$. The blue cloud represents the local wavefront, whose propagation direction is indicated by the unit propagation vector $\hat{e}$. The associated displacement field $\underline{u}_P$, shown in dark blue, is parallel to $\hat{e}$, consistently with the longitudinal polarization of P-waves. At the point of incidence $\underline{x}_0 \in \partial\Omega$, the displacement generally exhibits a non-vanishing tangential component, highlighted in red and given by $\underline{u}_\tau = (\underline{u}_P \cdot \hat{\tau}) \hat{\tau}$, where $\hat{\tau}$ denotes the tangent unit vector to the boundary.

Thus, enforcing homogeneous Dirichlet boundary conditions can be interpreted, in this geometric picture, as forcing the P-wave component to have a zero tangential component at the boundary. As a result, it is purely normal to $\partial\Omega$. Consequently, the S component, defined as $\underline{u}_S = \underline{u} - \underline{u}_P$ satisfies

$$\underline{u}_S \cdot \hat{\tau} = \underline{u} \cdot \hat{\tau} - \underline{u}_P \cdot \hat{\tau} = \underline{u} \cdot \hat{\tau} \quad \text{on } \partial\Omega \quad (6.3)$$

This geometric constraint arises from the mathematical formulation and provides a formal interpretation of the decomposition at the boundary. However, it does not correspond to a general physical property of elastic wave-fields, since the P-wave component of the displacement field may exhibit a non-vanishing tangential component at the boundary, as illustrated in figure 6.1. This leads to the following behavior. Consider a displacement field that is purely P, i.e.,

$$\underline{u} = \underline{u}_P, \quad \underline{u}_S = \underline{0}$$

When such a P-wave reaches the boundary of the domain, it generally exhibits a non-

vanishing tangential component, that is,

$$\underline{u} \cdot \hat{\tau} = \underline{u}_P \cdot \hat{\tau} \neq 0 \quad \text{on } \partial\Omega$$

Therefore, according to (6.3), this contribution is spuriously transferred to $\underline{u}_S$. Hence, when a purely compressional wave interacts with the boundary, one expects the appearance of numerical artifacts in the reconstructed S-wave component, localized near the portions of the boundary where the P-wave impinges.

This interpretation highlights a clear duality with respect to the Poisson–Neumann formulation, discussed in section 5.1.2, together with a fundamental difference in the underlying mechanism. In the Neumann case, the boundary conditions directly enforce the normal component of the reconstructed P-wave field, so that, when an S-wave impinges on $\partial\Omega$, the Poisson problem is activated through the boundary data, leading to the appearance of a spurious P component. In contrast, in the Dirichlet case, the constraint acts indirectly on the tangential component of the reconstructed P-wave field, imposing a geometric restriction that is not generally compatible with the intrinsic polarization of compressional waves. As a consequence, when a P-wave reaches the boundary, its tangential component cannot be represented and is transferred to the S component, giving rise to spurious shear contributions.

6.2. Numerical solution of the Poisson–Dirichlet problem

In this section, we address the numerical solution of the Poisson–Dirichlet problem for the P–S wave-field separation. As in the previous chapter, we restrict the analysis to the two-dimensional setting, so that the solenoidal component $\underline{u}_S$ coincides with the SV wave-field, and the decomposition takes the form of a P–SV separation.

An important feature of the Poisson–Dirichlet formulation is that, in rectangular domains, it admits an explicit analytical solution based on the spectral properties of the Dirichlet Laplacian. This observation naturally leads to a different perspective with respect to the Neumann formulation. Rather than discretizing differential operators, the solution is obtained by approximating its continuous spectral representation in a way consistent with the information available on the discrete grid. Although this change of viewpoint results in an algorithm that is, in practice, very similar to the one previously introduced in section 5.2.3, it has significant implications for the analytical interpretation and numerical properties of the method.

We first exploit the basic spectral properties of the continuous Dirichlet Laplacian to derive an analytical representation of the solution of the Poisson–Dirichlet problem. This representation is then specialized to rectangular domains, where it takes a particularly simple and explicit form.

Building upon this framework, we introduce the corresponding numerical approximation and define the complete P–SV separation algorithm, whose computational cost is briefly analyzed.

Finally, we investigate the boundary effects induced by the Dirichlet formulation, and show that the same mitigation strategy introduced in section 5.2.4 remains effective in this setting.

6.2.1. Application of the basic spectral properties of the continuous Dirichlet Laplacian to the analytical solution of the Poisson–Dirichlet problem

We first recall the basic spectral properties of the continuous Dirichlet Laplacian. We then use these properties to derive an abstract analytical representation of the solution of the Poisson–Dirichlet problem.

Let $\Omega \subset \mathbb{R}^n$ open, bounded and connected, such that $\partial\Omega \in \text{Lip}$. Let us consider the following eigenvalue problem:

$$\begin{cases} -\Delta\varphi = \lambda\varphi & \text{in } \Omega \\ \varphi = 0 & \text{on } \partial\Omega \end{cases} \quad (6.4)$$

From standard spectral theory of elliptic operators (see, e.g. chapter 9.8 in [4] and chapter 6.5 in [10]), problem (6.4) admits a sequence of eigenpairs $\{(\lambda_n, \varphi_n)\}_{n \in \mathbb{N}}$ such that

- The eigenvalues $\{\lambda_n\}_{n \in \mathbb{N}} \subset \mathbb{R}$ satisfy $0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \rightarrow +\infty$;
- The eigenfunctions $\{\varphi_n\}_{n \in \mathbb{N}} \subset H_0^1(\Omega)$ form, up to normalization, an orthonormal basis of $(L^2(\Omega), (\cdot, \cdot)_{L^2(\Omega)})$.

In the context of the Poisson–Dirichlet problem (6.1), we consider the right-hand side

$$b = -\operatorname{div}(\underline{u}) \in L^2(\Omega)$$

and the corresponding solution given by the scalar potential

$$f \in H_0^1(\Omega) \subset L^2(\Omega).$$

Therefore, both b and f can be expanded with respect to the basis of eigenfunctions of the Dirichlet Laplacian, namely

$$b = \sum_{n=1}^{+\infty} \hat{b}_n \varphi_n, \quad f = \sum_{n=1}^{+\infty} \hat{f}_n \varphi_n \quad (6.5)$$

in the sense that

$$\left\| b - \sum_{n=1}^k \hat{b}_n \varphi_n \right\|_{L^2(\Omega)} \longrightarrow 0, \quad \left\| f - \sum_{n=1}^k \hat{f}_n \varphi_n \right\|_{L^2(\Omega)} \longrightarrow 0, \quad k \rightarrow +\infty$$

where the coefficients $\{\hat{b}_n\}_{n \in \mathbb{N}}, \{\hat{f}_n\}_{n \in \mathbb{N}} \subset \mathbb{R}$ can be explicitly computed as

$$\hat{b}_n = (b, \varphi_n)_{L^2(\Omega)} = \int_{\Omega} b \varphi_n d\Omega, \quad \hat{f}_n = (f, \varphi_n)_{L^2(\Omega)} = \int_{\Omega} f \varphi_n d\Omega, \quad \forall n \in \mathbb{N}$$

To rigorously relate the expansion coefficients of the scalar potential to those of the right-hand side, we exploit the weak formulation of both the Poisson–Dirichlet problem (6.1) and of the eigenvalue problem (6.4).

By definition, each eigenfunction $\varphi_n \in H_0^1(\Omega)$ satisfies

$$\int_{\Omega} \nabla \varphi_n \cdot \nabla v d\Omega = \lambda_n \int_{\Omega} \varphi_n v d\Omega, \quad \forall v \in H_0^1(\Omega)$$

Choosing $v = f \in H_0^1(\Omega)$, we obtain

$$\int_{\Omega} \nabla \varphi_n \cdot \nabla f d\Omega = \lambda_n \int_{\Omega} \varphi_n f d\Omega = \lambda_n \hat{f}_n \quad (6.6)$$

On the other hand, since f is the weak solution of the Poisson–Dirichlet problem, it fulfills

$$\int_{\Omega} \nabla f \cdot \nabla v d\Omega = \int_{\Omega} b v d\Omega, \quad \forall v \in H_0^1(\Omega)$$

Thus, choosing $v = \varphi_n$, we get

$$\int_{\Omega} \nabla f \cdot \nabla \varphi_n d\Omega = \int_{\Omega} b \varphi_n d\Omega = \hat{b}_n \quad (6.7)$$

Combining equations (6.6) and (6.7), thanks to the arbitrariness of $n \in \mathbb{N}$, it follows that

$$\lambda_n \hat{f}_n = \hat{b}_n, \quad \forall n \in \mathbb{N}$$

Hence, recalling that $\lambda_n > 0$ for all $n \in \mathbb{N}$, we conclude

$$\hat{f}_n = \frac{\hat{b}_n}{\lambda_n}, \quad \forall n \in \mathbb{N} \quad (6.8)$$

We finally specify the form of the right-hand side expansion coefficients in the present setting, where $b = -\operatorname{div}(\underline{u})$. By applying the *generalized Gauss–Green formula* (see appendix B, theorem B.5), we get

$$\hat{b}_n = - \int_{\Omega} \operatorname{div}(\underline{u}) \varphi_n d\Omega = \int_{\Omega} \underline{u} \cdot \nabla \varphi_n d\Omega, \quad \forall n \in \mathbb{N} \quad (6.9)$$

where the boundary term vanishes since $\varphi_n \in H_0^1(\Omega)$.

This construction highlights a deep analogy with the discrete diagonalization procedures introduced in section 5.2.2. In both cases, the solution is obtained through a spectral decomposition with respect to the basis of eigenfunctions of the underlying operator. The fundamental difference lies in the level of the construction: here, the Dirichlet Laplacian is diagonalized as an operator on an infinite-dimensional space, while in the discrete setting of the previous chapter the same idea is applied to a finite-dimensional approximation of the Neumann Laplacian.

6.2.2. Analytical solution of the Poisson–Dirichlet problem in rectangular domains

In our setting, we consider the rectangular domain $\Omega = (0, L_x) \times (0, L_z) \subset \mathbb{R}^2$. In this case, the eigenvalue problem (6.4) can be solved explicitly by means of separation of variables, leading to closed-form expressions for the eigenvalues $\{\lambda_{n,m}\}_{(n,m) \in \mathbb{N}^2}$ and the corresponding eigenfunctions $\{\varphi_{n,m}\}_{(n,m) \in \mathbb{N}^2}$.

We postulate a solution of the form

$$\varphi(x, z) = \alpha(x)\beta(z), \quad \forall (x, z) \in \bar{\Omega} \quad (6.10)$$

Substituting the ansatz (6.10) into the equation of the eigenvalue problem (6.4) yields

$$-\alpha''(x)\beta(z) - \alpha(x)\beta''(z) = \lambda \alpha(x)\beta(z), \quad \forall (x, z) \in \Omega$$

Assuming that α and β are non-trivial, this identity implies that there exist constants $\lambda_x, \lambda_z \in \mathbb{R}$ such that

$$-\alpha''(x) = \lambda_x \alpha(x), \quad -\beta''(z) = \lambda_z \beta(z), \quad \lambda_x + \lambda_z = \lambda \quad (6.11)$$

where the equations hold in $(0, L_x)$ and $(0, L_z)$, respectively.

Imposing the homogeneous Dirichlet boundary condition $\varphi = 0$ on each side of the rectangle and excluding the trivial solution leads to

$$\alpha(0) = \alpha(L_x) = 0, \quad \beta(0) = \beta(L_z) = 0$$

Hence, the original two-dimensional eigenvalue problem can be decoupled into the following analogous one-dimensional eigenvalue problems:

$$\begin{cases} -\alpha''(x) = \lambda_x \alpha(x) & \text{in } (0, L_x) \\ \alpha(0) = \alpha(L_x) = 0 \end{cases} \quad \begin{cases} -\beta''(z) = \lambda_z \beta(z) & \text{in } (0, L_z) \\ \beta(0) = \beta(L_z) = 0 \end{cases}$$

The eigenpairs associated to these problems are classical and follow from standard theory of second-order linear ODEs with constant coefficients, namely

$$\begin{aligned} \lambda_{x,n} &= \left(\frac{n\pi}{L_x} \right)^2, \quad \alpha_n(x) = A_n \sin\left(\frac{n\pi}{L_x} x \right), \quad \forall n \in \mathbb{N} \\ \lambda_{z,m} &= \left(\frac{m\pi}{L_z} \right)^2, \quad \beta_m(z) = B_m \sin\left(\frac{m\pi}{L_z} z \right), \quad \forall m \in \mathbb{N} \end{aligned}$$

where $A_n, B_m \in \mathbb{R}$ are free normalization constants.

Then, according to (6.10) and (6.11), for all $(n, m) \in \mathbb{N}^2$, the eigenpairs of problem (6.4) are given by

$$\lambda_{n,m} = \left(\frac{n\pi}{L_x} \right)^2 + \left(\frac{m\pi}{L_z} \right)^2 \quad (6.12)$$

$$\varphi_{n,m}(x, z) = \frac{2}{\sqrt{L_x L_z}} \sin\left(\frac{n\pi}{L_x} x \right) \sin\left(\frac{m\pi}{L_z} z \right), \quad \forall (x, z) \in \bar{\Omega} \quad (6.13)$$

where the constant $C_{n,m} = A_n B_m = 2/\sqrt{L_x L_z}$ is chosen in order to guarantee $\|\varphi_{n,m}\|_{L^2(\Omega)} = 1$ for all $(n, m) \in \mathbb{N}^2$.

We now exploit the explicit characterization of the eigenpairs to derive the explicit rep-

resentation of the solution to the Poisson–Dirichlet problem (6.1).

By (6.9) and (6.13), the expansion coefficients of the right-hand side $b = -\operatorname{div}(\underline{u})$ can be computed as

$$\hat{b}_{n,m} = \int_{\Omega} \underline{u} \cdot \nabla \varphi_{n,m} d\Omega = \frac{n\pi}{L_x} \hat{u}_{x,n,m} + \frac{m\pi}{L_z} \hat{u}_{z,n,m}, \quad \forall (n, m) \in \mathbb{N}^2 \quad (6.14)$$

where we denoted, for all $(n, m) \in \mathbb{N}^2$,

$$\hat{u}_{x,n,m} = \frac{2}{\sqrt{L_x L_z}} \int_0^{L_x} \int_0^{L_z} u_x(x, z) \cos\left(\frac{n\pi}{L_x} x\right) \sin\left(\frac{m\pi}{L_z} z\right) dz dx \quad (6.15)$$

$$\hat{u}_{z,n,m} = \frac{2}{\sqrt{L_x L_z}} \int_0^{L_x} \int_0^{L_z} u_z(x, z) \sin\left(\frac{n\pi}{L_x} x\right) \cos\left(\frac{m\pi}{L_z} z\right) dz dx \quad (6.16)$$

Once the coefficients $\{\hat{b}_{n,m}\}_{(n,m) \in \mathbb{N}^2}$ have been computed, the corresponding coefficients of the scalar potential $\{\hat{f}_{n,m}\}_{(n,m) \in \mathbb{N}^2}$ follow from (6.8) together with (6.12).

Finally, the analytical solution of the Poisson–Dirichlet problem is given by (6.5) and (6.13), explicitly

$$f(x, z) = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{+\infty} \sum_{m=1}^{+\infty} \hat{f}_{n,m} \sin\left(\frac{n\pi}{L_x} x\right) \sin\left(\frac{m\pi}{L_z} z\right) \quad (6.17)$$

6.2.3. Description of the P–SV separation algorithm and computational cost analysis

We now describe the algorithm implementing the P–SV separation strategy based on the Poisson–Dirichlet problem, which arises from the approximation of the continuous spectral representation derived in the previous section with the information available on the discrete grid, together with a brief analysis of its computational cost. As in section 5.2.3, the analysis focuses on the asymptotic complexity of the main operations.

We consider the same staggered grid setup described in section 5.2.1. In this discrete setting, the spectral representation (6.17) is approximated by truncating the infinite series to the finite set of admissible wavenumbers supported by the grid. In particular, according to the *Nyquist sampling theorem*, the maximum resolvable wavenumbers are

$$k_{x,\max} = \frac{\pi}{h_x}, \quad k_{z,\max} = \frac{\pi}{h_z} \quad (6.18)$$

This imposes an upper bound on the spectral modes that can be represented without aliasing on the discrete grid, namely

$$k_{x,n} = \frac{n\pi}{L_x} \leq k_{x,\max} \Leftrightarrow n \leq N_x, \quad k_{z,m} = \frac{m\pi}{L_z} \leq k_{z,\max} \Leftrightarrow m \leq N_z$$

Thus, the truncated spectral representation is defined over the discrete set of admissible wavenumbers $(k_{x,n}, k_{z,m})$, with indices belonging to the set

$$\Sigma^{(s)} = \{1, \dots, N_x\} \times \{1, \dots, N_z\}$$

Finally, we remark that the computation of the approximated expansion coefficients of the displacement and the truncated reconstruction of the P-wave component can be efficiently carried out via mixed Discrete Cosine Transforms (DCT) and Discrete Sine Transforms (DST). Accordingly, as in section 5.2.3, the double summations appearing in the algorithm below are to be interpreted as FFT-based DCT/DST operations.

The Poisson–Dirichlet P–SV separation algorithm can be described through the following sequence of steps:

1. Approximate $\hat{u}_{x,n,m}$, as given by (6.15), for all $(n, m) \in \Sigma^{(s)}$ through the quadrature formula

$$\hat{u}_{n,m}^{(x)} = \frac{2}{\sqrt{L_x L_z}} \sum_{i=0}^{N_x} \sum_{j=0}^{N_z-1} w_i^{(x)} u_{i,j+1/2}^{(x)} \cos\left(\frac{n\pi}{N_x} i\right) \sin\left(\frac{m\pi}{N_z} (j+1/2)\right) h_x h_z \quad (6.19)$$

where the quadrature weights are

$$w_i^{(x)} = \begin{cases} \frac{1}{2} & i = 0 \vee i = N_x \\ 1 & i = 1, \dots, N_x - 1 \end{cases} \quad (6.20)$$

The computational cost of this step corresponds to that of a mixed two-dimensional transform, consisting of a DCT-I along the x direction and a DST-II along the z direction, implemented via two successive one-dimensional transforms:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

2. Approximate $\hat{u}_{z,n,m}$, as given by (6.16), for all $(n, m) \in \Sigma^{(s)}$ through the quadrature

formula

$$\hat{u}_{n,m}^{(z)} = \frac{2}{\sqrt{L_x L_z}} \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z} w_j^{(z)} u_{i+1/2,j}^{(z)} \sin\left(\frac{n\pi}{N_x}(i+1/2)\right) \cos\left(\frac{m\pi}{N_z}j\right) h_x h_z \quad (6.21)$$

where the quadrature weights are

$$w_j^{(z)} = \begin{cases} \frac{1}{2} & j = 0 \vee j = N_z \\ 1 & j = 1, \dots, N_z - 1 \end{cases} \quad (6.22)$$

The computational cost of this step is identical to that of the previous one, with the corresponding transforms applied along the opposite coordinate directions.

3. Approximate the expansion coefficients of the right-hand side $\hat{b}_{n,m}$, as given by (6.14), for all $(n, m) \in \Sigma^{(s)}$:

$$\hat{b}_{h,n,m} = \frac{n\pi}{L_x} \hat{u}_{n,m}^{(x)} + \frac{m\pi}{L_z} \hat{u}_{n,m}^{(z)}$$

The computational cost of this step amounts to that of a single sweep over the modes:

$$\mathcal{O}(N_x N_z)$$

4. Reconstruct the approximated expansion coefficients of the scalar potential $\hat{f}_{n,m}$, as given by (6.8), for all $(n, m) \in \Sigma^{(s)}$:

$$\hat{f}_{h,n,m} = \frac{\hat{b}_{h,n,m}}{\lambda_{n,m}}$$

The computational cost of this step amounts to that of a single sweep over the modes.

5. Approximate the expansion coefficients of $\underline{u}_P = \nabla f$ for all $(n, m) \in \Sigma^{(s)}$ by term-by-term differentiation of the truncated expansion of the scalar potential:

$$\hat{u}_{P,n,m}^{(x)} = \frac{n\pi}{L_x} \hat{f}_{h,n,m}, \quad \hat{u}_{P,n,m}^{(z)} = \frac{m\pi}{L_z} \hat{f}_{h,n,m}$$

The computational cost of this step amounts to that of a single sweep over the modes.

6. Reconstruct the degrees of freedom of the horizontal component of the P wave-field by evaluating the x -derivative of the truncated expansion of f at the corresponding

grid locations:

$$u_{P,i,j+1/2}^{(x)} = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{N_x} \sum_{m=1}^{N_z} \hat{u}_{P,n,m}^{(x)} \cos\left(\frac{n\pi}{N_x} i\right) \sin\left(\frac{m\pi}{N_z} (j + 1/2)\right), \quad \forall (i, j) \in \Sigma^{(v)}$$

The computational cost of this step corresponds to that of a mixed two-dimensional transform, consisting of a DCT-I (self-inverse, up to normalization) along the x direction and a DST-III (inverse of DST-II, up to normalization) along the z direction, implemented via two successive one-dimensional transforms:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

7. Reconstruct the degrees of freedom of the vertical component of the P wave-field by evaluating the z -derivative of the truncated expansion of f at the corresponding grid locations:

$$u_{P,i+1/2,j}^{(z)} = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{N_x} \sum_{m=1}^{N_z} \hat{u}_{P,n,m}^{(z)} \sin\left(\frac{n\pi}{N_x} (i + 1/2)\right) \cos\left(\frac{m\pi}{N_z} j\right), \quad \forall (i, j) \in \Sigma^{(h)}$$

The computational cost of this step is identical to that of the previous one, with the corresponding transforms applied along the opposite coordinate directions.

8. Compute the degrees of freedom of the SV component of the wave-field by subtraction:

$$\begin{aligned} u_{S,i,j+1/2}^{(x)} &= u_{i,j+1/2}^{(x)} - u_{P,i,j+1/2}^{(x)}, \quad \forall (i, j) \in \Sigma^{(v)} \\ u_{S,i+1/2,j}^{(z)} &= u_{i+1/2,j}^{(z)} - u_{P,i+1/2,j}^{(z)}, \quad \forall (i, j) \in \Sigma^{(h)} \end{aligned}$$

The computational cost of this step amounts to that of a single sweep over the computational grid:

$$\mathcal{O}(N_x N_z)$$

Hence, the overall asymptotic complexity of the proposed Poisson–Dirichlet P–SV separation algorithm is

$$\mathcal{O}(N_x N_z \log(N_x N_z))$$

with the dominant contribution arising from the DCT/DST-based steps one, two, six and seven.

6.2.4. Boundary effects and mitigation strategy

In this subsection, we investigate the boundary effects induced by the Poisson–Dirichlet formulation of the P–SV wave-field separation, and assess the effectiveness of the mitigation strategy introduced in section 5.2.4. As discussed in section 6.1.1, imposing homogeneous Dirichlet boundary conditions enforces an indirect constraint on the tangential component of the reconstructed P-wave field, which may lead to the generation of spurious contributions in the vicinity of the boundary. In particular, when a P-wave impinges on $\partial\Omega$, its tangential component cannot be represented by the scalar potential and may be spuriously transferred to the SV component.

The numerical test considered is identical to that presented in section 5.2.4. We employ the same homogeneous solid model and source configuration. To isolate and analyze the behavior of the separation procedure in the critical case of a P-wave interacting with the boundary, we consider a representative snapshot of the wave-field at $t \approx 1.25$ s, shown in figure 6.2. It captures the P-wave impinging on $\partial\Omega$, with the slower SV-wave still entirely contained within the interior of the computational domain. The resulting P and SV components obtained from the decomposition are shown in figures 6.3 and 6.4.

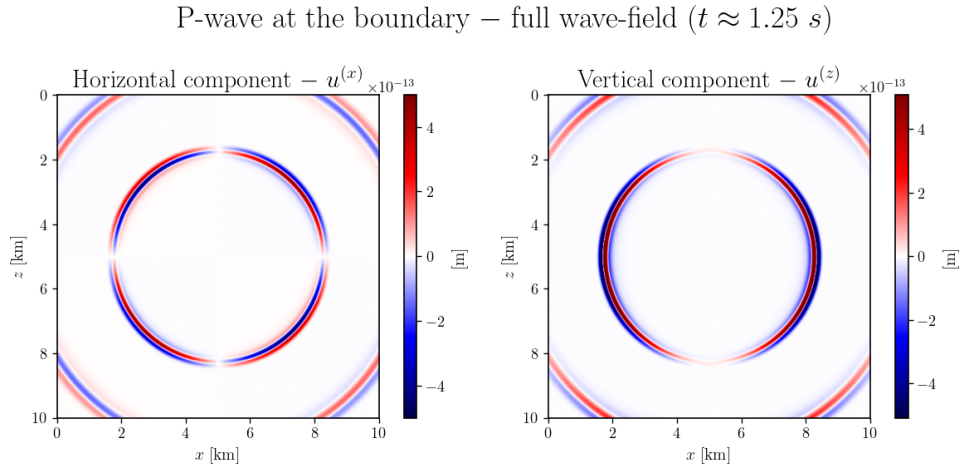


Figure 6.2: Snapshot of the full wave-field when the P-wave impinges on $\partial\Omega$ ($t \approx 1.25$ s). The horizontal (left) and vertical (right) components of the displacement field are shown.

As shown in the left panels of figure 6.3, the amplitude and structure of the P-wave are well captured in the domain’s bulk. However, the wavefront appears significantly distorted in the vicinity of the boundary, where the imposed constraint alters the local structure of the reconstructed field. Coherently, the SV component, reported in the left panels of figure 6.4, exhibits a non-vanishing contribution localized along the P incidence regions near the boundary. This spurious component is not physical, as the underlying

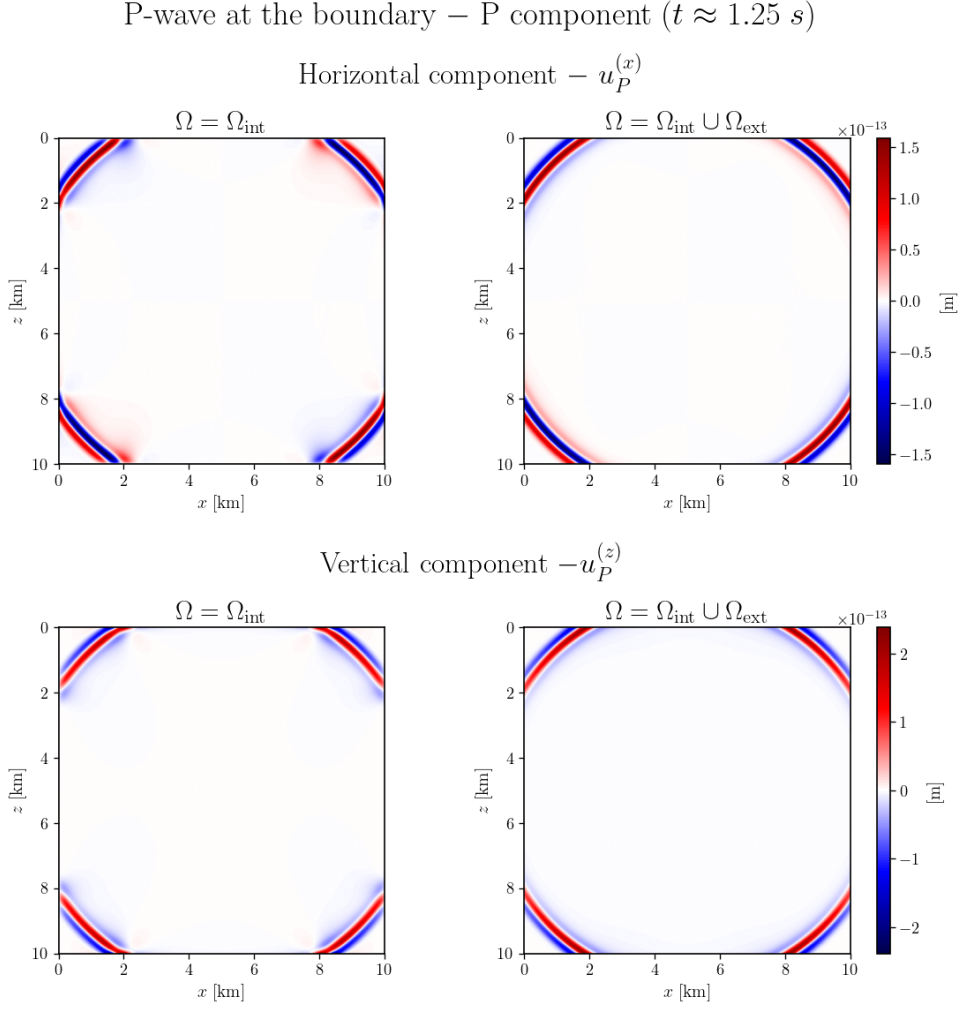


Figure 6.3: P component of the wave-field, when the P-wave impinges on $\partial\Omega$ ($t \approx 1.25$ s). Left: absorbing layers excluded ($\Omega = \Omega_{\text{int}}$). Right: absorbing layers included ($\Omega = \Omega_{\text{int}} \cup \Omega_{\text{ext}}$). The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

displacement field is purely compressional. Its presence is consistent with the geometric interpretation discussed in section 6.1.1: the homogeneous Dirichlet constraint on the scalar potential indirectly enforces a vanishing tangential component of the reconstructed P-wave at $\partial\Omega$, so that the tangential part of the incident P-wave is transferred to the SV component. As a result, a spurious shear contribution appears in correspondence with the P boundary interaction. When the separation is performed on the extended domain, the spurious SV component is significantly reduced inside Ω_{int} , as shown in the right panels of figure 6.4, to the point of not being visible. In particular, the non-physical contribution is mainly confined within Ω_{ext} , and the decomposition in the interior of the domain is effectively preserved.

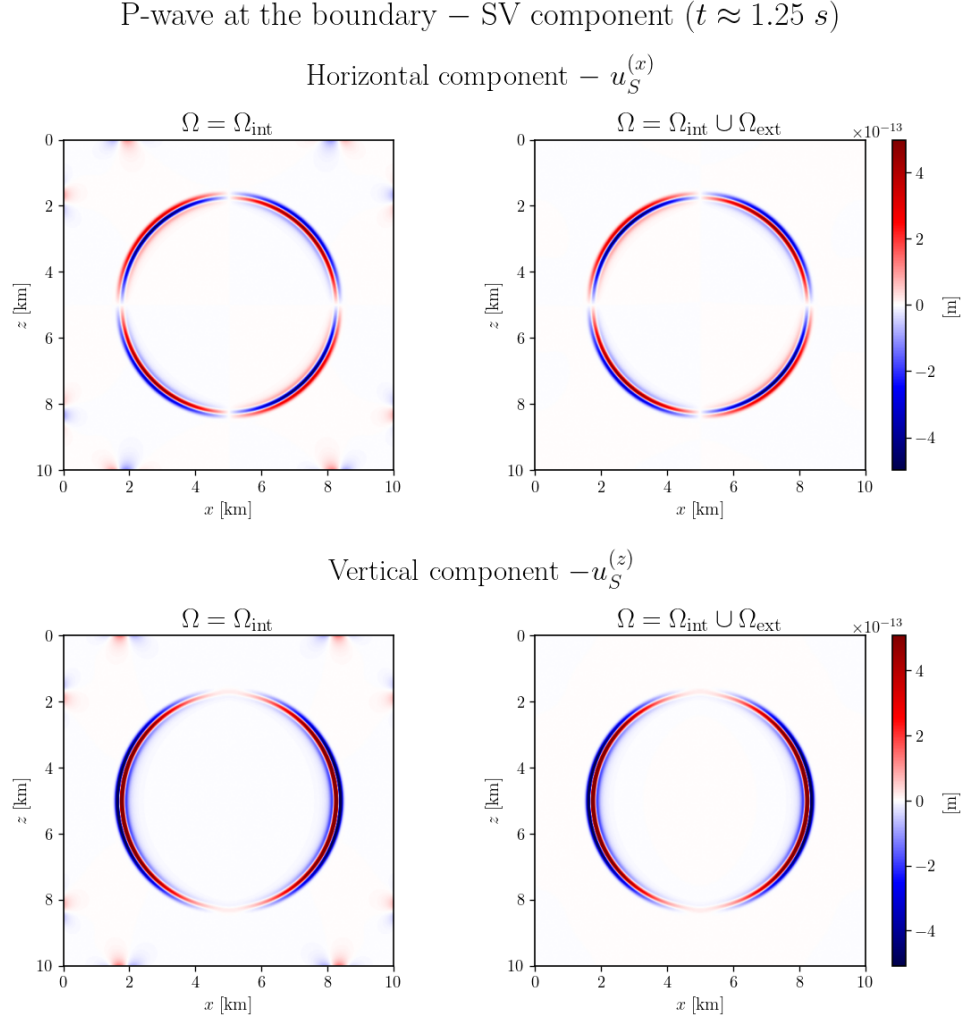


Figure 6.4: SV component of the wave-field, when the P-wave impinges on $\partial\Omega$ ($t \approx 1.25$ s). Left: absorbing layers excluded ($\Omega = \Omega_{\text{int}}$). Right: absorbing layers included ($\Omega = \Omega_{\text{int}} \cup \Omega_{\text{ext}}$). The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

The dual configuration, namely an SV-wave interacting with the boundary, does not introduce significant additional boundary-induced effects and is therefore not reported.

In light of these results, the Poisson–Dirichlet P–SV separation will be employed throughout the remainder of this work in combination with the domain extension strategy described in section 5.2.4, in order to mitigate the boundary-induced artifacts associated with wave interactions at $\partial\Omega$.

6.3. Insight on the accuracy of the numerical solution of the Poisson–Dirichlet problem

In this section, we investigate some properties of the Poisson–Dirichlet P–SV separation algorithm introduced in the previous section. In particular, the goal of this analysis is to identify the conditions under which the method is exact. To this end, we analyze the exactness of the algorithm in the idealized setting of band-limited displacement fields, where the modal content is fully resolved by the discrete grid. This allows us to isolate the role of the quadrature formulas and of the discrete trigonometric bases used in the construction of the method.

Overall, this analysis is intended to clarify the numerical and structural features of the proposed method that may support its use as a suitable approach for practical P–SV separation in grid-based wave propagation simulations.

6.3.1. Exactness in the band-limited case

In this subsection, we analyze the exactness of the Poisson–Dirichlet P–SV separation algorithm in the case of band-limited displacement fields. In particular, we aim to identify the conditions under which the discrete quadrature formulas used to approximate (6.15) and (6.16) recover the exact spectral representation of the wave-field.

Let us assume that the displacement components u_x and u_z belong to the following finite-dimensional spaces, respectively:

$$V_x = \text{span}\left(\{\xi_{n,m}\}_{(n,m) \in \Sigma^{(s)}}\right), \quad V_z = \text{span}\left(\{\eta_{n,m}\}_{(n,m) \in \Sigma^{(s)}}\right) \quad (6.23)$$

where, according to (6.15) and (6.16), we define

$$\begin{aligned} \xi_{n,m}(x, z) &= \frac{2}{\sqrt{L_x L_z}} \cos\left(\frac{n\pi}{L_x} x\right) \sin\left(\frac{m\pi}{L_z} z\right), \quad \forall (n, m) \in \Sigma^{(s)} \\ \eta_{n,m}(x, z) &= \frac{2}{\sqrt{L_x L_z}} \sin\left(\frac{n\pi}{L_x} x\right) \cos\left(\frac{m\pi}{L_z} z\right), \quad \forall (n, m) \in \Sigma^{(s)} \end{aligned}$$

In particular,

$$u_x(x, z) = \sum_{n=1}^{N_x} \sum_{m=1}^{N_z} \hat{u}_{x,n,m} \xi_{n,m}(x, z), \quad u_z(x, z) = \sum_{n=1}^{N_x} \sum_{m=1}^{N_z} \hat{u}_{z,n,m} \eta_{n,m}(x, z) \quad (6.24)$$

We refer to this assumption as *band-limitedness*, meaning that the modal coefficients $\hat{u}_{x,n,m}$ and $\hat{u}_{z,n,m}$ are identically null for all $n > N_x$ and/or $m > N_z$.

We now determine when the approximated modal coefficients (6.19) and (6.21) are exact, i.e.,

$$\begin{aligned}\hat{u}_{n,m}^{(x)} &= \sum_{i=0}^{N_x} \sum_{j=0}^{N_z-1} w_i^{(x)} u_x(x_i, z_{j+1/2}) \xi_{n,m}(x_i, z_{j+1/2}) h_x h_z = \hat{u}_{x,n,m} \\ \hat{u}_{n,m}^{(z)} &= \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z} w_j^{(z)} u_z(x_{i+1/2}, z_j) \eta_{n,m}(x_{i+1/2}, z_j) h_x h_z = \hat{u}_{z,n,m}\end{aligned}$$

where the quadrature weights $w_i^{(x)}$ and $w_j^{(z)}$ are given by (6.20) and (6.22), respectively.

We carry out the analysis for the horizontal component only, as the case of the vertical component follows analogously by interchanging the roles of the two coordinate directions. Substituting the expansion of u_x , given by (6.24), into the corresponding quadrature formula and rearranging the terms, we obtain

$$\begin{aligned}\hat{u}_{n,m}^{(x)} &= \frac{4}{L_x L_z} \sum_{p=1}^{N_x} \sum_{q=1}^{N_z} \hat{u}_{x,p,q} \left[\sum_{i=0}^{N_x} w_i^{(x)} \cos\left(\frac{p\pi}{N_x} i\right) \cos\left(\frac{n\pi}{N_x} i\right) h_x \right] \\ &\quad \cdot \left[\sum_{j=0}^{N_z-1} \sin\left(\frac{q\pi}{N_z} (j+1/2)\right) \sin\left(\frac{m\pi}{N_z} (j+1/2)\right) h_z \right]\end{aligned}$$

We now exploit the discrete orthogonality of the trigonometric bases:

$$\sum_{i=0}^{N_x} w_i^{(x)} \cos\left(\frac{p\pi}{N_x} i\right) \cos\left(\frac{n\pi}{N_x} i\right) = \frac{N_x}{2} \begin{cases} 2 & p = n = N_x \\ 1 & p = n = 1, \dots, N_x - 1 \\ 0 & p \neq n \end{cases} \quad (6.25)$$

$$\sum_{j=0}^{N_z-1} \sin\left(\frac{q\pi}{N_z} (j+1/2)\right) \sin\left(\frac{m\pi}{N_z} (j+1/2)\right) = \frac{N_z}{2} \begin{cases} 2 & q = m = N_z \\ 1 & q = m = 1, \dots, N_z - 1 \\ 0 & q \neq m \end{cases} \quad (6.26)$$

Applying (6.25) and (6.26) to the previous expression, we obtain that all terms vanish except for those corresponding to $p = n$ and $q = m$. Therefore, the approximated coefficients satisfy

$$\hat{u}_{n,m}^{(x)} = (1 + \delta_{n,N_x})(1 + \delta_{m,N_z}) \hat{u}_{x,n,m}, \quad \forall (n, m) \in \Sigma^{(s)}$$

Explicitly, this means

$$\hat{u}_{n,m}^{(x)} = \begin{cases} \hat{u}_{x,n,m} & n = 1, \dots, N_x - 1, m = 1, \dots, N_z - 1 \\ 2\hat{u}_{x,n,m} & n = N_x, m = 1, \dots, N_z - 1 \\ 2\hat{u}_{x,n,m} & n = 1, \dots, N_x - 1, m = N_z \\ 4\hat{u}_{x,n,m} & n = N_x, m = N_z \end{cases}$$

The same relation holds between $\hat{u}_{n,m}^{(z)}$ and $\hat{u}_{z,n,m}$.

In particular, the approximated coefficients coincide with the exact ones for all $n = 1, \dots, N_x - 1$ and $m = 1, \dots, N_z - 1$, i.e., for all modes strictly below the Nyquist limit in both coordinate directions. Therefore, if the displacement field is strictly sub-Nyquist band-limited, then the discrete quadrature formulas recover exactly all modal coefficients that are present in the expansion.

Thus, under this stricter assumption, the expansion coefficients of the right-hand side are also recovered exactly at the discrete level. Since the Poisson problem is inverted using the exact eigenvalues of the continuous Dirichlet Laplacian, the same holds for the scalar potential and, consequently, for the P-wave component. Finally, as no modes at or beyond the Nyquist limit are present, the truncated expansion coincides with the exact one. Hence, in floating-point arithmetic, the P and SV components are recovered exactly, up to machine precision, at their grid collocation points.

This shows that the proposed Poisson–Dirichlet P–SV separation algorithm is exact for strictly sub-Nyquist band-limited displacement fields whose modal coefficients vanish for all $n \geq N_x$ or $m \geq N_z$, i.e., at and beyond the Nyquist limit in both coordinate directions.

Remark 6.1.

The exactness property established above relies on the use of the eigenvalues of the continuous Dirichlet Laplacian in the inversion step. In particular, once the modal coefficients of the displacement field are exactly recovered, the spectral relation $\hat{f}_{n,m} = \hat{b}_{n,m}/\lambda_{n,m}$ ensures exact reconstruction of the scalar potential and, consequently, of the P-wave component.

An alternative implementation based on a second-order finite-difference discretization of the Dirichlet Laplacian, combined with a DST-based diagonalization, formally analogous to the approach used in the Poisson–Neumann case, would instead involve the corresponding discrete eigenvalues. From a spectral point of view, this amounts to replacing $\lambda_{n,m}$ with a modified quantity $\lambda_{h,n,m} = D(k_{x,n}, k_{z,m}) \lambda_{n,m}$, where the distortion factor $D \neq 1$ for non-negligible wavenumbers.

As a result, even in the band-limited setting considered above, such an approach would

introduce a systematic discrepancy in the inversion step, hindering the exact recovery of the scalar potential. Since, in practice, the relevant wave-fields can often be regarded as band-limited (see section 7.2), this observation provides a reason why the present spectral approach, although slightly more expensive (four trigonometric transforms instead of two), can be regarded as a reasonable alternative to a more direct finite-difference formulation.

7 | Comparison of the P–SV separation strategies in unbounded media

In the previous chapters, two alternative constructions of the P–SV wave-field separation have been introduced, based on the solution of a Poisson problem with either non-homogeneous Neumann or homogeneous Dirichlet boundary conditions. Their analytical properties have been discussed in detail, with particular attention to the mathematical and physical role of boundary conditions and to the exactness of the Dirichlet-based approach in the band-limited setting.

In this chapter, we focus on configurations in which all boundaries are equipped with absorbing layers, in order to mimic an effectively unbounded medium and reduce spurious reflections from the artificial boundaries. Moreover, as discussed in sections 5.2.4 and 6.2.4, the wave-field separations are performed in combination with the domain-extension mitigation strategy. Namely, the absorbing frame is included in the domain over which the separation is performed, so as to reduce boundary-induced artifacts in the separated fields.

The first part of the chapter is devoted to a qualitative comparison between the two approaches on heterogeneous elastic models. The objective is to evaluate their practical effectiveness in more realistic scenarios, highlighting possible differences in the reconstructed P and SV components when boundary effects are negligible.

In the second part, we investigate the physical relevance of the band-limitedness assumption underlying the exactness of the spectral Poisson–Dirichlet separation algorithm described in section 6.2.3. To this end, we introduce suitable quantitative indicators aimed at characterizing the spectral content of the numerical wave-fields generated in the simulations, and we verify whether such fields effectively satisfy the band-limitation conditions required by the spectral construction.

7.1. Qualitative comparison of the separation strategies

In this section, we present a series of numerical tests aimed at qualitatively comparing the two P–SV separation strategies introduced in the previous chapters, in order to assess the impact of the boundary conditions imposed on the auxiliary Poisson problem in effectively unbounded configurations.

We first consider a simple artificial bi-layer model (see appendix A.2.2), which provides a controlled setting to assess the behavior of the two approaches and to facilitate the interpretation of the resulting wave-field decompositions.

We then move to more realistic configurations, in order to evaluate the robustness of the separation procedures in geophysically relevant scenarios. To this end, we consider two benchmark models: a land section of the Marmousi-II model (see appendix A.2.3) and a section of the Sigsbee-Salt model (see appendix A.2.4).

Bi-layer model

The source term is defined as a vertical force with a Ricker wavelet temporal profile (see appendix A.1), with central frequency $f_0 = 10$ Hz, injected at $(x_s, z_s) = (5.0 \text{ km}, 2.5 \text{ km})$.

We first consider a representative snapshot of the wave-field extracted at $t \approx 1.67$ s and shown in figure 7.1. The corresponding Poisson–Neumann and Poisson–Dirichlet P–SV separations are shown in figures 7.2 and 7.3, respectively.

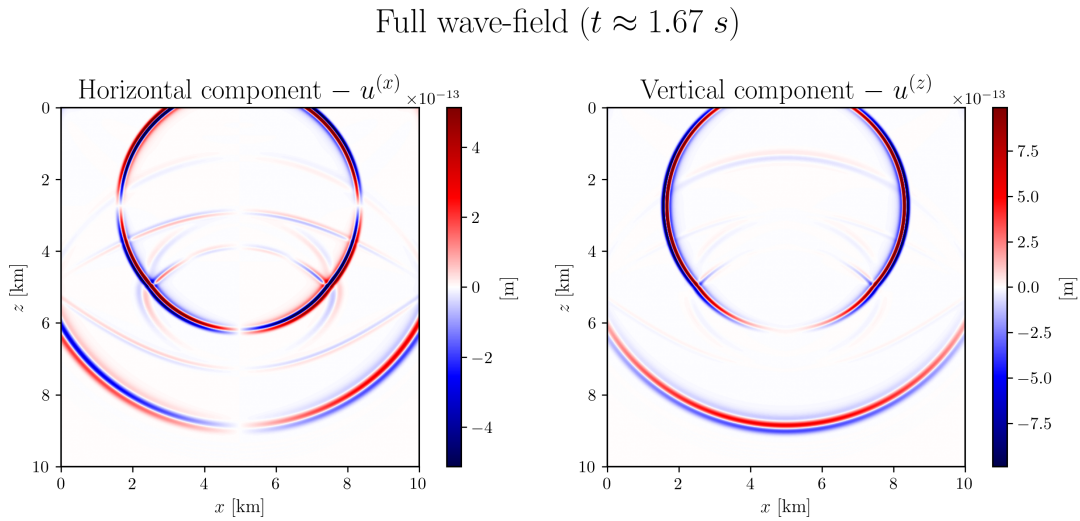


Figure 7.1: Snapshot of the full wave-field at $t \approx 1.67$ s. The horizontal (left) and vertical (right) components of the displacement field are shown.

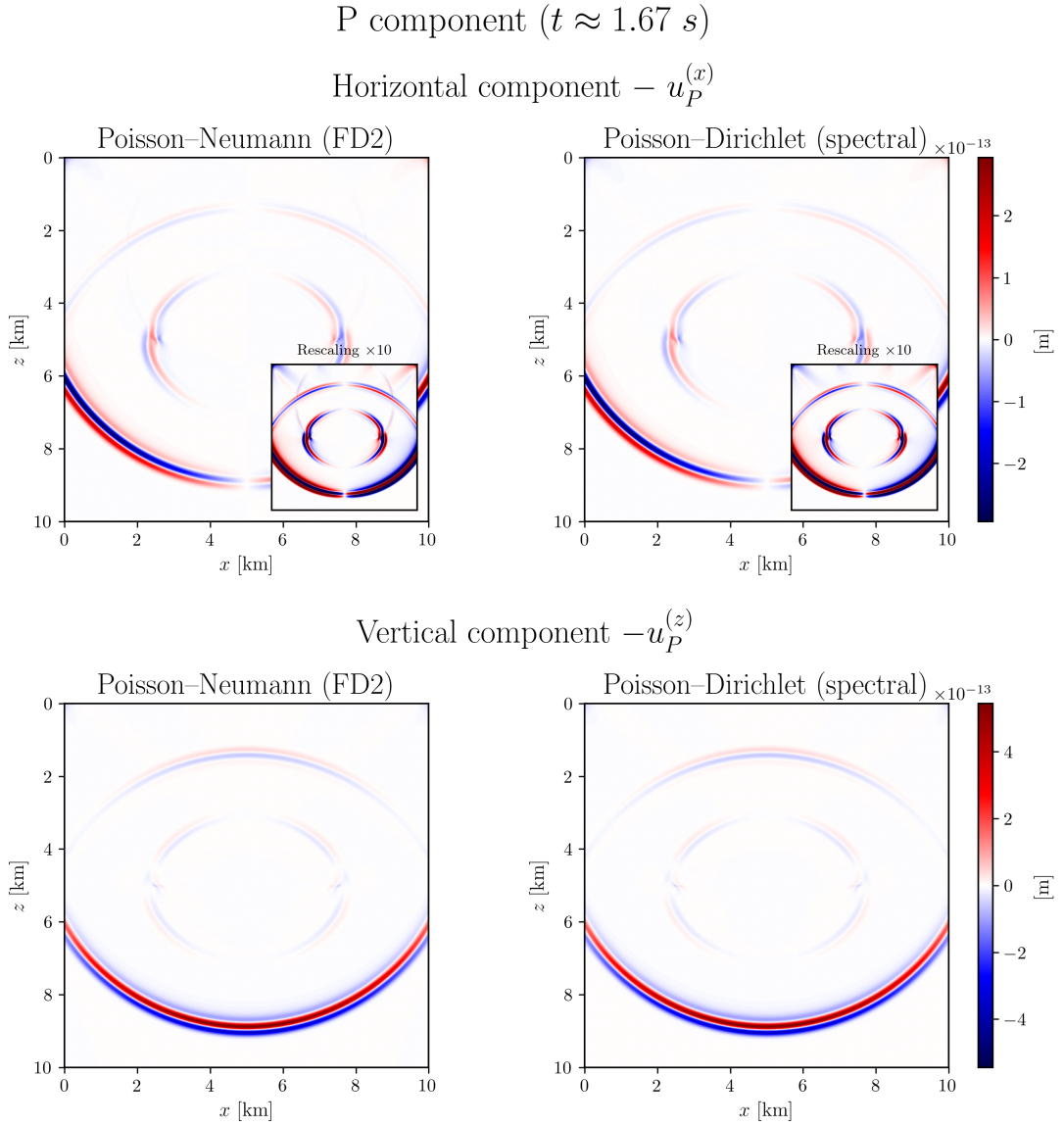


Figure 7.2: P component of the wave-field at $t \approx 1.67$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

The snapshot reported in figure 7.1 clearly shows the propagation of the direct P and SV wavefronts, together with the reflected and transmitted components generated at the interface. In particular, the faster P-wave and the slower SV-wave can be distinguished, as well as the mode conversions occurring upon interaction with the material discontinuity. The corresponding P–SV separations obtained with the two approaches are shown in figures 7.2 and 7.3. In both cases, the decomposition successfully separates the wave-field into its compressional and shear contributions, isolating both the direct and converted waves. Moreover, the amplitude, phase and spatial structure are preserved in a clean and

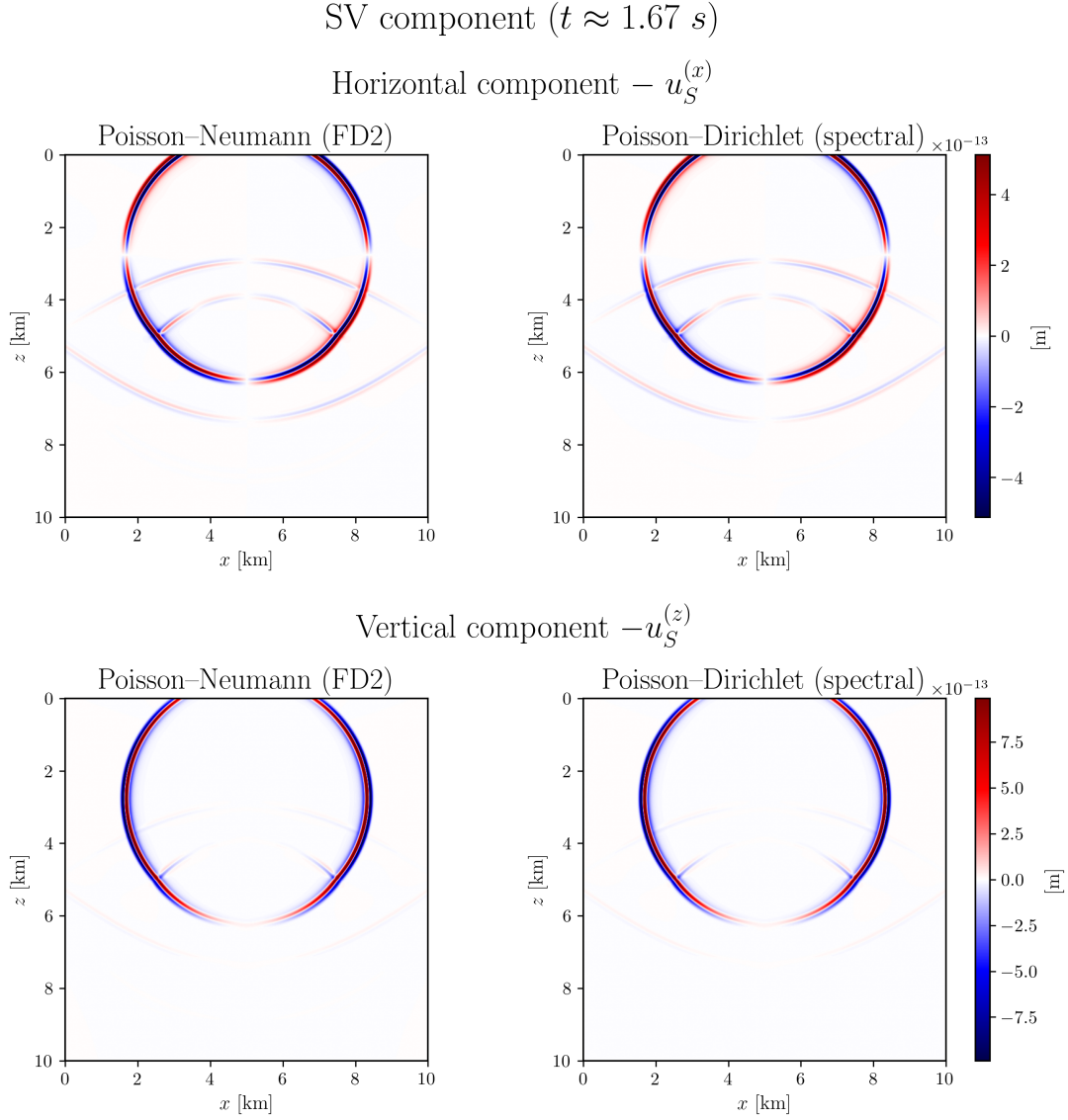


Figure 7.3: SV component of the wave-field at $t \approx 1.67$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

sharp way. A qualitative comparison between the two strategies shows that, in the bulk of the domain, the results are very similar, with no significant discrepancies in the reconstructed wave-fields. This indicates that, once boundary effects are mitigated, the two approaches exhibit a comparable behavior in terms of practical separation performance.

A closer inspection of the rescaled insets of the horizontal P component reveals additional features. In both approaches, weak spurious reflections emerging from the absorbing boundary can be observed, together with weak halos associated with the distortion of the

SV wave-field within the absorbing layers, consistently with the discussion in section 5.2.4. Moreover, in the Poisson–Neumann case, a residual ring reproducing the geometry of the SV wavefront is visible, with an amplitude only one order of magnitude smaller than the physical P-wave field. This feature is not appreciable in the corresponding Poisson–Dirichlet inset. This indicates a larger SV-to-P leakage in the finite-difference-based Poisson–Neumann separation, which can be attributed to the lower spectral accuracy of the discrete projection compared to the spectral Dirichlet construction.

To provide a global view over the entire simulated time interval and to better distinguish direct and reflected phases, we report the seismogram recorded at $z_r \approx 4.0$ km (i.e., 1 km above the interface and 1.5 km below the source), with explicitly labeled arrivals. Given the practical equivalence of the two approaches in the bulk, only the Poisson–Dirichlet separation is shown. Figure 7.4 confirms, over the whole simulation, the same behavior observed in the snapshot: the separation remains clean and stable throughout the bulk.

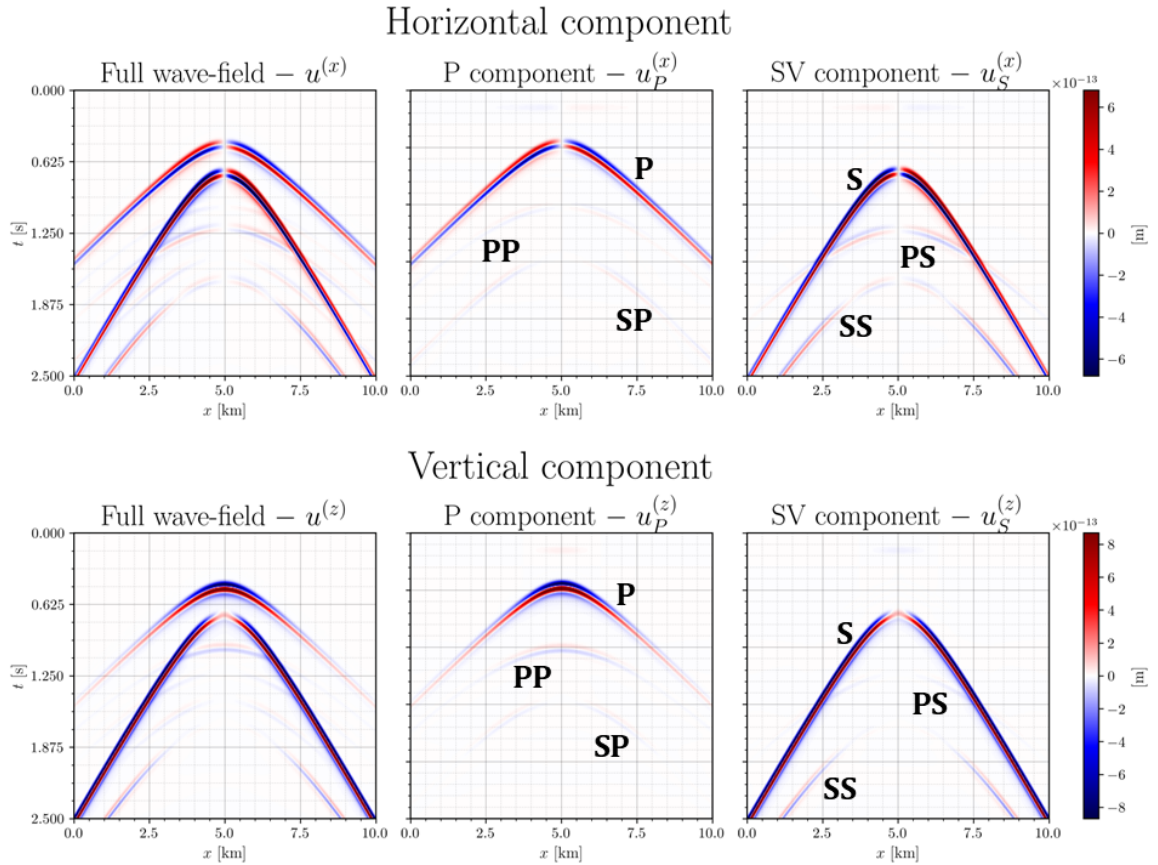


Figure 7.4: Seismograms recorded at $z_r \approx 4.0$ km. Left: full wave-field; center: P component; right: SV component. The horizontal (top) and vertical (bottom) components of the displacement field are shown. The separation is performed using the Poisson–Dirichlet approach, and the direct and reflected wave arrivals are explicitly labeled.

Land Marmousi-II model

The forcing term is an explosive source with the same temporal profile as in the previous test and injected at $(x_s, z_s) = (1.25 \text{ km}, 0.50 \text{ km})$. This test is not intended to provide a detailed analysis of the wave-field, but rather to assess the robustness of the two separation strategies in a more realistic, strongly layered solid medium. To this end, we simply report in figure 7.5 a representative snapshot of the wave-field at $t \approx 0.50 \text{ s}$, together with the associated Poisson–Neumann and Poisson–Dirichlet P–SV separations. For clarity, only the vertical component is shown, as it provides a representative view of the decomposition.

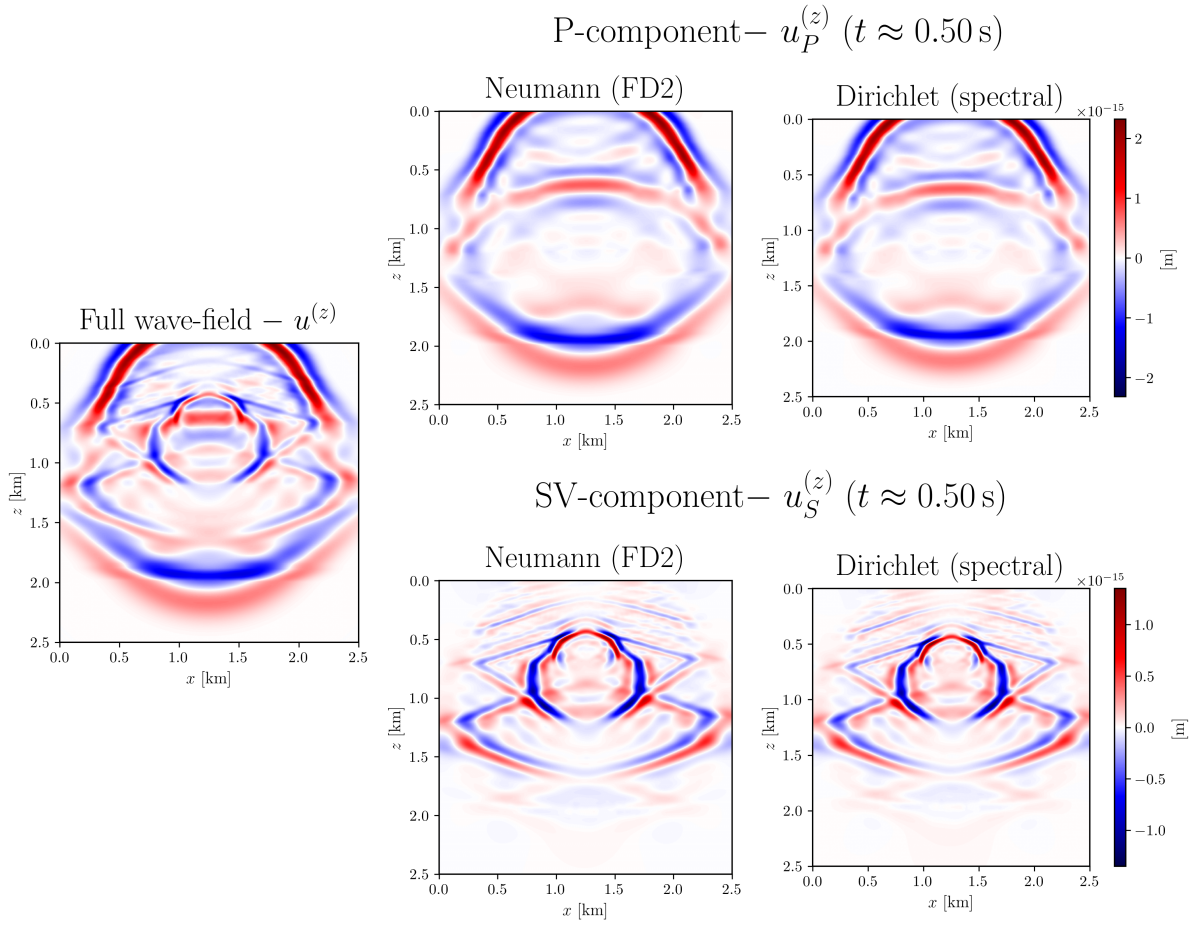


Figure 7.5: Snapshot of the wave-field and corresponding Poisson–Neumann and Poisson–Dirichlet P–SV separations at $t \approx 0.50 \text{ s}$. Left: full wave-field. Center: Poisson–Neumann separation. Right: Poisson–Dirichlet separation. For the separated fields, the P component is shown on the top row and the SV component on the bottom row. Only the vertical component is reported.

Figure 7.5 shows that both approaches remain numerically stable, in the sense that no spurious numerical artifacts or amplification of the separated fields are observed, and produce physically consistent and practically equivalent results in the physical bulk of the domain, i.e., in the region enclosed by the absorbing layers. The explosive source generates

a dominant direct P-wave, while the multiple reflections and conversions induced by the layered structure, clearly visible in the full wave-field, are effectively captured and properly localized within the P and SV components by both strategies, with amplitude, phase, and spatial structure accurately preserved.

Sigsbee–Salt model

We employ the same source as in the previous test, with central frequency $f_0 = 7.5$ Hz and injected at $(x_s, z_s) = (2.0 \text{ km}, 0.5 \text{ km})$. As a more challenging test, we consider a realistic configuration involving a salt structure, characterized by strong impedance contrasts and more complex interfaces. As before, we restrict the analysis to a representative snapshot of the vertical component of the wave-field and the corresponding P–SV decompositions, reported in figure 7.6, focusing on the overall robustness of the two strategies.

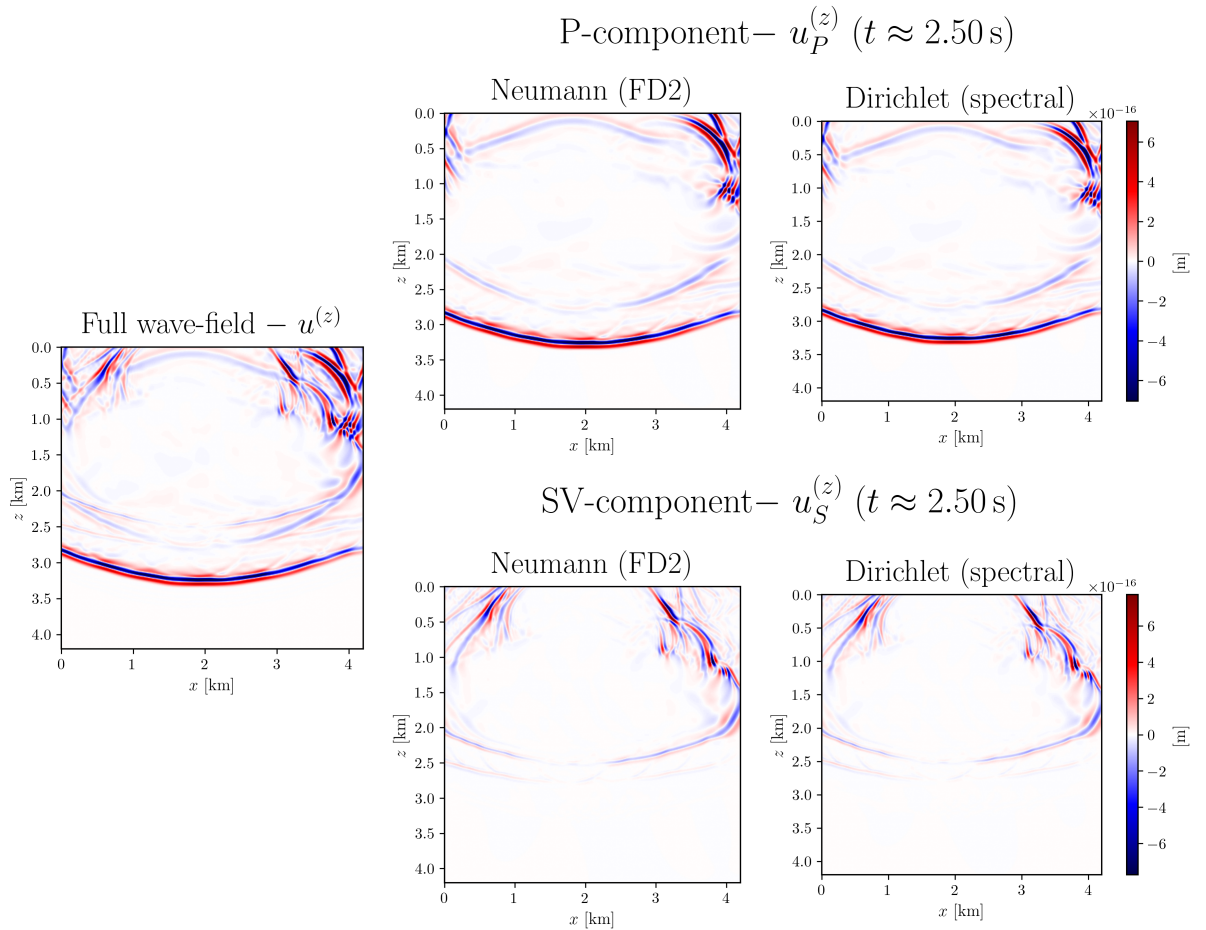


Figure 7.6: Snapshot of the wave-field and corresponding Poisson–Neumann and Poisson–Dirichlet P–SV separations at $t \approx 2.50$ s. Left: full wave-field. Center: Poisson–Neumann separation. Right: Poisson–Dirichlet separation. For the separated fields, the P component is shown on the top row and the SV component on the bottom row. Only the vertical component is reported.

In this setting, the strong contrasts associated with the salt dome give rise to significant mode conversions. These effects are clearly visible in the full wave-field and are consistently captured by both separation strategies, with the converted energy properly localized within the SV component. Even in the presence of such a highly complex wave-field, both separation strategies remain robust, producing physically consistent and practically equivalent results.

In summary, in effectively unbounded configurations where all boundaries of the computational domain are equipped with absorbing layers, the use of the domain extension mitigation strategy (see sections 5.2.4 and 6.2.4) ensures that the choice of the boundary conditions in the auxiliary Poisson problem has practically negligible impact on the quality of the separation. However, an exception is represented by the residual SV-to-P leakage observed in the Poisson–Neumann case, visible as a weak ring in the bi-layer test, which points to a slightly lower accuracy of the finite-difference projection compared to the spectral Dirichlet approach. Nevertheless, in scenarios of practical relevance, both methods remain stable and provide satisfactory and physically consistent decompositions.

7.2. Analysis of the spectral content of the elastic wave-fields

In this section, we investigate the spectral content of the numerical elastic wave-fields in order to assess the practical relevance of the band-limitedness assumption underlying the exactness of the spectral Poisson–Dirichlet separation (see section 6.3.1). To this end, we first discuss the physical mechanisms supporting such an assumption and then introduce quantitative indicators to characterize the distribution of energy in the wavenumber domain based on the simulated fields.

7.2.1. Physical relevance of the band-limitedness assumption

In practical applications, the band-limitedness of the wave-field is not only a mathematical idealization, but can be regarded as a physically meaningful assumption.

First, the displacement field is generated by source term with a prescribed temporal spectrum. The wavelets used in the simulations have essentially vanishing energy above a maximum frequency $f_{\max}$, so that the corresponding wavenumbers are bounded from above by

$$k_M \approx 2\pi \frac{f_{\max}}{V_{\min}}, \quad V_{\min} = \min_{\underline{x} \in \Omega} V_S(\underline{x})$$

In general, the natural evolution of the elastic wave equation does not spontaneously generate significant energy at wavenumbers much larger than k_M . As a consequence, the physical wave-field is not expected to contain arbitrarily high spatial frequencies: its energy is concentrated in a finite and bounded range of wavenumbers

$$0 \leq k \lesssim k_M$$

To numerically solve the elastic wave equation, we employed the numerical scheme presented in section 3.1.2. As discussed in section 3.2.2, in order for this scheme to have negligible numerical dispersion, equations (3.14) must be satisfied. Accordingly (see appendix A.2), to ensure a conservative choice, in our simulations we used

$$h_x = h_z = h = \frac{V_{\min}}{6 f_{\max}}$$

so that the maximum resolvable wavenumbers on the employed discrete grid are (see section 6.2.3)

$$k_{x,\max} = k_{z,\max} = 6\pi \frac{f_{\max}}{V_{\min}} = 3k_M$$

Hence, the numerical grid is able to resolve the physical wavenumber content of the wave-field with a significant spectral margin, ensuring that no physically meaningful component lies near the Nyquist limit of the grid.

In this sense, we expect $u^{(x)}$ and $u^{(z)}$ to be effectively band limited below $\sim k_M$, with all physically meaningful components fully represented by the chosen discretization.

7.2.2. Quantitative analysis of the spectral content of the elastic wave-field

To quantitatively assess the spectral content of the numerical wave-field, we introduce two indicators based on the discrete spectral representation of the displacement components.

According to equations (6.19) and (6.21), we denote by $\hat{u}_{n,m}^{(x)}$ and $\hat{u}_{n,m}^{(z)}$ the approximated modal coefficients of the horizontal and vertical displacement components, respectively. We define the modal energy as

$$e_{n,m} = |\hat{u}_{n,m}^{(x)}|^2 + |\hat{u}_{n,m}^{(z)}|^2, \quad \forall (n, m) \in \Sigma^{(s)}$$

and the total spectral energy as

$$E_{\text{tot}} = \sum_{n=1}^{N_x} \sum_{m=1}^{N_z} e_{n,m}$$

To assess the validity of the physical band-limitedness assumption, addressed in the previous subsection, we consider the fraction of modal energy contained below the physical cutoff wavenumber k_M :

$$\rho_M = \frac{1}{E_{\text{tot}}} \sum_{n=1}^{N_M^{(x)}} \sum_{m=1}^{N_M^{(z)}} e_{n,m}$$

where $N_M^{(x)} < N_x$ and $N_M^{(z)} < N_z$ are the maximum spectral indices such that $k_{x,n} \leq k_M$ and $k_{z,m} \leq k_M$, respectively. A value of ρ_M close to unity indicates that the wave-field is effectively band-limited below k_M .

In addition, it is important to quantify the energy contained in the highest resolvable modes, which are the critical ones for the accuracy of discrete spectral projections (see section 6.3.1). To this end, we introduce the fraction of energy associated with the Nyquist modes as

$$\eta_{\text{crit}} = \frac{1}{E_{\text{tot}}} \left[\sum_{m=1}^{N_z-1} e_{N_x,m} + \sum_{n=1}^{N_x-1} e_{n,N_z} + e_{N_x,N_z} \right]$$

The temporal evolution of the indicators ρ_M and η_{crit} over the simulated time intervals is reported in figures 7.7, 7.8 and 7.9 for the three models considered in the previous subsection. In each case, the indicators are shown together with the source time function, in order to highlight the correlation between the source injection phase and the transient deviation from the band-limited regime.

In all configurations, a consistent behavior is observed. During the source injection phase, both indicators exhibit a transient deviation from their asymptotic values, reflecting the broadband spectral content introduced by the source. However, once the source has injected its energy, the wave-field rapidly evolves towards a regime in which it is effectively band-limited. In particular, ρ_M approaches unity and remains close to one during the subsequent propagation, while η_{crit} quickly decays to negligible values.

The inset plots further show that, in the post-transient regime, the residual fluctuations of both indicators remain extremely small. In particular, $\rho_M > 99\%$, indicating that the spectral content of the numerical wave-field is effectively contained in the physically relevant wavenumber range, in agreement with the expected behavior. Most importantly, the values of η_{crit} are of the order of $\sim 10^{-7}$, indicating that the energy associated with

Bi-layer model

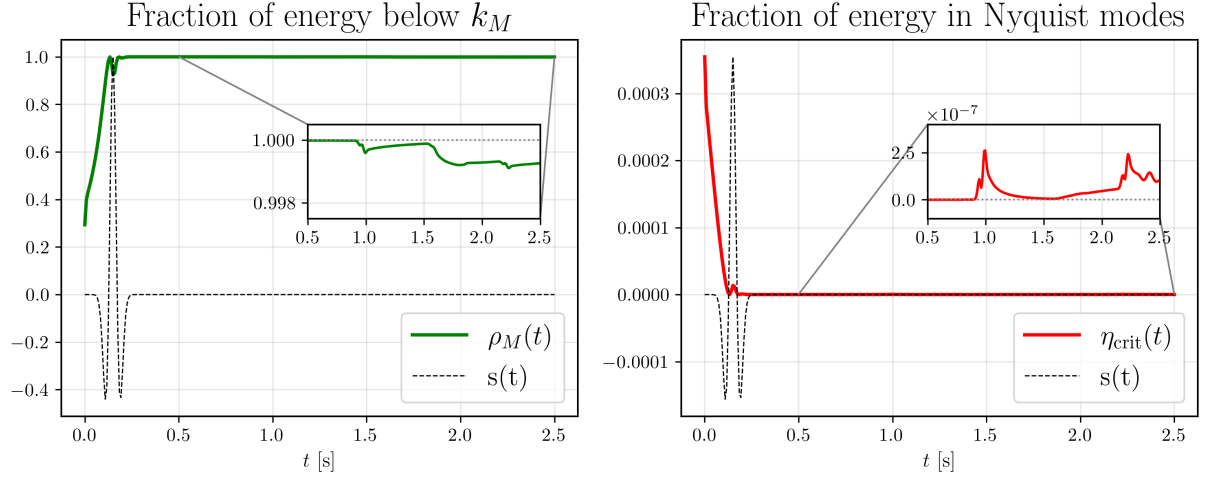


Figure 7.7: Time evolution of ρ_M (left) and η_{crit} (right) for the bi-layer model. The dashed curve represents the rescaled source wavelet. The inset plots show a zoom of the interval $t \in [0.5 \text{ s}, 2.5 \text{ s}]$.

Marmousi–II model

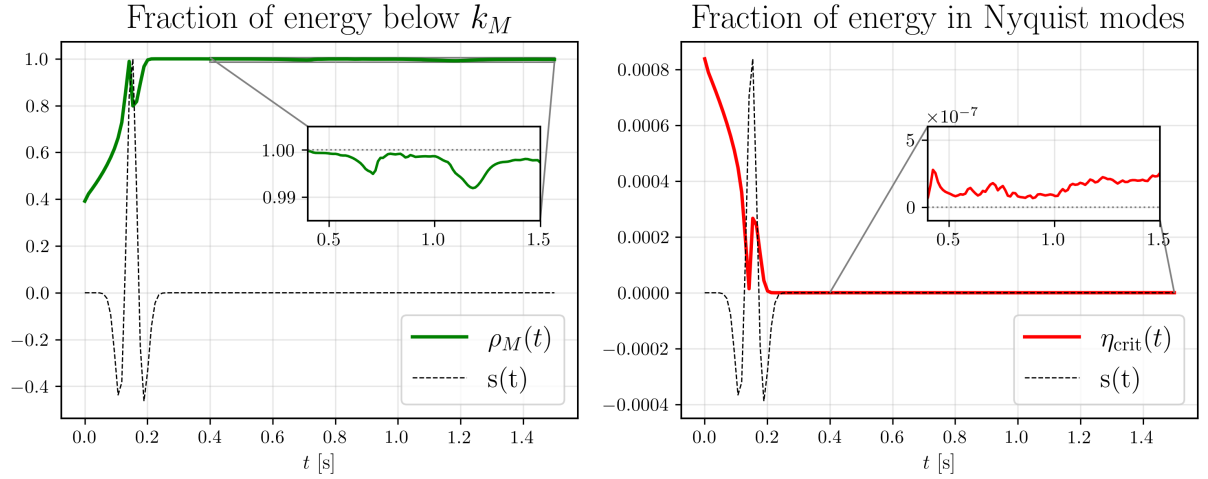


Figure 7.8: Time evolution of ρ_M (left) and η_{crit} (right) for the land Marmousi–II model. The dashed curve represents the rescaled source wavelet. The inset plots show a zoom of the interval $t \in [0.4 \text{ s}, 1.5 \text{ s}]$.

the Nyquist modes is negligible from a practical point of view.

These observations have a direct implication for the interpretation of the differences between the Poisson–Neumann and Poisson–Dirichlet approaches. In all considered config-

Sigsbee–Salt model

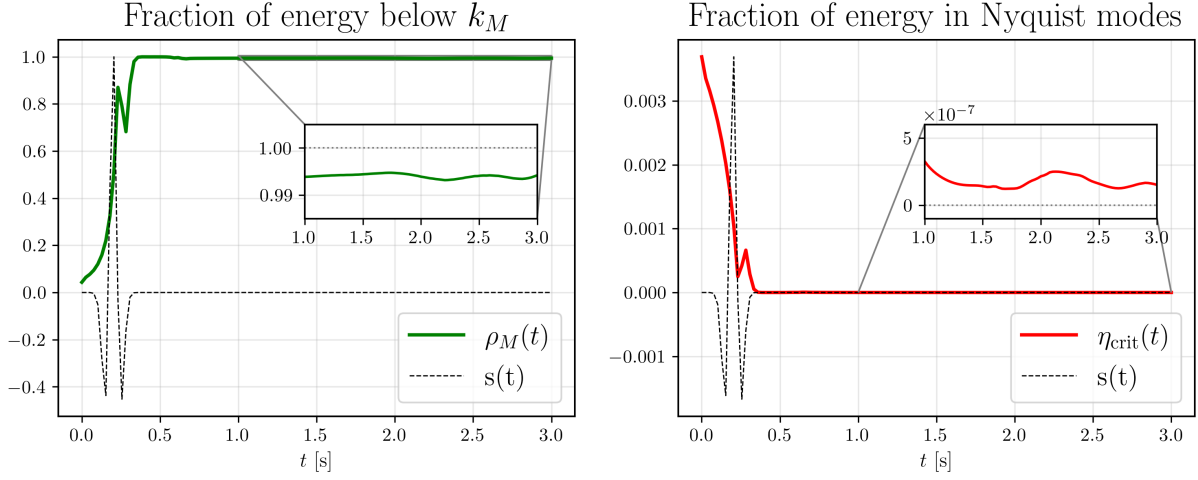


Figure 7.9: Time evolution of ρ_M (left) and η_{crit} (right) for the Sigsbee–Salt model. The dashed curve represents the rescaled source wavelet. The inset plots show a zoom of the interval $t \in [1.0 \text{ s}, 3.0 \text{ s}]$.

urations, the energy associated with the Nyquist modes remains several orders of magnitude smaller than the total spectral energy, so that the contribution of the highest resolvable modes can be regarded as negligible in practice. As a consequence, the spectral Dirichlet approach can be regarded as more accurate, since any quadrature errors in the computation of the modal coefficients are not expected to play a significant role in the resulting decomposition. In contrast, in the finite-difference Neumann formulation, the discrete differential operators do not reproduce exactly their continuous counterparts in the spectral domain. As a result, the method is affected by a systematic distortion of the spectral content, which is not limited to the highest wavenumbers, but also affects the intermediate-wavenumber components. This provides a plausible consistent interpretation of the spurious ring observed in the bi-layer configuration for the Neumann approach, and its absence in the spectral Dirichlet case.

8 | Influence of the free surface boundary condition

The numerical tests reported in the previous chapter indicate that, owing to the adoption of the domain extension mitigation strategy (see sections 5.2.4 and 6.2.4), the Poisson–Neumann and Poisson–Dirichlet separation strategies yield practically equivalent results in effectively unbounded media, i.e., when the boundaries of the computational domain are surrounded by absorbing layers. In this configuration, both approaches lead to clean wave-field separations within the physical core.

However, the presence of a free surface introduces additional complexity in the analysis of P–SV wave-field separation. In this setting, the behavior of the separation algorithms is strongly influenced by the interaction between the physical boundary condition at the free surface and the implicit constraints induced by the mathematical boundary conditions of the Poisson–Neumann and Poisson–Dirichlet auxiliary problems (see sections 5.2.1 and 6.1.1). The aim of this chapter is to investigate how the presence of a free surface affects the performance and physical consistency of the considered P–SV separation strategies.

The chapter is organized as follows. First, we briefly describe the numerical treatment of the free surface and discuss its interaction with the separation procedure. Then, we compare the behavior of the two separation strategies in the presence of a free surface, considering both solid and fluid configurations. Finally, we briefly revisit the limitations of the FFT-based decomposition method proposed in [47] in the presence of a fluid free surface. The artifacts observed in this case are consistent with those reported by the authors and can be attributed to the implicit periodic boundary conditions enforced by the FFT framework.

8.1. Free surface boundary condition and interaction with P–SV separation

In all the considered cases, the free surface is assumed to be horizontal and located at $z = 0$ m. In this case, the free surface boundary condition reduces to

$$\sigma_{xz} = \sigma_{zz} = 0, \quad \forall (x, z) \in [0, L_x] \times \{0\}$$

According to the staggered grid arrangement employed throughout this work (see section 3.1.1), it is imposed through the second-order stress-imaging method (see, e.g., [19]). This method relies on the introduction of auxiliary ghost nodes above the free surface and on an anti-symmetric mirroring of the stress tensor components with respect to the free surface plane, namely

$$\begin{aligned} \sigma_{i,0}^{(xz)} &= 0, \quad \sigma_{i,-1}^{(xz)} = -\sigma_{i,1}^{(xz)}, \quad \forall i \in \Sigma_i^{(n)} \\ \sigma_{i+1/2,-1/2}^{(zz)} &= -\sigma_{i+1/2,1/2}^{(zz)}, \quad \sigma_{i+1/2,-3/2}^{(zz)} = -\sigma_{i+1/2,3/2}^{(zz)}, \quad \forall i \in \Sigma_i^{(c)} \end{aligned}$$

The needed velocity components at the ghost nodes are then obtained consistently from these relations through the constitutive equations.

This approach provides a consistent numerical enforcement of the free surface condition without requiring modifications of the interior stencil. However, it does not by itself determine how the wave-field is decomposed into P and S components. The behavior of the separation is instead primarily governed by the interaction between the physical boundary condition at the free surface and the implicit constraints induced by the Poisson–Neumann and Poisson–Dirichlet separation strategies.

8.1.1. Interaction between free surface and P–SV separation

In this context, the boundary constraints implicitly enforced by the Poisson-based separation strategies play a non-negligible role when a free surface is present. In particular, as discussed in sections 5.2.1 and 6.1.1, the Poisson–Neumann formulation enforces a vanishing normal component of the SV wave-field at the boundary (i.e., $u_S^{(z)} = 0$ at the free surface), whereas the Poisson–Dirichlet formulation enforces a vanishing tangential component of the P displacement field (i.e., $u_P^{(x)} = 0$ at the free surface).

For a solid free surface, neither of these constraints is physically meaningful, as the traction-free condition does not translate into simple constraints on the displacement

components. To avoid introducing spurious boundary effects directly at the physical interface, the computational boundary used for the separation is therefore shifted one grid cell above the free surface, exploiting the ghost-node treatment required by the stress-imaging method.

In contrast, in the case of a fluid free surface, the condition imposed by the Poisson–Neumann formulation is consistent with the physical behavior of the wave-field, as no shear component can be sustained in the medium. As a result, the boundary of the computational domain can be made to coincide with the physical boundary where the free surface condition is applied.

8.2. Comparison of P–SV separation strategies in the presence of a free surface

In this section, we compare the behavior of the Poisson–Neumann and Poisson–Dirichlet separation strategies in the presence of a free surface. For the sake of clarity, only homogeneous models are considered, as their simplicity makes them an effective diagnostic framework to isolate and highlight the effects of the boundary condition. Two configurations are analyzed, corresponding to solid and fluid free surfaces. In the latter case, the discussion is complemented by a brief remark on the limitations of the FFT-based decomposition approach.

8.2.1. Solid free surface

We consider the homogeneous solid model introduced in appendix A.2.1. The forcing term is defined as an explosive source with a Ricker wavelet temporal profile (see appendix A.1), with central frequency $f_0 = 10$ Hz, injected at $(x_s, z_s) = (5.0 \text{ km}, 0.0 \text{ km})$.

We consider a representative snapshot of the wave-field, extracted at $t \approx 1.0$ s and shown in figure 8.1. The resulting P and SV components, for both the Poisson–Neumann and Poisson–Dirichlet separation strategies, are shown in figures 8.2 and 8.3, respectively.

The snapshot in figure 8.1 displays the full wave-field at an early stage of propagation. The fast P wave has already propagated to larger depths, forming the leading wavefront. Behind it, the slower SV wave is clearly visible as a secondary wavefront. In addition, a Rayleigh surface wave can be observed propagating along the free surface. This wave detaches from the SV front due to its lower propagation speed and is characterized by an amplitude that rapidly decays with depth. Finally, a weaker PS-head wave can be

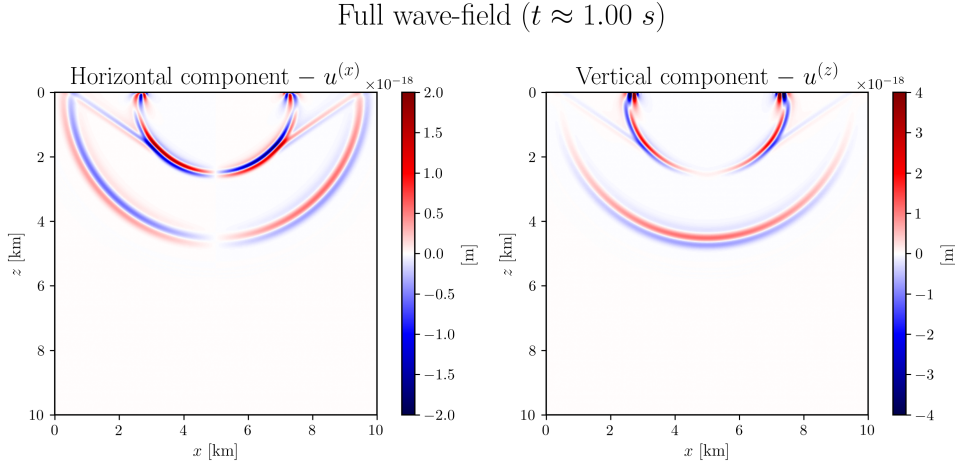


Figure 8.1: Snapshot of the full wave-field at $t \approx 1.0$ s. The horizontal (left) and vertical (right) components of the displacement field are shown.

identified, connecting the P and SV fronts.

Figures 8.2 and 8.3 highlight relevant differences in the near free surface behavior of the two decomposition strategies, emphasized in the rescaled insets. The most significant discrepancies concern how the two approaches handle the separation of the Rayleigh surface wave. In particular, the $u_P^{(x)}$ and $u_P^{(z)}$ components exhibit similar spatial structures in the two decompositions, but with reversed polarity. In addition, the $u_P^{(z)}$ component obtained from the Poisson–Dirichlet separation has smaller amplitudes.

Further minor differences can be observed in the superposition of the P and PS-head waves in the immediate vicinity of the free surface. In particular, a slight attenuation of the amplitude of the $u_P^{(x)}$ component is visible in the Poisson–Dirichlet case, which is not observed in the Poisson–Neumann decomposition.

Although only the homogeneous configuration is reported here for clarity, additional tests performed on heterogeneous media, including bi-layer and multi-layer models, as well as more complex benchmarks such as the land Marmousi–II and Sigsbee–Salt models, exhibit analogous differences between the two strategies. In such cases, their detailed structure naturally depends on the medium and on the employed forcing term, as different wave phenomena are involved in different configurations. Nevertheless, for a given medium, the two separation strategies systematically yield distinct near free surface decompositions, characterized by similar relative discrepancies.

Overall, this indicates that the origin of the observed differences can be primarily attributed to the interaction between the mathematical boundary conditions of the separation strategies and the physical free surface condition, while medium heterogeneity and

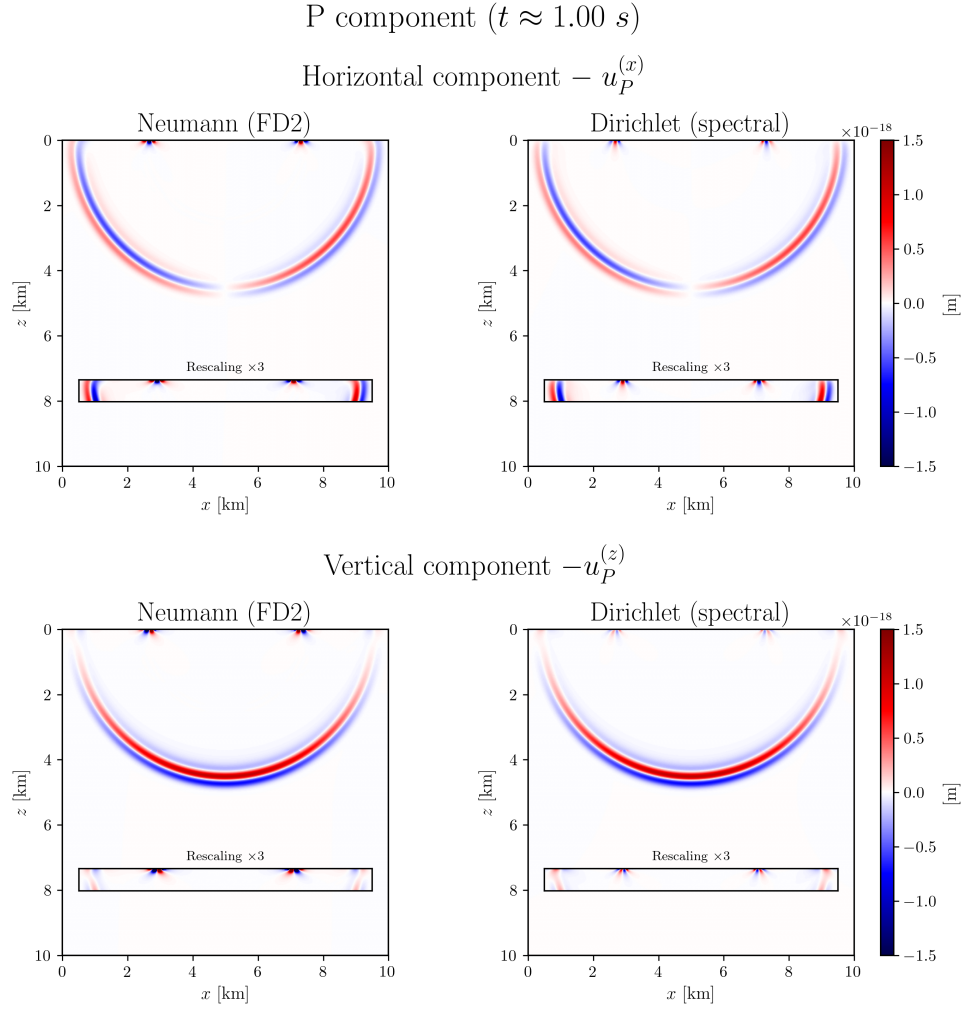


Figure 8.2: P component of the wave-field at $t \approx 1.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

the choice of the source mainly affect their specific manifestation. However, it is worth stressing that, in the solid free surface case, the observed discrepancies cannot be used to rank the two separation strategies, since P–SV coupling at the free surface is an intrinsic physical feature and no unequivocal reference separation exists.

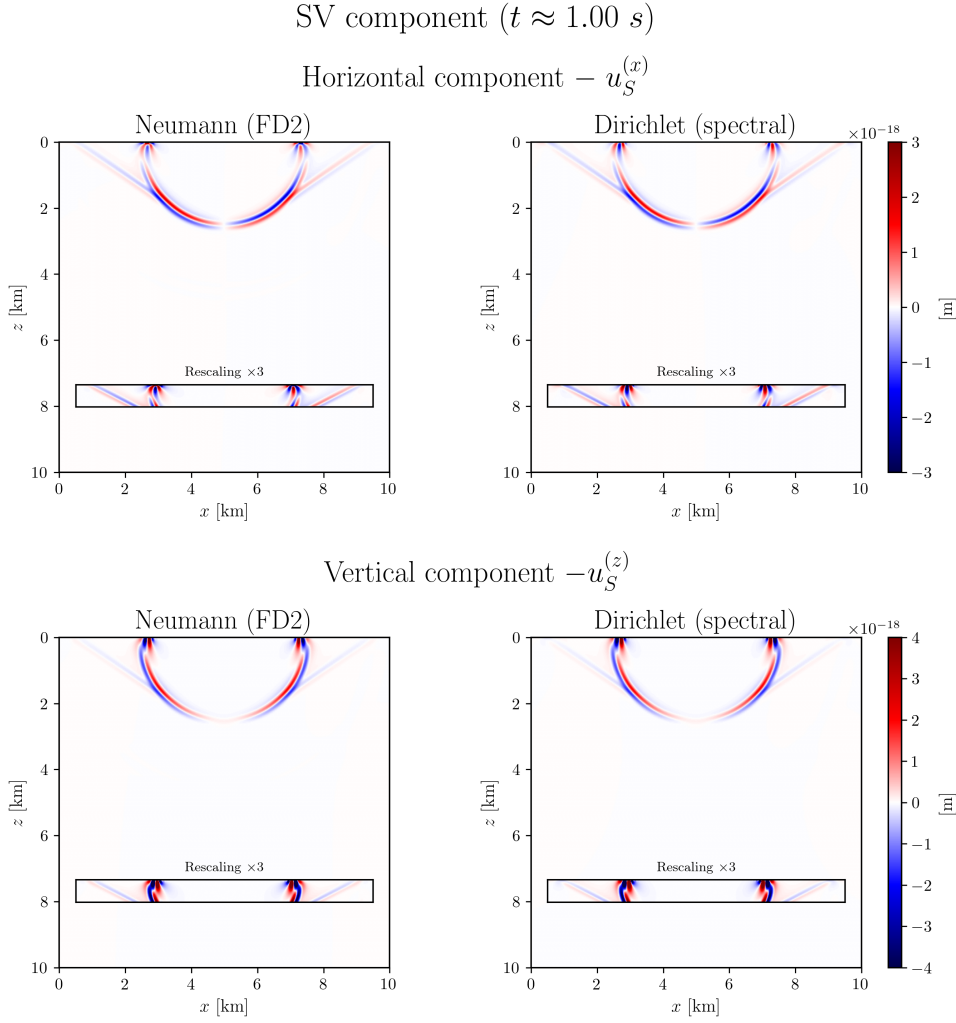


Figure 8.3: SV component of the wave-field at $t \approx 1.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

8.2.2. Fluid free surface

We consider the homogeneous fluid model introduced in appendix A.2.1. The forcing term is defined as in the previous test, with central frequency $f_0 = 5$ Hz and injected at $(x_s, z_s) = (5.0 \text{ km}, 1.5 \text{ km})$.

We consider a representative snapshot of the wave-field, extracted at $t \approx 2.0$ s and shown in figure 8.4. The resulting P and SV components, for both the Poisson–Neumann and Poisson–Dirichlet separation strategies, are shown in figures 8.5 and 8.6, respectively.

The snapshot in figure 8.4 displays a significantly simpler wave-field structure compared

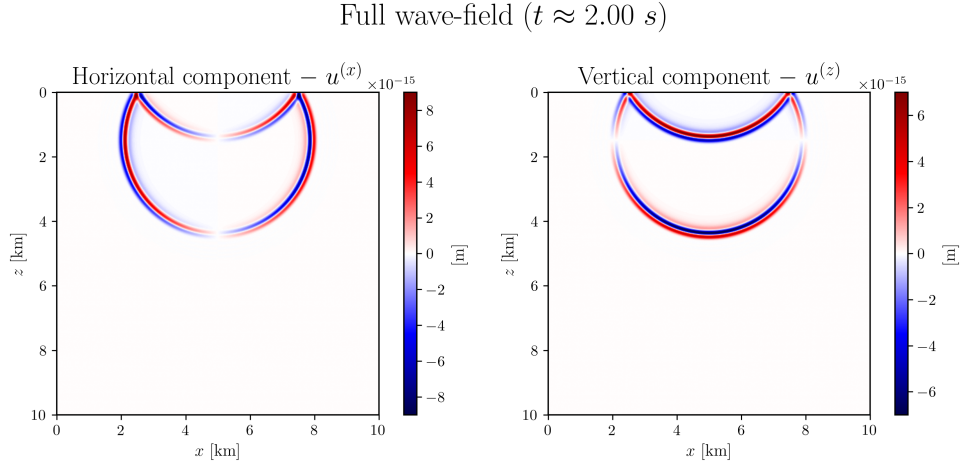


Figure 8.4: Snapshot of the full wave-field at $t \approx 2.0$ s. The horizontal (left) and vertical (right) components of the displacement field are shown.

to the solid case. Since the fluid medium does not support shear wave propagation, only the compressional wave is present. No mode conversion occurs as a result of the reflection at the free surface, and no surface waves are generated. As a result, the wave-field is characterized by a single wavefront associated with the P wave.

The separated P wave-fields reported in figure 8.5 show that the P components recovered by the Poisson–Neumann and Poisson–Dirichlet formulations are nearly indistinguishable at the scale of the figure. The main difference between the two strategies does not concern the reconstruction of the dominant P wave-field, but rather the amount and structure of the residual SV component.

The snapshot of the SV component of the wave-field, shown in figure 8.6, together with the rescaled insets, highlight a fundamental difference between the two separation strategies. In a fluid medium, shear waves cannot propagate; therefore, the SV-wave components displayed in the panels represent numerical leakage.

In particular, the Poisson–Dirichlet separation strategy induces spurious P-to-SV mode conversions, which manifest as localized bump-like features in the SV wave-field. These features propagate along the free surface following the incidence of the P-wave, consistent with a spurious conversion origin.

In contrast, as shown by the rescaled insets, the residual SV component obtained with the Poisson–Neumann separation is about one order of magnitude smaller in amplitude. Moreover, its spatial structure is fully consistent with that of the P wave-field. This behavior resembles the spurious ring observed in the bi-layer model test presented in section 7.1, suggesting that the observed SV component can be attributed to numerical

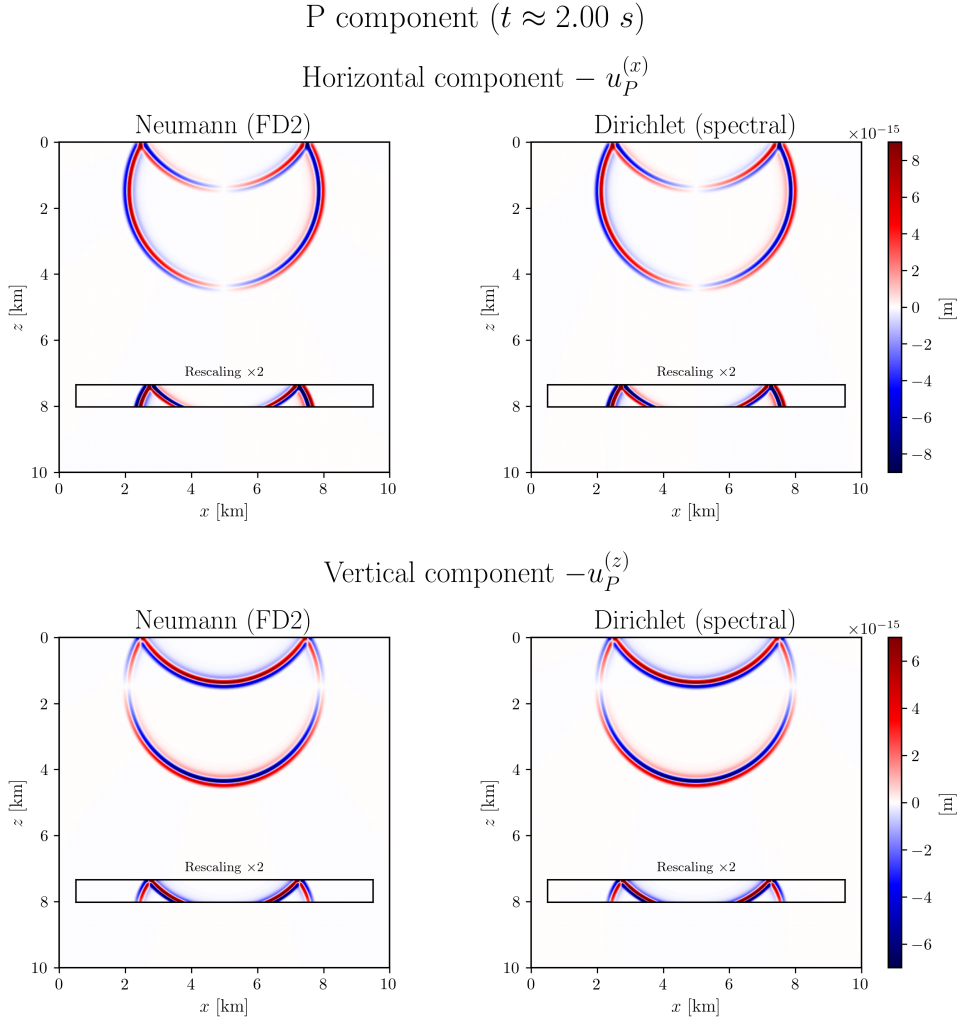


Figure 8.5: P component of the wave-field at $t \approx 2.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

errors, with no evidence of a boundary-induced or structural artifact associated with the separation method, which is consistent with the expected absence of shear waves in a fluid medium.

These observations can be directly related to the boundary constraints implicitly enforced by the two separation strategies. As already mentioned, in the Poisson–Neumann formulation, a vanishing normal component of the SV wave-field is imposed at the computational boundary. Since this condition is consistent with the physical behavior of a fluid medium, the computational boundary is made to coincide with the physical free surface. As a result, no spurious mode conversion is observed, and the residual SV component remains negligible. In contrast, the Poisson–Dirichlet formulation enforces a vanishing tangential

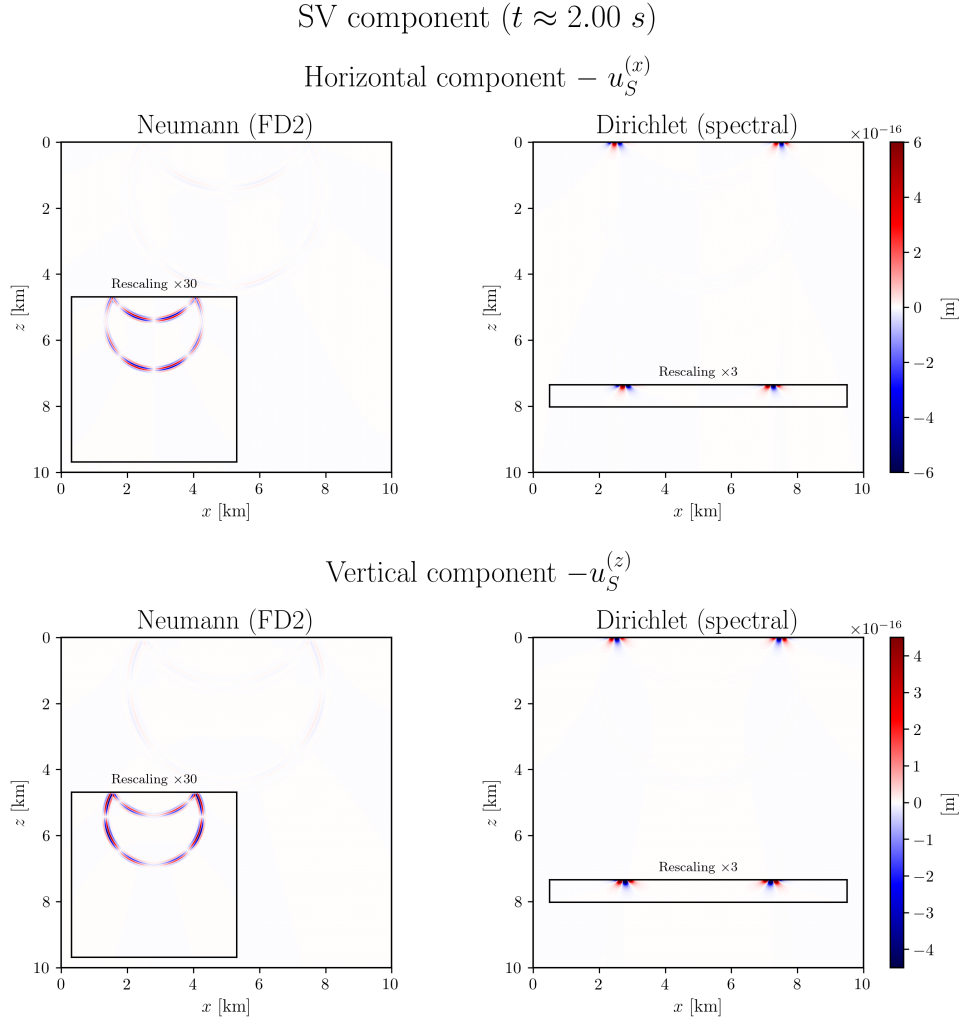


Figure 8.6: SV component of the wave-field at $t \approx 2.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–Dirichlet separation. The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

component of the P wave-field at the computational boundary. Since this requirement is not physically meaningful even in the fluid free surface case, the computational boundary used for the separation is shifted one grid cell above the physical free surface. Nevertheless, the presence of this non-physical constraint appears to be associated with visible artifacts in the separated fields, as evidenced by the spurious P-to-SV conversions observed near the free surface.

Although only the homogeneous configuration is reported here for clarity, additional tests performed on heterogeneous media exhibit the same behavior. In such cases, the detailed structure of the residual SV component depends on the medium and on the employed

source. Nevertheless, for a given medium, the Poisson–Neumann and Poisson–Dirichlet separation strategies systematically yield markedly different near free surface decompositions, characterized by localized spurious P-to-SV mode conversions in the Dirichlet case, which are absent in the Neumann formulation. A representative example in the realistic marine Marmousi–II benchmark model will be presented at the end of the following chapter.

Comparison with an FFT-based separation approach

For completeness, we also briefly discuss the behavior of the FFT-based wave-field separation approach proposed in [47]. The authors explicitly addressed the boundary artifacts induced by the implicit periodic extension of the FFT framework by introducing a mitigation strategy based on the extension of the computational domain. This idea is analogous to the domain extension mitigation strategy adopted in sections 5.2.4 and 6.2.4, which was inspired by their approach. Their results show that such a strategy works effectively when the artificial boundaries are equipped with absorbing layers, yielding clean separations in the physical core of the domain. However, the same authors reported the persistence of artifacts in the presence of a free surface, and in particular in fluid free surface configurations. For this reason, the comparison with the FFT-based approach is reported in the present chapter, where the interaction between the implicit boundary conditions of the separation method and the physical free surface condition becomes critical.

We tested this approach in all configurations. In the presence of a solid free surface, this method exhibits a behavior qualitatively similar to that of the Poisson–Dirichlet separation strategy, with comparable near-surface features. In the fluid free surface case, consistently with the observations reported by the authors, the FFT-based approach generates spurious SV components analogous to those observed in the Poisson–Dirichlet case. In addition, a further limitation arises in this configuration. When direct or reflected P waves impinge on the free surface, the combination of the implicitly imposed periodic boundary conditions inherent to the FFT formulation and the strong discontinuity of the wave-field and its gradient between the upper boundary (fluid free surface) and the lower boundary (treated as coincident by the periodic extension) leads to the onset of numerical instabilities in both the P and SV components. These instabilities develop along the free surface and, due to periodicity, appear simultaneously at the lower boundary of the computational domain. A representative snapshot for the homogeneous fluid model is reported in figure 8.7 to illustrate this behavior.

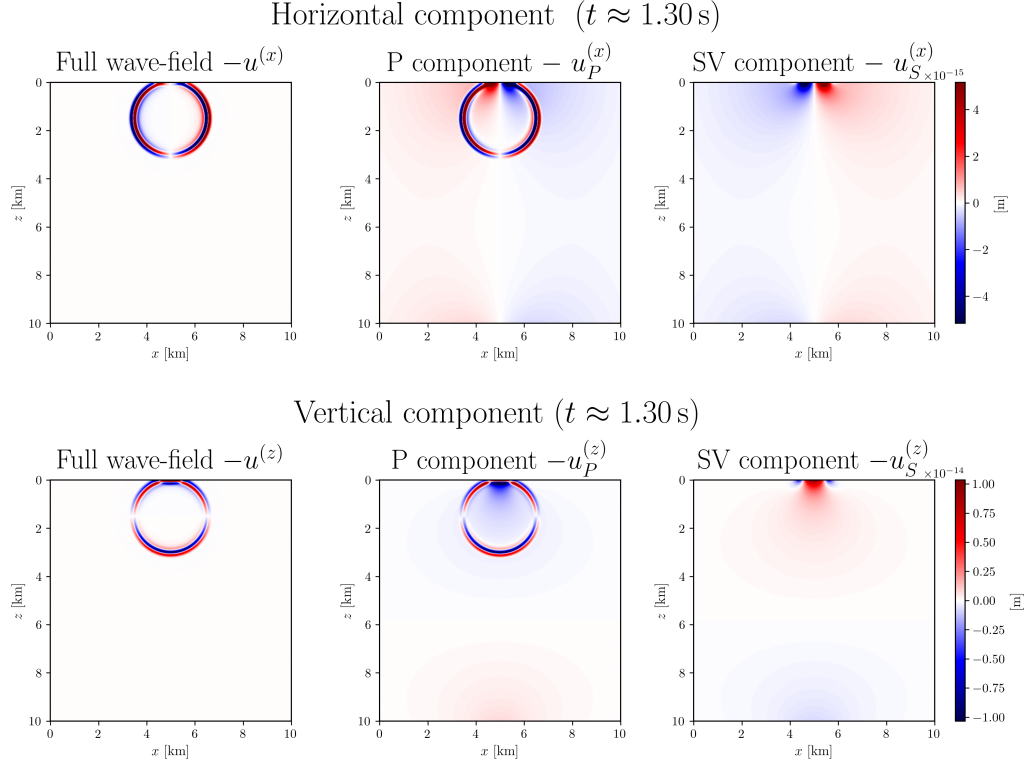


Figure 8.7: Snapshot and FFT-based separation at $t \approx 1.30$ s. Left: full wave-field. Center: P component. Right: SV component. The horizontal (top) and vertical (bottom) components of the full, P and SV displacement field are shown.

As shown in figure 8.7, the resulting artifacts are sufficiently strong to emerge from the absorbing layers near the bottom boundary and remain visible even when the absorbing frame is excluded from the visualization.

These observations indicate that the FFT-based approach exhibits inherent limitations in the presence of a fluid free surface, which prevent it from providing a clean separation. Given that its asymptotic computational complexity is comparable to that of the Poisson–Neumann separation strategy (both scaling as $\mathcal{O}(N_x N_z \log(N_x N_z))$), this limitation makes the FFT-based approach less effective in the considered fluid free surface configurations.

9 | P–S separation with mixed boundary conditions

The analysis carried out in the previous chapters highlights complementary strengths and limitations of the Poisson–Neumann and Poisson–Dirichlet formulations for the P–S wave-field separation. On the one hand, the numerical experiments presented in chapter 7 show that, in effectively unbounded configurations, where all the boundaries of the computational domain are preceded by absorbing layers and the domain extension mitigation strategy is employed, the specific choice of boundary conditions has no significant practical influence on the separation in the interior of the domain. On the other hand, the analysis of chapter 8 reveals that this no longer holds in the presence of a free surface. In particular, in the fluid free surface case, the imposition of non-homogeneous Neumann boundary conditions proves to be able to preserve physical consistency, as it prevents the appearance of spurious P-to-SV conversions at the free surface, which are instead observed when homogeneous Dirichlet conditions are enforced. Finally, the discussion in sections 6.3.1 and 7.2 suggests that, for band-limited wave-fields, the spectral construction underlying the Poisson–Dirichlet formulation is expected to provide a higher level of accuracy than the standard second-order finite-difference discretization adopted in the Poisson–Neumann case. This is supported by the numerical test in the unbounded bi-layer configuration (see section 7.1), where the Neumann formulation exhibits a weak SV-to-P leakage in the bulk, which is not observed in the corresponding Dirichlet results.

These observations motivate the construction of a hybrid approach, aimed at combining the favorable properties of the two formulations. In particular, the goal is to retain the expected improved accuracy associated with the spectral approach adopted in the Dirichlet construction in the interior of the domain, while enforcing non-homogeneous Neumann boundary conditions at the free surface in order to preserve the correct physical behavior at fluid free surfaces. To this end, we consider an auxiliary Poisson problem with mixed boundary conditions, consisting of homogeneous Dirichlet boundary conditions on the boundaries preceded by absorbing layers, and non-homogeneous Neumann boundary conditions at the free surface. Although such mixed boundary conditions do not arise

directly from the *Helmholtz–Weyl decomposition theorem* (see theorem 4.2), this choice is guided by engineering considerations. A key advantage of this formulation is that, in rectangular domains, one is able to obtain an analytical representation of the solution by introducing a suitable harmonic lifting of the non-homogeneous Neumann datum. This makes it possible to retain the same approach adopted in the Dirichlet case, avoiding the explicit discretization of differential operators and instead approximating directly the analytical solution. As a consequence, the proposed mixed formulation is expected to inherit both the improved accuracy of the spectral Dirichlet approach and the physically consistent behavior of the Neumann formulation at the fluid free surface.

The chapter is organized as follows. We first introduce the Poisson–mixed problem, together with the harmonic lifting of the non-homogeneous Neumann datum, and briefly discuss its well-posedness. We then address its numerical solution, showing how, in rectangular domains, the spectral properties of the mixed Laplacian enable an explicit analytical representation of the solution, which leads to the construction of the corresponding discrete algorithm. Finally, we assess the proposed approach by comparing the resulting separation with that obtained with the Poisson–Neumann and Poisson–Dirichlet formulations, focusing on the case of a fluid free surface.

9.1. The Poisson–mixed problem

Let $\underline{u} = \underline{u}(t) \in V \subset [H^1(\Omega)]^n$ be a snapshot of the wave-field, as introduced in (4.9). In this chapter, we define the scalar potential f as the solution of the following Poisson problem with mixed boundary conditions:

$$\begin{cases} -\Delta f = -\operatorname{div}(\underline{u}) & \text{in } \Omega \\ f = 0 & \text{on } \Gamma_D \\ \nabla f \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} & \text{on } \Gamma_N \end{cases} \quad (9.1)$$

where $\Gamma_D \subset \partial\Omega$ denotes the portion of the boundary equipped with absorbing layers, and $\Gamma_N = \partial\Omega \setminus \Gamma_D$ is the part of the boundary associated with the free surface.

9.1.1. Harmonic lifting of the non-homogeneous Neumann datum

In order to recast problem (9.1) into an equivalent formulation with homogeneous boundary conditions, which allows for an explicit representation of the solution in rectangular

domains, we introduce the following auxiliary lifting of the non-homogeneous Neumann datum:

$$f = f_1 + f_0$$

where f_1 is defined as the solution of the following auxiliary harmonic problem, referred to as the *lifting problem*:

$$\begin{cases} -\Delta f_1 = 0 & \text{in } \Omega \\ f_1 = 0 & \text{on } \Gamma_D \\ \nabla f_1 \cdot \hat{\nu} = \underline{u} \cdot \hat{\nu} & \text{on } \Gamma_N \end{cases} \quad (9.2)$$

Accordingly, f_0 solves the following problem:

$$\begin{cases} -\Delta f_0 = -\operatorname{div}(\underline{u}) & \text{in } \Omega \\ f_0 = 0 & \text{on } \Gamma_D \\ \nabla f_0 \cdot \hat{\nu} = 0 & \text{on } \Gamma_N \end{cases} \quad (9.3)$$

We now manipulate problem (9.3) in order to obtain an equivalent and more convenient formulation. To this purpose, we define the auxiliary variables

$$\underline{u}_1 = \nabla f_1, \quad \tilde{\underline{u}} = \underline{u} - \underline{u}_1 \quad (9.4)$$

Formally, since f_1 solves the homogeneous Laplace problem (9.2), it is harmonic, so that $\operatorname{div}(\underline{u}_1) = 0$, and therefore

$$\operatorname{div}(\tilde{\underline{u}}) = \operatorname{div}(\underline{u}) \quad \text{in } \Omega$$

Accordingly, we can rewrite problem (9.3) in the following equivalent formulation, referred to as the *lifted problem*:

$$\begin{cases} -\Delta f_0 = -\operatorname{div}(\tilde{\underline{u}}) & \text{in } \Omega \\ f_0 = 0 & \text{on } \Gamma_D \\ \nabla f_0 \cdot \hat{\nu} = 0 & \text{on } \Gamma_N \end{cases} \quad (9.5)$$

To understand the advantage of formulation (9.5) with respect to formulation (9.3), we observe that, by construction of the harmonic lifting, the normal trace of $\underline{u}_1$ matches that of $\underline{u}$ on Γ_N , which implies, according to (9.4),

$$\gamma_\nu(\tilde{\underline{u}})|_{\Gamma_N} = 0 \quad \text{in } H^{-1/2}(\Gamma_N) \quad (9.6)$$

This property holds for $\tilde{u}$, but not for $\underline{u}$, and makes formulation (9.5) more suitable for the subsequent analysis, as it allows to eliminate the boundary contribution in the spectral representation of the right-hand side.

Once the *lifting problem* (9.2) and the *lifted problem* (9.5) are solved, in analogy with chapters 5 and 6, we define the P and S component of the wave-field according to (5.5), namely

$$\underline{u}_P = \nabla f = \nabla f_0 + \nabla f_1, \quad \underline{u}_S = \underline{u} - \underline{u}_P \quad (9.7)$$

thus realizing the projection operators Π_P and $\Pi_S = \text{Id} - \Pi_P$.

Remark 9.1.

The harmonic lifting of non-homogeneous Neumann data cannot, in general, be applied in the Poisson–Neumann case (see chapter 5), where fully non-homogeneous Neumann boundary conditions are prescribed. Indeed, both the harmonic lifting problem and the associated lifted problem would require a global compatibility condition for solvability (see theorem 5.1). In general, such a condition is not satisfied by the data, so that neither problem is guaranteed to admit a solution.

By contrast, in the mixed Dirichlet–Neumann setting, no compatibility condition is required, thanks to the presence of a Dirichlet portion of the boundary. This allows for the construction of the lifting and the subsequent spectral formulation without additional constraints.

9.1.2. Well-posedness of the mixed formulation

We now briefly assess the well-posedness of problems (9.1), (9.2) and (9.5). The analysis is based on the *Lax–Milgram Lemma* (see appendix B, theorem B.6).

The weak formulation of problem (9.1) reads as follows:

Find $f \in H_{\Gamma_D}^1(\Omega)$ such that

$$\int_{\Omega} \nabla f \cdot \nabla v \, d\Omega = - \int_{\Omega} \text{div}(\underline{u}) v \, d\Omega + \langle \gamma_{\nu}(\underline{u})|_{\Gamma_N}, \gamma_0(v)|_{\Gamma_N} \rangle, \quad \forall v \in H_{\Gamma_D}^1(\Omega)$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^{-1/2}(\Gamma_N)$ and $H^{1/2}(\Gamma_N)$, and

$$H_{\Gamma_D}^1(\Omega) = \{f \in H^1(\Omega) \mid \gamma_0(f)|_{\Gamma_D} = 0\}$$

which is a Hilbert space when endowed with the standard $H^1(\Omega)$ scalar product.

The continuity and coercivity of the bilinear form

$$a : H_{\Gamma_D}^1(\Omega) \times H_{\Gamma_D}^1(\Omega) \rightarrow \mathbb{R}, \quad a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega$$

can be proved analogously as in section 5.1.1.

We now assess the continuity of the linear functional

$$F : H_{\Gamma_D}^1(\Omega) \rightarrow \mathbb{R}, \quad \langle F, v \rangle = - \int_{\Omega} \operatorname{div}(\underline{u}) v \, d\Omega + \langle \gamma_{\nu}(\underline{u})|_{\Gamma_N}, \gamma_0(v)|_{\Gamma_N} \rangle$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing either between $(H_{\Gamma_D}^1(\Omega))^*$ and $H_{\Gamma_D}^1(\Omega)$ or between $H^{-1/2}(\Gamma_N)$ and $H^{1/2}(\Gamma_N)$, with the meaning being clear from the context. Using the *Cauchy–Schwarz inequality* for the volumetric term, together with the definition of the dual norm and the continuity of the trace operator γ_0 , we obtain, for all $v \in H_{\Gamma_D}^1(\Omega)$,

$$|\langle F, v \rangle| \leq \left(\|\operatorname{div}(\underline{u})\|_{L^2(\Omega)} + C_T \|\gamma_{\nu}(\underline{u})\|_{H^{-1/2}(\Gamma_N)} \right) \|v\|_{H^1(\Omega)}$$

where $C_T > 0$ denotes the continuity constant of the trace operator.

Hence, by the *Lax–Milgram lemma*, there exists a unique weak solution $f \in H_{\Gamma_D}^1(\Omega)$ to the Poisson–mixed problem (9.1).

The same argument applies, with minor simplifications, to the *lifting problem* (9.2) and to the *lifted problem* (9.5). Hence, the decomposition $f = f_1 + f_0$ is well-defined and recovers, by uniqueness, the solution of the original mixed problem (9.1).

9.2. Numerical solution of the Poisson–mixed problem and computational cost analysis

In this section, we address the numerical solution of the Poisson–mixed problem for the P–S wave-field separation. As in chapters 5 and 6, we restrict the analysis to the two-dimensional setting, so that the solenoidal component $\underline{u}_S$ coincides with the SV wave-field, and the decomposition takes the form of a P–SV separation.

Relying on the lifting strategy introduced in section 9.1.1, the solution f is decomposed into a lifting contribution f_1 and a residual term f_0 . We first exploit the spectral properties of the continuous mixed Laplacian to derive an analytical representation of the solution of the *lifted problem* (9.5). We then specialize this representation to rectangular domains, where it takes a particularly simple form, and derive the corresponding analytical solution

for the *lifting problem* (9.2).

This framework allows us to construct the numerical solution by approximating the analytical representations of f_1 and f_0 , rather than discretizing differential operators. The resulting algorithm mirrors the Poisson–Dirichlet approach, while incorporating the non-homogeneous Neumann boundary condition through the lifting term. Finally, we outline the complete P–SV separation procedure and briefly discuss its computational cost.

9.2.1. Application of the basic spectral properties of the continuous mixed Laplacian to the analytical solution of the *lifted problem*

We first recall the spectral properties of the continuous mixed Laplacian. We then use these properties to derive an abstract analytical representation of the solution of the *lifted problem*.

Let $\Omega \subset \mathbb{R}^n$ open, bounded and connected, such that $\partial\Omega \in \text{Lip}$. Let $\partial\Omega = \Gamma_D \cup \Gamma_N$, with $\Gamma_D \cap \Gamma_N = \emptyset$ and $|\Gamma_D| > 0$. We consider the following eigenvalue problem:

$$\begin{cases} -\Delta\varphi = \lambda\varphi & \text{in } \Omega \\ \varphi = 0 & \text{on } \Gamma_D \\ \nabla\varphi \cdot \hat{\nu} = 0 & \text{on } \Gamma_N \end{cases} \quad (9.8)$$

The spectral properties discussed in section 6.2.1 for the continuous Dirichlet Laplacian extend to the present mixed boundary setting. This follows from the same functional-analytic framework, based on the continuity and coercivity of the associated bilinear form on $H_{\Gamma_D}^1(\Omega)$ and the compactness of the embedding $H_{\Gamma_D}^1(\Omega) \hookrightarrow L^2(\Omega)$.

Hence, problem (9.8) admits a sequence of eigenpairs $\{(\lambda_n, \varphi_n)\}_{n \in \mathbb{N}}$ such that

- The eigenvalues $\{\lambda_n\}_{n \in \mathbb{N}} \subset \mathbb{R}$ satisfy $0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \rightarrow +\infty$;
- The eigenfunctions $\{\varphi_n\}_{n \in \mathbb{N}} \subset H_{\Gamma_D}^1(\Omega)$ form, up to normalization, an orthonormal basis of $(L^2(\Omega), (\cdot, \cdot)_{L^2(\Omega)})$.

In the context of the *lifted problem* (9.5), we consider as right-hand side and corresponding solution

$$b = -\operatorname{div}(\tilde{\underline{u}}) \in L^2(\Omega), \quad f_0 \in H_{\Gamma_D}^1(\Omega) \subset L^2(\Omega)$$

Therefore, both b and f_0 can be expanded with respect to the basis of eigenfunctions of

the mixed Laplacian, namely

$$b = \sum_{n=1}^{+\infty} \hat{b}_n \varphi_n, \quad f_0 = \sum_{n=1}^{+\infty} \hat{f}_{0,n} \varphi_n \quad (9.9)$$

where the series converge in the $L^2(\Omega)$ norm and the coefficients $\{\hat{b}_n\}_{n \in \mathbb{N}}, \{\hat{f}_{0,n}\}_{n \in \mathbb{N}} \subset \mathbb{R}$ can be explicitly computed as

$$\hat{b}_n = (b, \varphi_n)_{L^2(\Omega)} = \int_{\Omega} b \varphi_n d\Omega, \quad \hat{f}_{0,n} = (f_0, \varphi_n)_{L^2(\Omega)} = \int_{\Omega} f_0 \varphi_n d\Omega, \quad \forall n \in \mathbb{N}$$

The relation between the expansion coefficients of the solution and those of the right-hand side coincides with the one obtained in the Poisson–Dirichlet case (see section 6.2.1), namely

$$\hat{f}_{0,n} = \frac{\hat{b}_n}{\lambda_n}, \quad \forall n \in \mathbb{N} \quad (9.10)$$

We now specify the form of the expansion coefficients of the right-hand side in the present setting, where $b = -\operatorname{div}(\tilde{\underline{u}})$. By applying the *generalized Gauss–Green formula* (see appendix B, theorem B.5), we obtain

$$\hat{b}_n = - \int_{\Omega} \operatorname{div}(\tilde{\underline{u}}) \varphi_n d\Omega = \int_{\Omega} \tilde{\underline{u}} \cdot \nabla \varphi_n d\Omega \quad (9.11)$$

where the boundary contribution vanishes. Indeed, on Γ_D , we have $\gamma_0(\varphi_n)|_{\Gamma_D} = 0$, since $\varphi_n \in H_{\Gamma_D}^1(\Omega)$, while, on Γ_N , according to equation (9.6), we have $\gamma_\nu(\tilde{\underline{u}})|_{\Gamma_N} = 0$.

In light of this result, the advantage of introducing the auxiliary variable $\tilde{\underline{u}}$ becomes clear. Indeed, thanks to property (9.6), the boundary contribution on Γ_N vanishes in the expression of the coefficients $\{\hat{b}_n\}_{n \in \mathbb{N}}$. By contrast, if the original field $\underline{u}$ were used, such a contribution would persist. In practice, in preliminary numerical tests based on the direct use of $\underline{u}$, the explicit discretization of this boundary contribution was observed to generate numerical artifacts within the spectral framework considered in this work.

9.2.2. Analytical solution of the *lifted* and *lifting problems* in rectangular domains

In our setting, we consider the rectangular domain $\Omega = (0, L_x) \times (0, L_z) \subset \mathbb{R}^2$, and we assume a free surface located at $z = 0$ m, so that $\Gamma_N = [0, L_x] \times \{0\}$ and $\Gamma_D = \partial\Omega \setminus \Gamma_N$. In this case, separation of variables can be employed both to solve explicitly the eigenvalue problem (9.8), leading to closed-form expressions for the eigenvalues and the corresponding

eigenfunctions, which are used to construct the solution of the *lifted problem* f_0 , and to derive an explicit expression for the solution of the *lifting problem* f_1 .

Solution of the *lifted problem*

Proceeding as in section 6.2.2, the two-dimensional eigenvalue problem (9.8) can be decoupled into the following one-dimensional eigenvalue problems:

$$\begin{cases} -\alpha''(x) = \lambda_x \alpha(x) & \text{in } (0, L_x) \\ \alpha(0) = \alpha(L_x) = 0 \end{cases} \quad \begin{cases} -\beta''(z) = \lambda_z \beta(z) & \text{in } (0, L_z) \\ \beta'(0) = 0 \\ \beta(L_z) = 0 \end{cases}$$

The eigenpairs associated to these problems are classical and follow from standard theory of second-order linear ODEs with constant coefficients, namely

$$\begin{aligned} \lambda_{x,n} &= \left(\frac{n\pi}{L_x}\right)^2, \quad \alpha_n(x) = A_n \sin\left(\frac{n\pi}{L_x}x\right), \quad \forall n \in \mathbb{N} \\ \lambda_{z,m} &= \left[\left(m + \frac{1}{2}\right) \frac{\pi}{L_z}\right]^2, \quad \beta_m(z) = B_m \cos\left(\left(m + \frac{1}{2}\right) \frac{\pi}{L_z}z\right), \quad \forall m \in \mathbb{N} \cup \{0\} \end{aligned}$$

where $A_n, B_m \in \mathbb{R}$ are free normalization constants.

Then, for all $n \in \mathbb{N}$ and $m \in \mathbb{N} \cup \{0\}$, the eigenpairs of problem (9.8) are given by

$$\lambda_{n,m} = \left(\frac{n\pi}{L_x}\right)^2 + \left[\left(m + \frac{1}{2}\right) \frac{\pi}{L_z}\right]^2 \quad (9.12)$$

$$\varphi_{n,m}(x, z) = \frac{2}{\sqrt{L_x L_z}} \sin\left(\frac{n\pi}{L_x}x\right) \cos\left(\left(m + \frac{1}{2}\right) \frac{\pi}{L_z}z\right), \quad \forall (x, z) \in \bar{\Omega} \quad (9.13)$$

where the constant $C_{n,m} = A_n B_m = 2/\sqrt{L_x L_z}$ is chosen in order to guarantee $\|\varphi_{n,m}\|_{L^2(\Omega)} = 1$ for all $n \in \mathbb{N}$ and $m \in \mathbb{N} \cup \{0\}$.

We now exploit the explicit characterization of the eigenpairs to derive the explicit representation of the solution of the *lifted problem* (9.5).

By (9.11) and (9.12), the expansion coefficients of the right-hand side $b = -\operatorname{div}(\tilde{u})$ can be computed as

$$\hat{b}_{n,m} = \int_{\Omega} \tilde{u} \cdot \nabla \varphi_{n,m} d\Omega = \frac{n\pi}{L_x} \hat{u}_{x,n,m} - \left(m + \frac{1}{2}\right) \frac{\pi}{L_z} \hat{u}_{z,n,m}, \quad \forall n \in \mathbb{N}, \forall m \in \mathbb{N} \cup \{0\} \quad (9.14)$$

where we denoted, for all $n \in \mathbb{N}$ and $m \in \mathbb{N} \cup \{0\}$,

$$\hat{u}_{x,n,m} = \frac{2}{\sqrt{L_x L_z}} \int_0^{L_x} \int_0^{L_z} \tilde{u}_x(x, z) \cos\left(\frac{n\pi}{L_x} x\right) \cos\left(\left(m + \frac{1}{2}\right) \frac{\pi}{L_z} z\right) dz dx \quad (9.15)$$

$$\hat{u}_{z,n,m} = \frac{2}{\sqrt{L_x L_z}} \int_0^{L_x} \int_0^{L_z} \tilde{u}_z(x, z) \sin\left(\frac{n\pi}{L_x} x\right) \sin\left(\left(m + \frac{1}{2}\right) \frac{\pi}{L_z} z\right) dz dx \quad (9.16)$$

Once the coefficients of the right-hand side have been computed, the corresponding coefficients of f_0 follow from (9.10) together with (9.12).

Finally, the analytical solution of the *lifted problem* is given by (9.9) and (9.13), explicitly

$$f_0(x, z) = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{+\infty} \sum_{m=0}^{+\infty} \hat{f}_{0,n,m} \sin\left(\frac{n\pi}{L_x} x\right) \cos\left(\left(m + \frac{1}{2}\right) \frac{\pi}{L_z} z\right) \quad (9.17)$$

Solution of the *lifting problem*

In this paragraph, the derivations are carried out at a formal level. All manipulations can be rigorously justified within the appropriate Sobolev space framework. For the sake of conciseness, such technical details are omitted, as the focus is on the construction of an explicit solution procedure.

We seek solutions to the *lifting problem* (9.2) of the form

$$f_1(x, z) = \gamma(x)\delta(z), \quad \forall (x, z) \in \bar{\Omega} \quad (9.18)$$

Substituting this ansatz into the Laplace equation and separating variables yields

$$-\gamma''(x) = \mu \gamma(x), \quad \delta''(z) - \mu \delta(z) = 0$$

for some constant $\mu \in \mathbb{R}$, with the equations holding in $(0, L_x)$ and $(0, L_z)$, respectively.

Analogously to section 6.2.2, imposing the homogeneous Dirichlet boundary conditions on the left and right boundaries yields

$$\mu_n = \left(\frac{n\pi}{L_x}\right)^2, \quad \gamma_n(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n\pi}{L_x} x\right), \quad \forall n \in \mathbb{N} \quad (9.19)$$

where the constant $A_n = \sqrt{2/L_x}$ is chosen in order to guarantee $\|\gamma_n\|_{L^2(0, L_x)} = 1$ for all $n \in \mathbb{N}$.

For each mode $n \in \mathbb{N}$, δ_n solves

$$\delta_n''(z) - \mu_n \delta_n(z) = 0 \quad \text{in } (0, L_z)$$

whose general solution is

$$\delta_n(z) = C_n \cosh(\sqrt{\mu_n} z) + D_n \sinh(\sqrt{\mu_n} z)$$

where $C_n, D_n \in \mathbb{R}$ are free normalization constants.

Imposing the homogeneous Dirichlet boundary condition at the bottom boundary ($z = L_z$) leads to

$$\delta_n(z) = D_n [\sinh(\sqrt{\mu_n} z) - \tanh(\sqrt{\mu_n} L_z) \cosh(\sqrt{\mu_n} z)] \quad (9.20)$$

Since the equation of the *lifting problem* (9.2) is linear, thanks to the superposition principle, we infer, according to (9.18), that its general form is

$$f_1(x, z) = \sum_{n=1}^{+\infty} \gamma_n(x) \delta_n(z) \quad (9.21)$$

We now determine the form of the constants $\{D_n\}_{n \in \mathbb{N}} \subset \mathbb{R}$ by imposing the non-homogeneous Neumann boundary condition on Γ_N . In the present configuration, this reduces to

$$\frac{\partial f_1}{\partial z}(x, 0) = u_z(x, 0) \quad \text{in } (0, L_x) \quad (9.22)$$

Taking the derivative with respect to z of expression (9.21) and evaluating at $z = 0$ yields

$$\frac{\partial f_1}{\partial z}(x, 0) = \sum_{n=1}^{+\infty} \gamma_n(x) \delta_n'(0) = \sum_{n=1}^{+\infty} \sqrt{\mu_n} D_n \gamma_n(x) \quad (9.23)$$

We now expand the Neumann datum with respect to the basis $\{\gamma_n\}_{n \in \mathbb{N}} \subset L^2(0, L_x)$ as

$$u_z(x, 0) = \sum_{n=1}^{+\infty} \hat{u}_{z,n} \gamma_n(x) \quad (9.24)$$

where the coefficients $\{\hat{u}_{z,n}\} \subset \mathbb{R}$ can be explicitly computed as

$$\hat{u}_{z,n} = (u_z(\cdot, 0), \gamma_n)_{L^2(0, L_x)} = \sqrt{\frac{2}{L_x}} \int_0^{L_x} u_z(x, 0) \sin\left(\frac{n\pi}{L_x} x\right) dx, \quad \forall n \in \mathbb{N} \quad (9.25)$$

Substituting (9.23) and (9.24) into (9.22), we obtain

$$\sum_{n=1}^{+\infty} \left(\sqrt{\mu_n} D_n - \hat{u}_{z,n} \right) \gamma_n(x) = 0 \quad \text{in } (0, L_x)$$

By orthogonality of $\{\gamma_n\}_{n \in \mathbb{N}}$, it follows that

$$D_n = \frac{\hat{u}_{z,n}}{\sqrt{\mu_n}}, \quad \forall n \in \mathbb{N} \quad (9.26)$$

Substituting (9.19), (9.20) and (9.26) into (9.21), we obtain an explicit representation of the harmonic lifting f_1 , which depends only on the non-homogeneous Neumann boundary datum:

$$f_1(x, z) = \sqrt{\frac{2}{L_x}} \sum_{n=1}^{+\infty} \hat{u}_{z,n} \sin\left(\frac{n\pi}{L_x} x\right) K_n(z) \quad (9.27)$$

where the hyperbolic kernel K_n is defined as

$$K_n(z) = \frac{L_x}{n\pi} \left[\sinh\left(\frac{n\pi}{L_x} z\right) - \tanh\left(\frac{n\pi}{L_x} L_z\right) \cosh\left(\frac{n\pi}{L_x} z\right) \right], \quad \forall n \in \mathbb{N} \quad (9.28)$$

9.2.3. Description of the P–SV separation algorithm and computational cost analysis

We now describe the algorithm implementing the P–SV separation strategy based on the Poisson–mixed problem. The algorithm is obtained by approximating the continuous spectral representations of f_1 and f_0 derived in the previous section using the information available on the discrete grid. We also provide a brief analysis of its computational cost. As in sections 5.2.3 and 6.2.3, the analysis focuses on the asymptotic complexity of the main operations.

We consider the same staggered-grid setup described in section 5.2.1. In this discrete setting, as discussed in section 6.2.3, the *Nyquist sampling theorem* implies that the maximum resolvable wavenumbers are given by (6.18). Therefore, the spectral modes that can be represented without aliasing satisfy

$$k_{x,n} = \frac{n\pi}{L_x} \leq k_{x,\max} \Leftrightarrow n \leq N_x, \quad k_{z,m} = \left(m + \frac{1}{2}\right) \frac{\pi}{L_z} \leq k_{z,\max} \Leftrightarrow m \leq N_z - 1$$

Accordingly, the truncated spectral representation of the solution of the *lifted problem* f_0

is defined over the discrete set of admissible wavenumbers $(k_{x,n}, k_{z,m})$, with indices

$$\tilde{\Sigma}^{(s)} = \{1, \dots, N_x\} \times \{0, \dots, N_z - 1\}$$

Similarly, the spectral representation of the solution of the *lifting problem* f_1 is truncated to the horizontal wavenumbers $k_{x,n}$ with indices

$$\tilde{\Sigma}_i^{(s)} = \{1, \dots, N_x\}$$

Finally, as in sections 5.2.3 and 6.2.3, we remark that the double summations appearing in the algorithm below are implemented via FFT-based DCT/DST operations, rather than as direct matrix–vector products.

The Poisson–mixed P–SV separation algorithm can be divided into three parts and described through the following sequence of steps.

Approximation of the *lifting problem*

1. Approximate $\hat{u}_{z,n}$, as given by (9.25), for all $n \in \tilde{\Sigma}_i^{(s)}$ through the quadrature formula

$$\hat{u}_n^{(z)} = \sqrt{\frac{2}{L_x}} \sum_{i=0}^{N_x-1} u_{i+1/2,0}^{(z)} \sin\left(\frac{n\pi}{N_x}(i+1/2)\right) h_x$$

The computational cost of this step corresponds to that of a one-dimensional DST-II along the x direction:

$$\mathcal{O}(N_x \log(N_x))$$

2. Reconstruct the degrees of freedom of the horizontal component of the auxiliary variable $\underline{u}_1 = \nabla f_1$ by evaluating the x -derivative of the truncated expansion of f_1 at the corresponding grid locations:

$$u_{1,i,j+1/2}^{(x)} = \sqrt{\frac{2}{L_x}} \sum_{n=1}^{N_x} \hat{u}_n^{(z)} \xi_n(j+1/2) \cos\left(\frac{n\pi}{N_x}i\right), \quad \forall (i, j) \in \Sigma^{(v)}$$

where we denoted, for all $j \in \Sigma_j^{(v)}$,

$$\xi_n(j+1/2) = \sinh\left(\frac{n\pi}{L_x}h_z(j+1/2)\right) - \tanh\left(\frac{n\pi}{L_x}L_z\right) \cosh\left(\frac{n\pi}{L_x}h_z(j+1/2)\right)$$

The computational cost of this step corresponds to that of a one-dimensional DCT-I

(self-inverse, up to normalization) along the x direction, for each value of $j \in \Sigma_j^{(v)}$:

$$\mathcal{O}(N_z N_x \log(N_x))$$

3. Reconstruct the degrees of freedom of the vertical component of the auxiliary variable $\underline{u}_1 = \nabla f_1$ by evaluating the z -derivative of the truncated expansion of f_1 at the corresponding grid locations:

$$u_{1,i+1/2,j}^{(z)} = \sqrt{\frac{2}{L_x}} \sum_{n=1}^{N_x} \hat{u}_n^{(z)} \eta_n(j) \sin\left(\frac{n\pi}{N_x}(i+1/2)\right), \quad \forall (i, j) \in \Sigma^{(h)}$$

where we denoted, for all $j \in \Sigma_j^{(h)}$,

$$\eta_n(j) = \cosh\left(\frac{n\pi}{L_x} h_z j\right) - \tanh\left(\frac{n\pi}{L_x} L_z\right) \sinh\left(\frac{n\pi}{L_x} h_z j\right)$$

The computational cost of this step is identical to that of the previous one, as it consists of a one-dimensional DST-III (inverse of DST-II, up to normalization) applied along the x direction for each $j \in \Sigma_j^{(h)}$.

Hence, the overall asymptotic complexity of the numerical approximation of the solution of the *lifting problem* is

$$\mathcal{O}(N_z N_x \log(N_x)) \tag{9.29}$$

with the dominant contribution arising from the DCT/DST-based steps two and three.

We remark that the analytical expressions of ξ_n and η_n involve hyperbolic functions and may suffer from overflow for large values of $(n\pi/L_x)L_z$. Then, in the implementation, we evaluate ξ_n and η_n using the following equivalent exponential forms:

$$\begin{aligned} \xi_n(j+1/2) &= -e^{-\frac{n\pi}{L_x} h_z (j+1/2)} \frac{1 - e^{-2\frac{n\pi}{L_x} (L_z - h_z (j+1/2))}}{1 + e^{-2\frac{n\pi}{L_x} L_z}} \\ \eta_n(j) &= e^{-\frac{n\pi}{L_x} h_z j} \frac{1 + e^{-2\frac{n\pi}{L_x} (L_z - h_z j)}}{1 + e^{-2\frac{n\pi}{L_x} L_z}} \end{aligned}$$

These expressions only involve decaying exponentials for $z \in [0, L_z]$ and are therefore numerically stable.

Approximation of the *lifted problem*

1. Compute the degrees of freedom of the auxiliary variable $\tilde{u}$ by subtraction:

$$\begin{aligned}\tilde{u}_{i,j+1/2}^{(x)} &= u_{i,j+1/2}^{(x)} - u_{1,i,j+1/2}^{(x)}, \quad \forall (i, j) \in \Sigma^{(v)} \\ \tilde{u}_{i+1/2,j}^{(z)} &= u_{i+1/2,j}^{(z)} - u_{1,i+1/2,j}^{(z)}, \quad \forall (i, j) \in \Sigma^{(h)}\end{aligned}$$

The computational cost of this step amounts to that of a single sweep over the computational grid:

$$\mathcal{O}(N_x N_z)$$

2. Approximate $\hat{\tilde{u}}_{x,n,m}$, as given by (9.15), for all $(n, m) \in \tilde{\Sigma}^{(s)}$ through the quadrature formula

$$\hat{\tilde{u}}_{n,m}^{(x)} = \frac{2}{\sqrt{L_x L_z}} \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} w_i^{(x)} \tilde{u}_{i,j+1/2}^{(x)} \cos\left(\frac{n\pi}{N_x} i\right) \cos\left((m+1/2)\frac{\pi}{N_z}(j+1/2)\right) h_x h_z$$

where the quadrature weights are given by (6.20).

The computational cost of this step corresponds to that of a mixed two-dimensional transform, consisting of a DCT-I along the x direction and a DCT-IV along the z direction, implemented via two successive one-dimensional transforms:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

3. Approximate $\hat{\tilde{u}}_{z,n,m}$, as given by (9.16), for all $(n, m) \in \tilde{\Sigma}^{(s)}$ through the quadrature formula

$$\hat{\tilde{u}}_{n,m}^{(z)} = \frac{2}{\sqrt{L_x L_z}} \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_z-1} w_j^{(z)} \tilde{u}_{i+1/2,j}^{(z)} \sin\left(\frac{n\pi}{N_x}(i+1/2)\right) \sin\left((m+1/2)\frac{\pi}{N_z} j\right) h_x h_z$$

where the quadrature weights are given by (6.22).

The computational cost of this step is identical to that of the previous one, as it consists of a one-dimensional DST-II applied along the x direction and a one-dimensional DST-III applied along the z direction, performed subsequently.

4. Approximate the expansion coefficients of the right-hand side $\hat{b}_{n,m}$, as given by (9.14), for all $(n, m) \in \tilde{\Sigma}^{(s)}$:

$$\hat{b}_{h,n,m} = \frac{n\pi}{L_x} \hat{\tilde{u}}_{n,m}^{(x)} - (m+1/2) \frac{\pi}{L_z} \hat{\tilde{u}}_{n,m}^{(z)}$$

The computational cost of this step amounts to that of a single sweep over the modes:

$$\mathcal{O}(N_x N_z)$$

5. Reconstruct the approximated expansion coefficients of the solution of the *lifted problem* $\hat{f}_{0,n,m}$, as given by (9.10), for all $(n, m) \in \tilde{\Sigma}^{(s)}$:

$$\hat{f}_{h,0,n,m} = \frac{\hat{b}_{h,n,m}}{\lambda_{n,m}}$$

The computational cost of this step amounts to that of a single sweep over the modes.

6. Approximate the expansion coefficients of the auxiliary variable $\underline{u}_0 = \nabla f_0$ for all $(n, m) \in \tilde{\Sigma}^{(s)}$ by term-by-term differentiation of the truncated expansion of the solution of the *lifted problem*:

$$\hat{u}_{0,n,m}^{(x)} = \frac{n\pi}{L_x} \hat{f}_{h,0,n,m}, \quad \hat{u}_{0,n,m}^{(z)} = -(m+1/2) \frac{\pi}{L_z} \hat{f}_{h,0,n,m}$$

The computational cost of this step amounts to that of a single sweep over the modes.

7. Reconstruct the degrees of freedom of the horizontal component of $\underline{u}_0$ by evaluating the x -derivative of the truncated expansion of f_0 at the corresponding grid locations:

$$u_{0,i,j+1/2}^{(x)} = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{N_x} \sum_{m=0}^{N_z-1} \hat{u}_{0,n,m}^{(x)} \cos\left(\frac{n\pi}{N_x} i\right) \cos\left((m+1/2) \frac{\pi}{N_z} (j+1/2)\right)$$

for all $(i, j) \in \Sigma^{(v)}$.

The computational cost of this step corresponds to that of a mixed two-dimensional transform, consisting of a DCT-I (self-inverse, up to normalization) along the x direction and a DCT-IV (self-inverse, up to normalization) along the z direction, implemented via two successive one-dimensional transforms:

$$\mathcal{O}(N_z N_x \log(N_x)) + \mathcal{O}(N_x N_z \log(N_z)) = \mathcal{O}(N_x N_z \log(N_x N_z))$$

8. Reconstruct the degrees of freedom of the vertical component of $\underline{u}_0$ by evaluating

the z -derivative of the truncated expansion of f_0 at the corresponding grid locations:

$$u_{0,i+1/2,j}^{(z)} = \frac{2}{\sqrt{L_x L_z}} \sum_{n=1}^{N_x} \sum_{m=0}^{N_z-1} \hat{u}_{0,n,m}^{(z)} \sin\left(\frac{n\pi}{N_x}(i+1/2)\right) \sin\left((m+1/2)\frac{\pi}{N_z}j\right)$$

for all $(i, j) \in \Sigma^{(h)}$.

The computational cost of this step is identical to that of the previous one, as it consists of a one-dimensional DST-III (inverse of DST-II, up to normalization) applied along the x direction and a one-dimensional DST-II (inverse of DST-III, up to normalization) applied along the z direction, performed subsequently.

Hence, the overall asymptotic complexity of the numerical approximation of the solution of the *lifted problem* is

$$\mathcal{O}(N_x N_z \log(N_x N_z)) \quad (9.30)$$

with the dominant contribution arising from the DCT/DST-based steps two, three, seven and eight.

Reconstruction of the separated wave-field

Once the auxiliary lifting and lifted fields $\underline{u}_1 = \nabla f_1$ and $\underline{u}_0 = \nabla f_0$ have been approximated, the reconstruction of the degrees of freedom of the P and SV components of the wave-field follow straightforwardly from (9.7), namely

$$\begin{aligned} u_{P,i,j+1/2}^{(x)} &= u_{0,i,j+1/2}^{(x)} + u_{1,i,j+1/2}^{(x)}, & u_{S,i,j+1/2}^{(x)} &= u_{i,j+1/2}^{(x)} - u_{P,i,j+1/2}^{(x)}, & \forall (i, j) \in \Sigma^{(v)} \\ u_{P,i+1/2,j}^{(z)} &= u_{0,i+1/2,j}^{(z)} + u_{1,i+1/2,j}^{(z)}, & u_{S,i+1/2,j}^{(z)} &= u_{i+1/2,j}^{(z)} - u_{P,i+1/2,j}^{(z)}, & \forall (i, j) \in \Sigma^{(h)} \end{aligned}$$

The computational cost of this step amounts to that of a single sweep over the computational grid:

$$\mathcal{O}(N_x N_z) \quad (9.31)$$

Therefore, according to (9.29), (9.30) and (9.31), the overall cost is dominated by the approximation of the *lifted problem*, in particular by the two-dimensional DCT/DST-based steps. Hence, the asymptotic complexity of the proposed Poisson–mixed P–SV separation algorithm is

$$\mathcal{O}(N_x N_z \log(N_x N_z))$$

This matches the complexity of the Poisson–Neumann and Poisson–Dirichlet algorithms proposed in sections 5.2.3 and 6.2.3, respectively, although it includes an additional stage associated with the preliminary computation of the harmonic lifting.

9.3. Numerical validation of the Poisson–mixed formulation

In this section, we qualitatively assess the performance of the Poisson–mixed P–SV separation strategy through a set of numerical experiments. The goal is to verify that the proposed formulation effectively combines the main advantages of the Poisson–Neumann and Poisson–Dirichlet approaches discussed in the previous chapters.

To this end, we consider two representative configurations. In both tests, the models are equipped with a fluid free surface located at $z = 0$ m. We first analyze a homogeneous fluid model (see appendix A.2.1), analogous to the test case introduced in section 8.2.2, in order to verify that the mixed formulation correctly reproduces the physically consistent behavior of the Poisson–Neumann separation at the fluid free surface, and to assess the residual SV leakage. We then consider a more realistic heterogeneous configuration based on the marine Marmousi–II model (see appendix A.2.3), where we compare the Poisson–mixed approach with both the Poisson–Neumann and Poisson–Dirichlet formulations.

These tests are intended to provide a qualitative and comparative assessment of the proposed method, with particular attention to the behavior near the free surface and to the consistency of the separation in the interior of the domain.

Homogeneous fluid model

The source configuration is the same as in the test proposed in section 8.2.2, namely an explosive source with a Ricker wavelet temporal profile (see appendix A.1), with central frequency $f_0 = 5$ Hz and injected at $(x_s, z_s) = (5.0 \text{ km}, 1.5 \text{ km})$. We also consider the same representative snapshot of the wave-field at $t \approx 2.0$ s, shown in figure 8.4. The resulting P and SV components, both for the Poisson–Neumann and Poisson–mixed separation strategies, are displayed in figures 9.1 and 9.2.

In such a fluid medium, shear waves are not physically supported. As a consequence, the SV component obtained from the separation can be entirely interpreted as a numerical leakage associated with the discrete projection procedure.

As can be observed from figure 9.2, and more clearly from the corresponding rescaled insets, both the Poisson–Neumann and the Poisson–mixed approaches exhibit a residual SV component whose spatial structure closely resembles that of the P wave-field with no evidence of spurious P-to-SV conversions at the free surface, suggesting that the observed leakage can be attributed to numerical errors. This behavior is fully consistent with the observations reported in section 8.2.2 for the Poisson–Neumann formulation, and

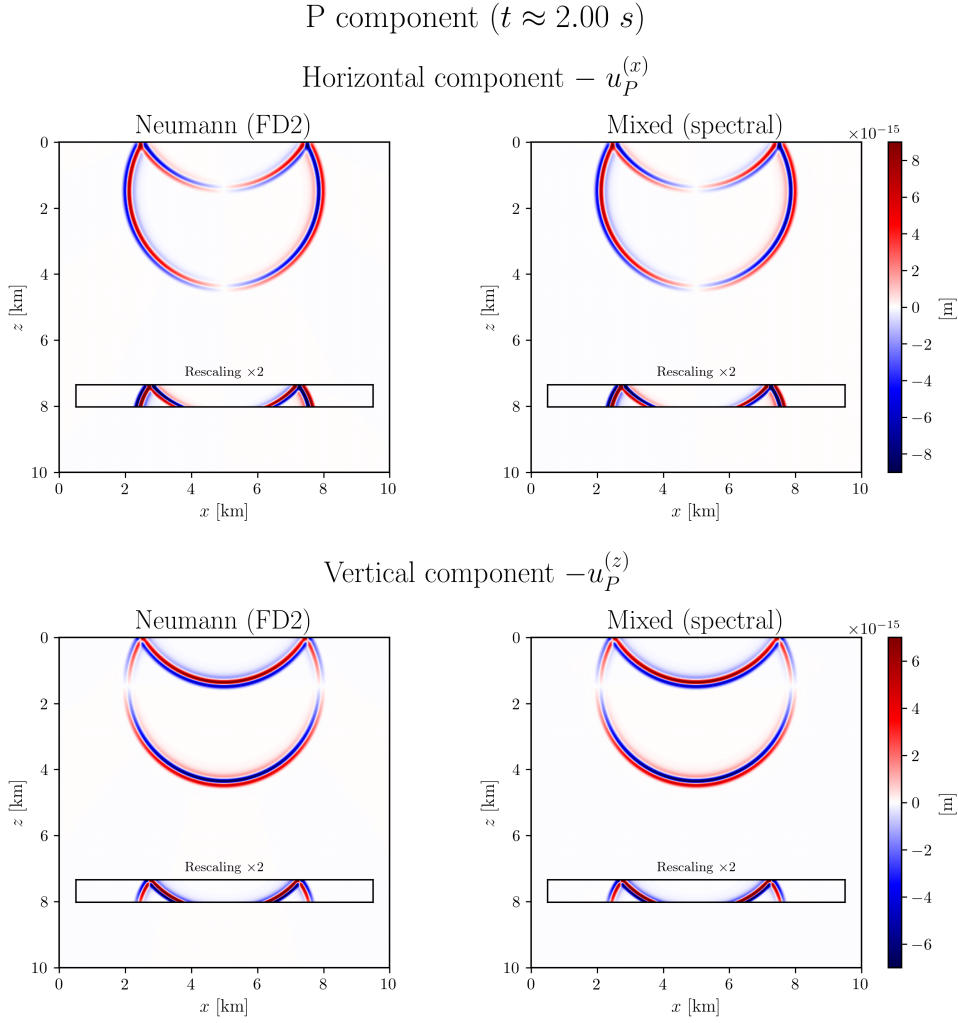


Figure 9.1: P component of the wave-field at $t \approx 2.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–mixed separation. The horizontal (top) and vertical (bottom) components of the P displacement field are shown.

can be explained by the fact that the Poisson–mixed approach enforces the same non-homogeneous Neumann boundary condition at the fluid free surface, which implies a vanishing normal component of the SV field, in agreement with the underlying physical model.

A more detailed comparison, based on the rescaled insets, indicates that the amplitude of the residual SV component obtained with the Poisson–mixed formulation is approximately one order of magnitude smaller than that produced by the second-order finite-difference

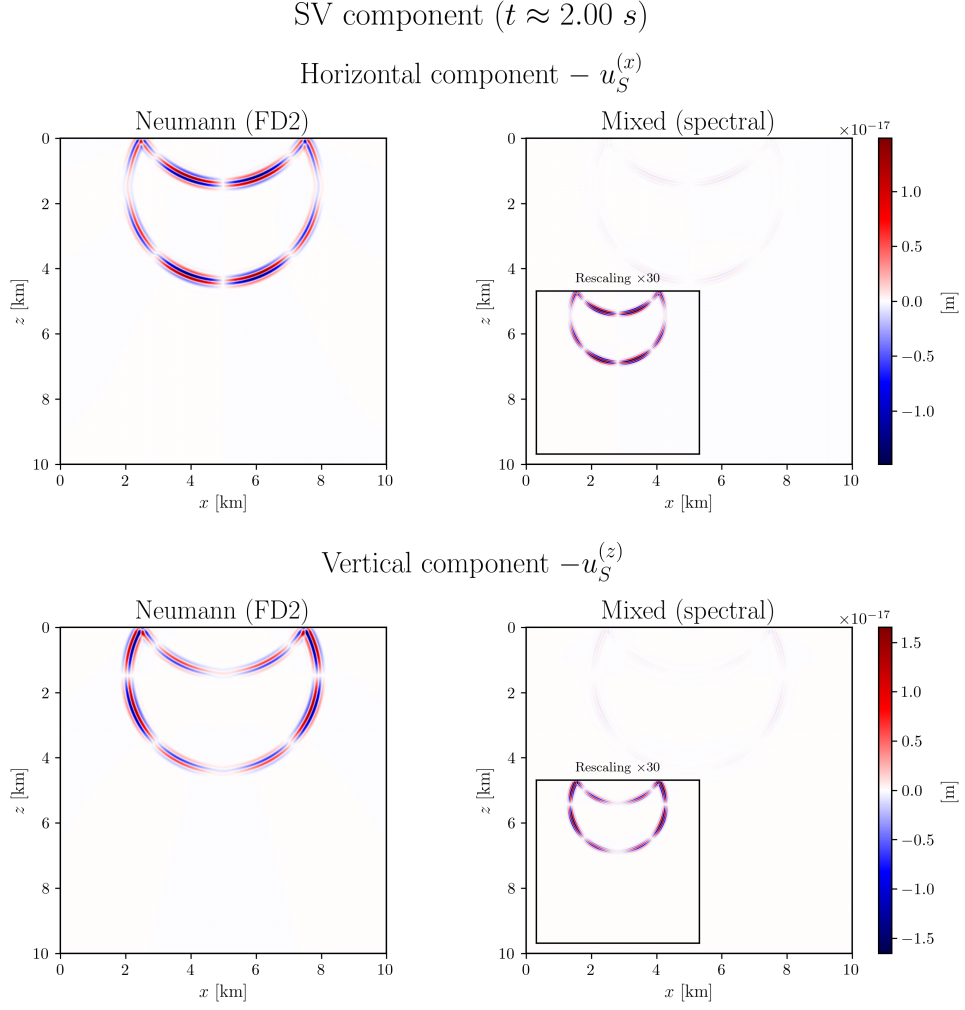


Figure 9.2: SV component of the wave-field at $t \approx 2.0$ s. Left: second-order finite-difference Poisson–Neumann separation. Right: spectral Poisson–mixed separation. The horizontal (top) and vertical (bottom) components of the SV displacement field are shown.

Poisson–Neumann approach. In particular:

$$\text{Poisson–Neumann: } \max_{(i,j) \in \Sigma^{(v)}} \left| u_{S,i,j+1/2}^{(x)} \right| \approx 1.6 \cdot 10^{-17}, \quad \max_{(i,j) \in \Sigma^{(h)}} \left| u_{S,i+1/2,j}^{(z)} \right| \approx 1.6 \cdot 10^{-17}$$

$$\text{Poisson–mixed: } \max_{(i,j) \in \Sigma^{(v)}} \left| u_{S,i,j+1/2}^{(x)} \right| \approx 1.9 \cdot 10^{-18}, \quad \max_{(i,j) \in \Sigma^{(h)}} \left| u_{S,i+1/2,j}^{(z)} \right| \approx 8.7 \cdot 10^{-19}$$

This observation is consistent with the higher level of accuracy expected from the spectral construction underlying the mixed formulation, in line with the behavior previously observed for the Poisson–Dirichlet approach.

Overall, this test confirms that the proposed Poisson–mixed strategy is able to reproduce the physically consistent behavior of the Poisson–Neumann separation at a fluid free

surface, while exhibiting a reduced level of residual P-to-SV leakage, without increasing the asymptotic computational complexity.

Marine Marmousi–II model

We employ the same source as in the previous test, with central frequency $f_0 = 7.5$ Hz and injected at $(x_s, z_s) = (1.250 \text{ km}, 0.045 \text{ km})$. We consider a representative snapshot of the wave-field, extracted at $t \approx 0.90$ s and shown in figure 9.3. The resulting P and SV components, obtained through the Poisson–Neumann, Poisson–Dirichlet and Poisson–mixed separation strategies, are shown in figures 9.4 and 9.5.

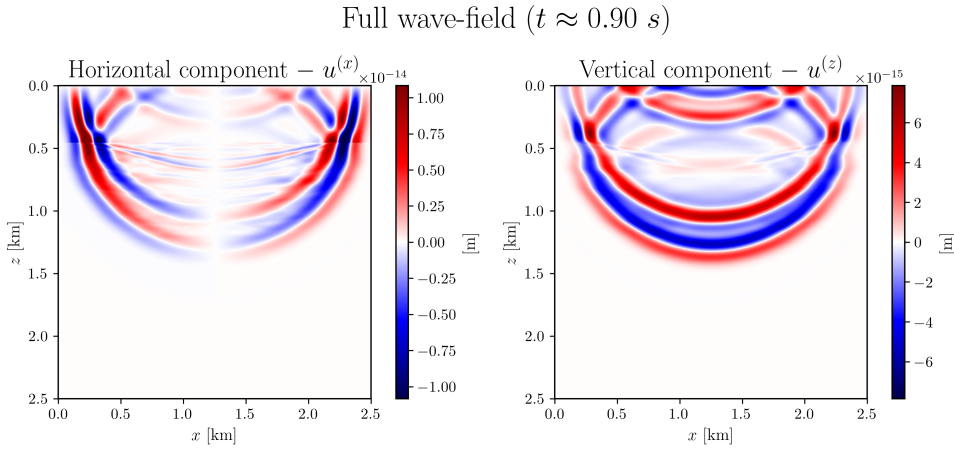


Figure 9.3: Snapshot of the full wave-field at $t \approx 0.90$ s. The horizontal (left) and vertical (right) components of the displacement field are shown.

In this configuration, the presence of a fluid upper layer implies that shear waves are not physically supported in this portion of the medium. As a consequence, any SV component observed in the separated wave-field above $z \approx 0.45$ km must be interpreted as artifacts.

A first qualitative observation, based on the upper panels of figures 9.4 and 9.5, is that all three approaches provide a consistent reconstruction of the P wave-field in the interior of the domain. In particular, the main wavefronts and their interactions with the heterogeneous structure are accurately captured by all methods, with no visible discrepancies at the macroscopic level. This behavior is consistent with the observations reported in chapter 7, and confirms that, in effectively unbounded regions, the choice of boundary conditions has a negligible impact on the separation in the bulk of the domain.

More relevant differences emerge in the analysis of the SV component. As can be observed from the lower panels of figures 9.4 and 9.5, both the Poisson–Neumann and the Poisson–mixed approaches exhibit a lower level of SV contamination in the upper fluid layer than the Poisson–Dirichlet formulation, with no evidence of spurious conversions at the

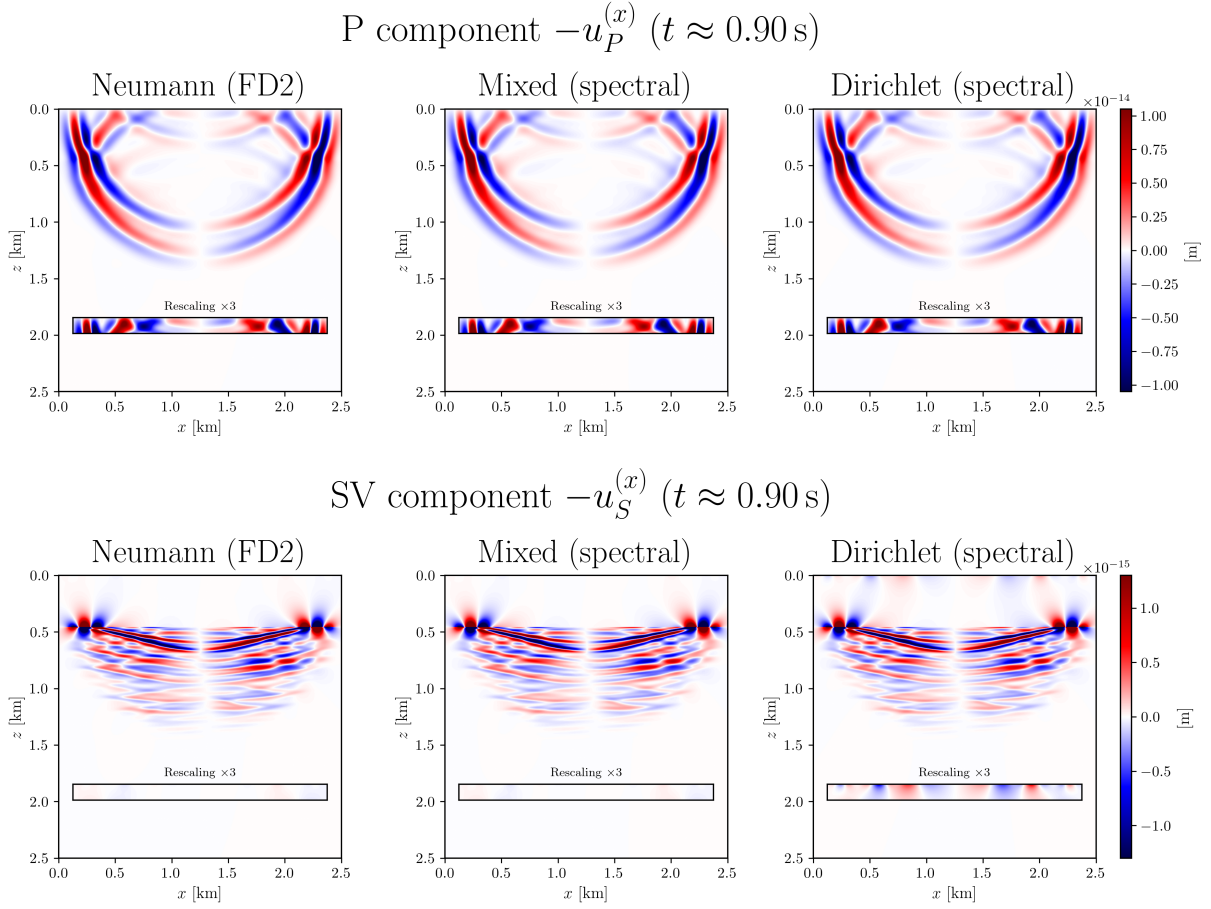


Figure 9.4: Horizontal component of the separated wave-field at $t \approx 0.90$ s. Left: Poisson–Neumann separation. Center: Poisson–mixed separation. Right: Poisson–Dirichlet separation. The P (top) and SV (bottom) components of the horizontal displacement field are shown.

free surface. This behavior is consistent with the physically correct boundary constraint implicitly enforced in both formulations, namely a vanishing normal component of the SV field at the fluid free surface. In contrast, as expected by the discussion in section 8.2.2, the Poisson–Dirichlet approach produces a residual SV component that is more pronounced near the free surface, as highlighted by the rescaled insets. This can be attributed to the fact that the Dirichlet formulation does not enforce a boundary constraint consistent with the physical model at the fluid interface, which may induce spurious near surface contributions in the separated SV field.

In addition to the spurious P-to-SV conversions at the fluid free surface induced by the Poisson–Dirichlet approach, a further feature can be observed in all three separation results, namely the presence of oscillatory artifacts in the SV component generated at the fluid–solid interface and propagating within the overlying fluid layer. These instabilities

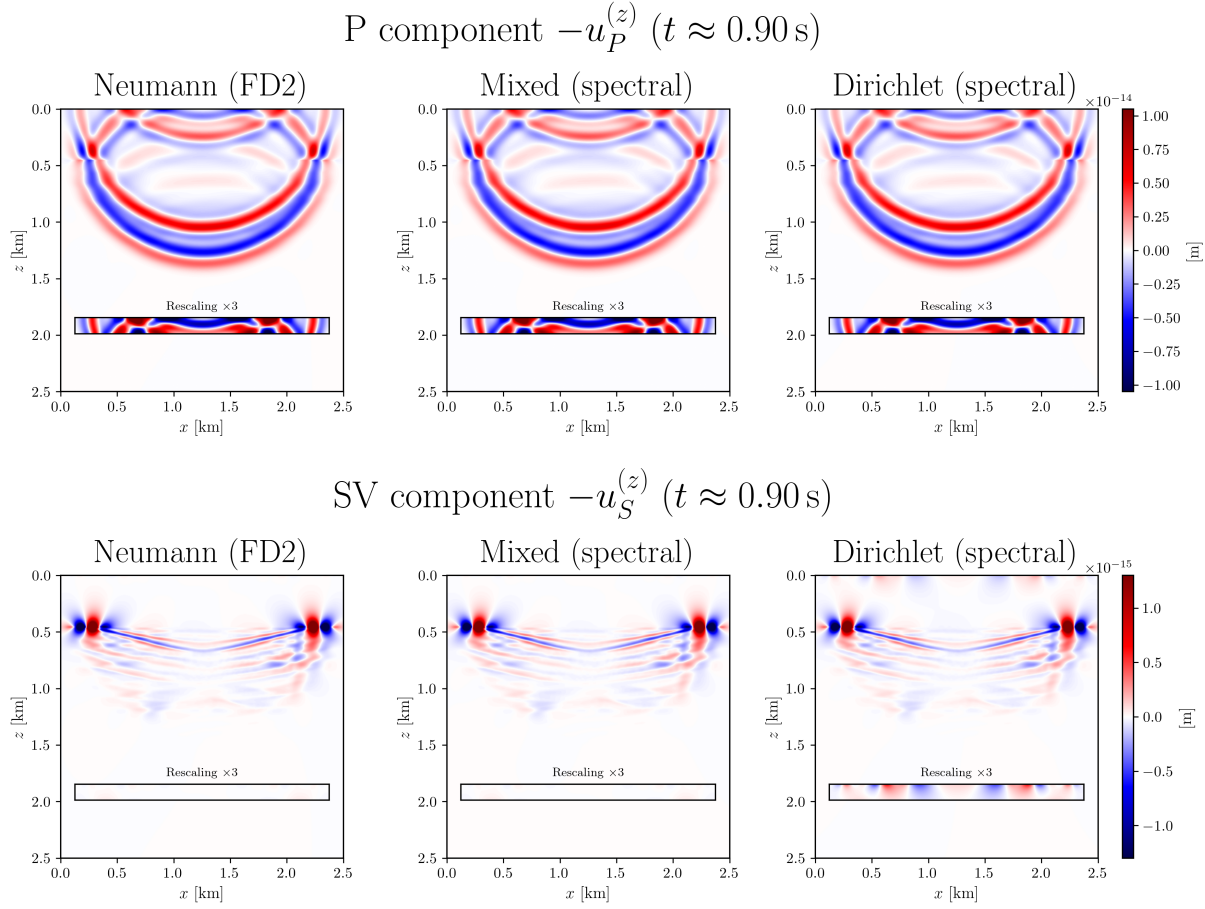


Figure 9.5: Vertical component of the separated wave-field at $t \approx 0.90$ s. Left: Poisson–Neumann separation. Center: Poisson–mixed separation. Right: Poisson–Dirichlet separation. The P (top) and SV (bottom) components of the vertical displacement field are shown.

are observed to originate when the incident P-waves interact with the fluid–solid interface, and are more pronounced when the first, high-amplitude incident wavefront reaches the interface, while becoming progressively weaker for later reflected waves of lower amplitude. Once generated, these artifacts propagate as rather unstructured numerical noise far from the interface within the overlying fluid layer and, in the case of the Poisson–Neumann and Poisson–mixed approaches, may eventually reach the free surface. Conversely, in the Poisson–Dirichlet case, the near free-surface region is mainly affected by spurious P-to-SV conversions, which appear to be the dominant contribution in that region, compared with the interface-generated numerical noise.

However, the qualitative similarity of such instabilities across all three approaches suggests that they are unlikely to be primarily related to the P–SV separation itself, to the choice of boundary conditions, or to the numerical technique used to solve the auxiliary Poisson

problem. A plausible explanation is that these artifacts originate from small numerical oscillations generated when the incident P waves interact with the sharp discontinuity of the elastic parameters at the fluid–solid interface, where the shear modulus vanishes on the fluid side. In the present work, the fluid–solid interface is treated within the heterogeneous staggered-grid finite-difference approach described in section 3.3.2, following the effective-medium averaging strategy of Moczo et al. [29]. This approach represents material discontinuities through local arithmetic or harmonic averages of the physical parameters and relies on simplified continuity assumptions, rather than on an explicit acoustic–elastic formulation in which the interface conditions are imposed directly. A more detailed investigation of the interface-generated artifacts observed here may therefore require a comparison with a numerical framework specifically designed for coupled acoustic–elastic wave propagation. In this respect, spectral element methods for coupled acoustic–elastic media (see, e.g., [21]) provide a natural reference, since the corresponding interface conditions can be incorporated at the variational level.

Overall, the results presented in this section show that the Poisson–mixed formulation provides a robust and physically consistent P–SV separation strategy, effectively combining the advantages of the Poisson–Neumann and Poisson–Dirichlet approaches.

10 | Application to the Elastic Full Waveform Inversion

The analysis developed in the previous chapters has established a mathematically grounded and numerically consistent framework for the separation of elastic isotropic wave-fields into their compressional and shear components. Starting from the *Helmholtz–Weyl decomposition theorem*, we have introduced projection operators that allow a consistent decomposition of the displacement field into its irrotational and solenoidal parts, and we have shown how these operators can be constructed and implemented through the solution of auxiliary Poisson problems under different boundary conditions. Their theoretical properties and numerical behavior have been thoroughly investigated, with particular attention to the role of boundary conditions and to the mitigation of boundary-induced artifacts.

A natural question is whether this separation framework can be exploited beyond wave-field analysis, and, in particular, within inverse problems based on elastic wave propagation. In this context, Elastic Full Waveform Inversion (E-FWI) represents a natural and highly relevant setting. Indeed, FWI has proven to be a powerful technique for the reconstruction of high-resolution subsurface properties by exploiting the full waveform content of seismic data (see, e.g., [35, 39]). The extension from acoustic to elastic formulations allows the inversion to incorporate both compressional and shear effects, enabling the simultaneous reconstruction of the P-wave and S-wave velocities, which carry complementary physical information and are of fundamental importance in many applications.

However, this increased level of physical realism comes at the cost of a significantly more challenging inverse problem. In particular, the simultaneous inversion for multiple elastic parameters increases the nonlinearity of FWI and makes it more vulnerable to parameter trade-offs, commonly referred to as cross-talk, especially between the P-wave and S-wave velocities (e.g., [30]). These coupling effects may lead to spurious updates in the reconstructed models and reduce the interpretability and reliability of the inversion results. A considerable body of work has been devoted to mitigating these issues, for

instance through the use of alternative parametrizations (see, e.g., [15]) or accounting for the inverse Hessian operator within the optimization scheme (see, e.g., [28]).

In this work, we adopt a different perspective, based on the physical decomposition of the elastic wave-field. The key idea is to exploit the separation of the displacement field into its P and S components in order to selectively extract the information associated with compressional and shear waves. Similar P–S decoupling strategies have been successfully employed in elastic reverse time migration to obtain physically interpretable images free from imaging cross-talk (e.g., in [40, 44]). In the context of elastic full waveform inversion, mode-decomposition-based approaches have also been proposed to precondition the adjoint-state gradients and mitigate parameter trade-offs (see, e.g., [41]).

The objective of this chapter is not only to incorporate the P–S separation into the inversion workflow, but, more importantly, to analyze the structural mechanisms through which it modifies the adjoint-state gradient and affects the coupling between the V_P and V_S parameters. In particular, we aim to provide a structural and physically motivated interpretation of the asymmetric behavior of the cross-talk observed in practice, whereby the introduction of the separation is found to significantly reduce the $V_P \rightarrow V_S$ leakage, while the opposite $V_S \rightarrow V_P$ coupling remains substantially unaffected.

The chapter is organized as follows. We first briefly recall the basic concepts of time-domain multi-parameter elastic inversion in the adjoint-state formulation, reviewing the structure of the associated gradients. Next, we introduce the P–S separation within the gradient computation and analyze its effect on the coupling mechanisms between the elastic parameters, both from a structural and a physical perspective. Finally, we present numerical inversion experiments that validate the theoretical findings and illustrate the impact of the proposed approach on the reconstructed models and on the convergence behavior of the inversion process.

10.1. Basic concepts of time-domain elastic multi-parameter inversion

In this section, we briefly recall the basic formulation of time-domain E–FWI. We do not aim at providing a complete and rigorous derivation of the method; rather, we focus on introducing the fundamental mechanism and establishing the notation used in the subsequent developments.

E–FWI is based on the iterative update of the material parameters describing the elastic model, with the objective of minimizing a suitable measure of the discrepancy between

observed and simulated data. This general structure provides the framework within which the *forward* and *adjoint problems*, the misfit functional and the associated gradient are defined.

Throughout this section and the following ones, the analysis is carried out at a formal level. All the objects involved are assumed to be sufficiently regular to justify the manipulations and properties required in the derivations.

Forward problem and solution operator

Let us consider a suitable domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, and the time interval $I = (0, T)$.

Let $\mathcal{M}$ denote the space of admissible material parameters and $\underline{m} = (\rho, \mu, \lambda) \in \mathcal{M}$, $\underline{m} : \Omega \rightarrow \mathbb{R}^3$ a generic model vector.

Let $\mathcal{F}$ denote the space of admissible forcing terms and $\underline{f} \in \mathcal{F}$, $\underline{f} : I \times \Omega \rightarrow \mathbb{R}^n$ a prescribed source term, assumed fixed throughout the inversion process.

Given the prescribed $\underline{f} \in \mathcal{F}$ and a generic $\underline{m} \in \mathcal{M}$, we recall the elastic wave equation in its *displacement-only formulation* for linear elastic and isotropic media (see section 2.1):

$$\begin{cases} \rho \frac{\partial^2 \underline{u}}{\partial t^2} - \operatorname{div} \left(2\mu \bar{\bar{\varepsilon}}(\underline{u}) + \lambda \operatorname{div}(\underline{u}) \bar{\bar{\mathbf{I}}} \right) = \underline{f} & \text{in } I \times \Omega \\ \underline{u} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{u} = \frac{\partial \underline{u}}{\partial t} = \underline{0} & \text{in } \{0\} \times \bar{\Omega} \end{cases} \quad (10.1)$$

For simplicity, we consider homogeneous Dirichlet boundary conditions on $\partial\Omega$ and vanishing initial conditions.

We denote by $\mathcal{U}$ the space of displacement fields $\underline{u} : I \times \Omega \rightarrow \mathbb{R}^n$ solving problem (10.1) in a suitable sense. Assuming that, for the prescribed source term $\underline{f} \in \mathcal{F}$, problem (10.1) admits a unique solution $\underline{u} \in \mathcal{U}$ for all $\underline{m} \in \mathcal{M}$, the associated solution operator is well defined as

$$S_f : \mathcal{M} \rightarrow \mathcal{U}, \quad \underline{m} \mapsto \underline{u} = S_f(\underline{m})$$

which associates to the model parameters $\underline{m}$ the corresponding predicted displacement field $\underline{u}$. In the context of E-FWI, problem (10.1) is referred to as the *forward problem*, while its solution $\underline{u} = S_f(\underline{m})$ is called the *forward wave-field*.

Remark 10.1.

According to the classical theory of second-order linear evolutionary equations, problem (10.1) is well-posed, and, therefore, the solution operator S_f is well defined, under suitable

minimal regularity assumptions on the coefficients and the data (see section 4.1).

However, since the present chapter is intended to provide structural and interpretative insight rather than a complete functional-analytic treatment, the analysis will be carried out at a formal level, and these technical considerations will be omitted.

Observation and misfit functional

Let $\mathcal{V}$ denote the space of admissible observable wave-fields $\underline{v} : I \times \Omega \rightarrow \mathbb{R}^n$, with $\mathcal{U} \subset \mathcal{V}$. We denote by $\mathcal{Y}$ the space of data $\underline{y} : I \rightarrow \mathbb{R}^{nN_r}$ (where N_r denotes the number of receivers), i.e., the space where the recorded measurements take values. Then, we introduce the observation operator

$$O : \mathcal{V} \rightarrow \mathcal{Y}, \quad \underline{v} \mapsto \underline{v}^{\text{obs}} = O(\underline{v})$$

which associates to a wave-field $\underline{v}$ its observations at the receivers' locations $\underline{v}^{\text{obs}}$.

We also introduce the adjoint observation operator. Assuming that $\mathcal{V}$ and $\mathcal{Y}$ are Hilbert spaces, endowed with scalar products $(\cdot, \cdot)_{\mathcal{V}}$ and $(\cdot, \cdot)_{\mathcal{Y}}$, respectively, the adjoint observation operator

$$O^* : \mathcal{Y} \rightarrow \mathcal{V}$$

is formally defined by the relation

$$(O(\underline{v}), \underline{y})_{\mathcal{Y}} = (\underline{v}, O^*(\underline{y}))_{\mathcal{V}}, \quad \forall \underline{v} \in \mathcal{V}, \quad \forall \underline{y} \in \mathcal{Y}$$

A possible choice is to take $\mathcal{V} = L^2(I; [L^2(\Omega)]^n)$ and $\mathcal{Y} = [L^2(I)]^{nN_r}$, and to interpret O as a (possibly regularized) sampling operator at the receivers' locations.

Let us now introduce the reduced operator

$$F : \mathcal{M} \rightarrow \mathcal{Y}, \quad F = O \circ S_f, \quad \underline{m} \mapsto \underline{u}^{\text{obs}} = F(\underline{m}) = O(S_f(\underline{m}))$$

which maps the model parameters $\underline{m}$ to the corresponding synthetic measurements at the receivers' locations $\underline{u}^{\text{obs}}$.

Let $\underline{d} \in \mathcal{Y}$ denote the observed data, i.e., the measurements recorded at the receivers. Then, for a given model $\underline{m} \in \mathcal{M}$, we define the data residual as

$$\underline{r}(\underline{m}) = F(\underline{m}) - \underline{d} = \underline{u}^{\text{obs}} - \underline{d} \in \mathcal{Y}$$

which is the difference between the synthetic measurements $\underline{u}^{\text{obs}}$ and the observed data $\underline{d}$.

Finally, we introduce the misfit functional. In the following, we adopt the standard L^2 -type data misfit, which is defined as

$$\chi : \mathcal{M} \rightarrow \mathbb{R}, \quad \underline{m} \mapsto \chi(\underline{m}) = \frac{1}{2} \|\underline{r}(\underline{m})\|_{\mathcal{Y}}^2$$

It represents the chosen measure of the discrepancy between predicted (simulated) and observed data. Its minimization drives the inversion process towards model parameters that best fit the data with respect to this adopted metric in the data space. If $\mathcal{Y} = [L^2(I)]^{nN_r}$, as suggested above, then the functional χ takes the explicit form

$$\chi(\underline{m}) = \frac{1}{2} \int_0^T \|\underline{r}(\underline{m})\|_{\mathbb{R}^{nN_r}}^2 dt = \frac{1}{2} \int_0^T \sum_{i=1}^{nN_r} r_i(\underline{m})^2 dt \quad (10.2)$$

Adjoint-state formulation and gradient expression

We now recall the expression of the gradient of the misfit functional within the adjoint-state framework (see, e.g., [14, 36] and chapter 8 in [13]). Consistently with the choice of the space of observable wave-fields $\mathcal{V}$ suggested above and the use of the adjoint-state formulation, the Gâteaux derivative of (10.2) can be expressed as

$$\begin{aligned} D\chi(\underline{m})[\delta\underline{m}] = & - \int_0^T \int_{\Omega} \delta\rho \frac{\partial \underline{u}}{\partial t} \cdot \frac{\partial \underline{p}}{\partial t} d\Omega dt + \int_0^T \int_{\Omega} 2\delta\mu \bar{\bar{\varepsilon}}(\underline{u}) : \bar{\bar{\varepsilon}}(\underline{p}) d\Omega dt + \\ & + \int_0^T \int_{\Omega} \delta\lambda \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) d\Omega dt \end{aligned} \quad (10.3)$$

where $\underline{u} = S_f(\underline{m}) \in \mathcal{U}$ is the *forward wave-field*, while $\underline{p}$, called the *adjoint wave-field*, denotes the solution of the following problem, called the *adjoint problem*:

$$\begin{cases} \rho \frac{\partial^2 \underline{p}}{\partial t^2} - \operatorname{div} \left(2\mu \bar{\bar{\varepsilon}}(\underline{p}) + \lambda \operatorname{div}(\underline{p}) \bar{\bar{\mathbf{I}}} \right) = \underline{g} & \text{in } I \times \Omega \\ \underline{p} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{p} = \frac{\partial \underline{p}}{\partial t} = \underline{0} & \text{in } \{T\} \times \bar{\Omega} \end{cases} \quad (10.4)$$

where $\underline{g} = O^*(\underline{r}(\underline{m})) \in \mathcal{V}$ is the so-called *adjoint source*.

To keep the notation compact, let us denote by $\tilde{\mathcal{U}}$ the space of *adjoint wave-fields* $p : I \times \Omega \rightarrow \mathbb{R}^n$ solving the *adjoint problem* (10.4) in a suitable sense. Assuming that, for the *adjoint source* $\underline{g} \in \mathcal{V}$, problem (10.4) admits a unique solution $\underline{p} \in \tilde{\mathcal{U}}$ for all $\underline{m} \in \mathcal{M}$,

the associated solution operator is well defined as

$$\tilde{S}_g : \mathcal{M} \rightarrow \tilde{\mathcal{U}}, \quad \underline{m} \mapsto \underline{p} = \tilde{S}_g(\underline{m})$$

which associates to the model parameters $\underline{m}$ the corresponding *adjoint wave-field* $\underline{p}$.

Gradient structure and first cross-talk mechanism

To investigate the cross-talk between the parameters V_P and V_S , we introduce the physical parametrization

$$\underline{m}' = (\rho, V_P, V_S) \in \mathcal{M}'$$

which is related to the original parametrization $\underline{m} = (\rho, \mu, \lambda) \in \mathcal{M}$ through the map

$$\Phi : \mathcal{M}' \rightarrow \mathcal{M}, \quad \underline{m} = \Phi(\underline{m}'), \quad \underline{m} = (\rho, \mu, \lambda) = \left(\rho, \rho V_S^2, \rho(V_P^2 - 2V_S^2) \right)$$

Therefore, a perturbation $\delta \underline{m}' = (\delta \rho, \delta V_P, \delta V_S)$ of the parameters $\underline{m}' = (\rho, V_P, V_S)$, induces a variation $\delta \underline{m} = (\delta \rho, \delta \mu, \delta \lambda)$ given by the Gâteaux derivative of Φ evaluated at the point $\underline{m}'$ along the direction $\delta \underline{m}'$:

$$\delta \underline{m} = D\Phi(\underline{m}')[\delta \underline{m}']$$

Explicitly, we obtain

$$\delta \mu = V_S^2 \delta \rho + 2V_S \rho \delta V_S$$

$$\delta \lambda = (V_P^2 - 2V_S^2) \delta \rho + 2\rho V_P \delta V_P - 4\rho V_S \delta V_S$$

To account for this change of parametrization, we introduce the corresponding solution operators for the *forward* and *adjoint problems*, together with the associated misfit functional:

$$S'_f : \mathcal{M}' \rightarrow \mathcal{U}, \quad S'_f = S_f \circ \Phi, \quad \underline{m}' \mapsto \underline{u} = S'_f(\underline{m}') = S_f(\Phi(\underline{m}'))$$

$$\tilde{S}'_g : \mathcal{M}' \rightarrow \tilde{\mathcal{U}}, \quad \tilde{S}'_g = \tilde{S}_g \circ \Phi, \quad \underline{m}' \mapsto \underline{p} = \tilde{S}'_g(\underline{m}') = \tilde{S}_g(\Phi(\underline{m}'))$$

$$\chi' : \mathcal{M}' \rightarrow \mathbb{R}, \quad \chi' = \chi \circ \Phi, \quad \underline{m}' \mapsto \chi'(\underline{m}') = \chi(\Phi(\underline{m}'))$$

Hence, applying the chain rule, the Gâteaux derivative of the misfit functional χ' at the point $\underline{m}' = (\rho, V_P, V_S)$, along the direction $\delta \underline{m}' = (\delta \rho, \delta V_P, \delta V_S)$ is given by

$$D\chi'(\underline{m}')[\delta \underline{m}'] = D(\chi \circ \Phi)(\underline{m}')[\delta \underline{m}'] = D\chi(\Phi(\underline{m}'))[D\Phi(\underline{m}')[\delta \underline{m}']]$$

Explicitly, we get

$$\begin{aligned}
D\chi'(\underline{m}')[\delta\underline{m}'] = & - \int_0^T \int_{\Omega} \left(\frac{\partial \underline{u}}{\partial t} \cdot \frac{\partial \underline{p}}{\partial t} - 2V_S^2 \bar{\varepsilon}(\underline{u}) : \bar{\varepsilon}(\underline{p}) - (V_P^2 - 2V_S^2) \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \right) \delta\rho \, d\Omega \, dt + \\
& + \int_0^T \int_{\Omega} 2\rho V_P \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \delta V_P \, d\Omega \, dt + \\
& + \int_0^T \int_{\Omega} 4\rho V_S \left(\bar{\varepsilon}(\underline{u}) : \bar{\varepsilon}(\underline{p}) - \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \right) \delta V_S \, d\Omega \, dt
\end{aligned}$$

To lighten the notation, we rewrite it in compact form as

$$D\chi'(\underline{m}')[\delta\underline{m}'] = \int_{\Omega} \nabla\chi'(\underline{m}') \cdot \delta\underline{m}' \, d\Omega$$

where we denote

$$\nabla\chi'(\underline{m}') = \left(\partial_{\rho}\chi'(\underline{m}'), \partial_{V_P}\chi'(\underline{m}'), \partial_{V_S}\chi'(\underline{m}') \right)$$

$$\begin{aligned}
\partial_{\rho}\chi'(\underline{m}') = & - \int_0^T \left(\frac{\partial \underline{u}}{\partial t} \cdot \frac{\partial \underline{p}}{\partial t} - 2V_S^2 \bar{\varepsilon}(\underline{u}) : \bar{\varepsilon}(\underline{p}) - (V_P^2 - 2V_S^2) \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \right) dt \\
\partial_{V_P}\chi'(\underline{m}') = & 2\rho V_P \int_0^T \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \, dt \tag{10.5}
\end{aligned}$$

$$\partial_{V_S}\chi'(\underline{m}') = 4\rho V_S \int_0^T \left(\bar{\varepsilon}(\underline{u}) : \bar{\varepsilon}(\underline{p}) - \operatorname{div}(\underline{u}) \operatorname{div}(\underline{p}) \right) dt \tag{10.6}$$

The above equations allow one to identify the gradient of the misfit functional with respect to the model parameters. In particular, the components of the gradient are given by the coefficients multiplying the variations $\delta\rho$, δV_P , and δV_S . This formulation shows that the gradient can be expressed in terms of time cross-correlations between the *forward* and *adjoint wave-fields*. More precisely, each component of the gradient is given by the interaction between specific features of the *forward wave-field* $\underline{u}$ and the *adjoint wave-field* $\underline{p}$, which encode the sensitivity of the misfit functional to perturbations of the corresponding physical parameters.

A more detailed inspection of the gradient components reveals that this structure may induce non-trivial coupling effects between the physical parameters. In particular, equations

(10.5) and (10.6) show that $\partial_{V_S}\chi'(\underline{m}')$ can be rewritten as

$$\partial_{V_S}\chi'(\underline{m}') = 4\rho V_S \int_0^T \bar{\bar{\varepsilon}}(\underline{u}) : \bar{\bar{\varepsilon}}(\underline{p}) dt - 2\frac{V_S}{V_P}\partial_{V_P}\chi'(\underline{m}') \quad (10.7)$$

This representation highlights that the gradient of the misfit functional with respect to V_S contains a contribution that is proportional to the gradient with respect to V_P . Moreover, the proportionality factor depends on V_P itself. This reveals a first intrinsic coupling mechanism through which variations of V_P directly affect the V_S update, thus providing a structural source of the $V_P \rightarrow V_S$ cross-talk observed in practice.

10.2. Incorporation of the P–S separation into gradient computation and its effect on the $V_P - V_S$ coupling

We now investigate how the P–S separation introduced in the previous chapters can be incorporated into the adjoint-state gradient computation.

Let us denote by Π_P and $\Pi_S = \text{Id} - \Pi_P$ the projection operators associated with the chosen P–S decomposition of the displacement field. Consistently with the framework introduced in section 4.2.2, these operators extract, respectively, the irrotational and solenoidal components of any decomposable vector field.

Making reference to the *forward wave-field* $\underline{u} = S'_f(\underline{m}') \in \mathcal{U}$ and *adjoint wave-field* $\underline{p} = \tilde{S}'_g(\underline{m}') \in \tilde{\mathcal{U}}$, we assume, as always, that $\underline{u}(t), \underline{p}(t) \in V \subset [H^1(\Omega)]^n$ for every $t \in I$. We then write

$$\begin{aligned} \underline{u}_P(t) &= \Pi_P(\underline{u}(t)) \in \mathcal{U}_P, & \underline{u}_S(t) &= \Pi_S(\underline{u}(t)) = \underline{u}(t) - \underline{u}_P(t) \in \mathcal{U}_S \\ \underline{p}_P(t) &= \Pi_P(\underline{p}(t)) \in \mathcal{U}_P, & \underline{p}_S(t) &= \Pi_S(\underline{p}(t)) = \underline{p}(t) - \underline{p}_P(t) \in \mathcal{U}_S \end{aligned}$$

Here, $\mathcal{U}_P$ and $\mathcal{U}_S$ denote the spatial spaces of irrotational and solenoidal fields introduced in section 4.2.2.

The concrete construction of the projection operators depends on the boundary conditions imposed on the auxiliary Poisson problem defining the action of Π_P , as discussed in chapters 5–9. However, in the present section, the specific choice of boundary conditions is not essential for the structural analysis of the gradient. We rely only on the defining

properties of the separated fields; in particular, for every $t \in I$,

$$\operatorname{div}(\underline{u}_S(t)) = \operatorname{div}(\underline{p}_S(t)) = 0 \quad (10.8)$$

Consequently, for every $t \in I$,

$$\operatorname{div}(\underline{u}(t)) = \operatorname{div}(\underline{u}_P(t)), \quad \operatorname{div}(\underline{p}(t)) = \operatorname{div}(\underline{p}_P(t)) \quad (10.9)$$

We now describe how this decomposition is incorporated into the computation of the gradients of the misfit functional. The *forward* and *adjoint problems* are not modified: the wave-fields $\underline{u}$ and $\underline{p}$ are still obtained by solving the standard forward and adjoint elastic equations (10.1) and (10.4). The P–S separation is instead applied a posteriori, at each time level, and only affects the wave-field temporal cross-correlations used to assemble the gradient.

At an algorithmic level, the incorporation of the P–S separation into the computation of the adjoint-state gradients proceeds as follows:

1. Solve the *forward problem* (10.1) to obtain the *forward wave-field*

$$\underline{u} = S'_f(\underline{m}')$$

2. Apply the P–S separation to the *forward wave-field*, pointwise in time, obtaining

$$\underline{u}_P(t) = \Pi_P(\underline{u}(t)), \quad \underline{u}_S(t) = \Pi_S(\underline{u}(t)), \quad \forall t \in I$$

3. Solve the *adjoint problem* (10.4) to obtain the *adjoint wave-field*

$$\underline{p} = \tilde{S}'_g(\underline{m}')$$

4. Apply the P–S separation to the *adjoint wave-field*, pointwise in time, obtaining

$$\underline{p}_P(t) = \Pi_P(\underline{p}(t)), \quad \underline{p}_S(t) = \Pi_S(\underline{p}(t)), \quad \forall t \in I$$

5. Compute the separation-based V_P -gradient component by retaining only the P–P cross-correlation:

$$J_{V_P}^{(\text{PP})}(\underline{m}') = 2\rho V_P \int_0^T \operatorname{div}(\underline{u}_P) \operatorname{div}(\underline{p}_P) dt \quad (10.10)$$

6. Compute the separation-based V_S -gradient component by retaining the P–S, S–P and S–S cross-correlations:

$$J_{V_S}^{(\text{PS,SP,SS})}(\underline{m}') = 4\rho V_S \int_0^T \left(\bar{\bar{\varepsilon}}(\underline{u}_P) : \bar{\bar{\varepsilon}}(\underline{p}_S) + \bar{\bar{\varepsilon}}(\underline{u}_S) : \bar{\bar{\varepsilon}}(\underline{p}_P) + \bar{\bar{\varepsilon}}(\underline{u}_S) : \bar{\bar{\varepsilon}}(\underline{p}_S) \right) dt \quad (10.11)$$

Remark 10.2.

The quantities introduced in the last two steps are modified gradient components obtained by retaining only selected modal interaction blocks. They are not introduced as exact partial derivatives of a newly defined misfit functional. For this reason, we denote them by J , rather than by $\partial\chi'$.

We now inspect how the introduction of the P–S separation modifies the structure of the adjoint-state gradients. First, comparing expression (10.5) with the modified component (10.10) in light of equation (10.9), it immediately follows that

$$J_{V_P}^{(\text{PP})}(\underline{m}') = \partial_{V_P}\chi'(\underline{m}'), \quad \forall \underline{m}' \in \mathcal{M}' \quad (10.12)$$

Therefore, at the level of the ideal continuous decomposition, the introduction of the separation does not modify the gradient of the misfit functional with respect to V_P .

On the other hand, the situation for V_S -gradient component is different. Starting from equation (10.6), we decompose the *forward* and *adjoint wave-fields* into their P and S components and retain only the P–S, S–P and S–S interaction blocks. Then, thanks to property (10.8), this leads to the modified separation-based component $J_{V_S}^{(\text{PS,SP,SS})}(\underline{m}')$ defined in equation (10.11). Comparing it with the exact gradient component $\partial_{V_S}\chi'(\underline{m}')$, and in particular with its rewritten form in equation (10.7), we observe that the modified component does not contain the explicit divergence contribution which, in the complete gradient, is proportional to $\partial_{V_P}\chi'(\underline{m}')$. As a consequence, the introduction of the P–S separation removes, at the level of the gradient assembly, the contribution responsible for the direct structural coupling between the exact V_P -gradient component and the V_S -update direction identified above. In other words, the separation suppresses this first source of $V_P \rightarrow V_S$ leakage in the modified adjoint-state gradient.

However, the contribution discussed above is not the only source of coupling between the V_P and V_S updates. In fact, even after the introduction of the P–S separation, $J_{V_P}^{(\text{PP})}$, which coincides with the exact V_P -gradient component, still depends in general on V_S , while $J_{V_S}^{(\text{PS,SP,SS})}$ may still depend on V_P through the *forward* and *adjoint wave-fields*.

Indeed,

$$\underline{u}_P(t) = \Pi_P(\underline{u}(t)), \quad \underline{u}_S(t) = \Pi_S(\underline{u}(t)), \quad \underline{u} = S'_f(\underline{m}')$$

$$\underline{p}_P(t) = \Pi_P(\underline{p}(t)), \quad \underline{p}_S(t) = \Pi_S(\underline{p}(t)), \quad \underline{p} = \tilde{S}'_g(\underline{m}')$$

Therefore, the separated *forward* and *adjoint wave-fields* still depend implicitly on the full elastic model $\underline{m}'$, and hence, in general, on both V_P and V_S . Thus, although the separation suppresses the explicit $V_P \rightarrow V_S$ contribution identified above, a residual coupling remains through the intrinsic dependence of the wave-fields on the complete elastic model.

10.2.1. Heuristic analysis of the residual coupling

We now provide a heuristic analysis of the residual coupling mechanisms identified above, relying on structural arguments. In particular, we focus on the cross-parameter sensitivities of the modified separation-based gradient components that remain after the introduction of the P–S separation in the gradient computation.

Sensitivity fields

To this end, we introduce the *sensitivity fields* associated with perturbations of the model parameters; these fields describe the first variations of the *forward* and *adjoint wave-fields* induced by infinitesimal perturbations of the elastic model.

Let us first consider a perturbation of V_S only. Given an increment δV_S , we define the *forward* and *adjoint sensitivity fields*

$$\underline{w} = D\underline{u}(\underline{m}')[(0, 0, \delta V_S)] = DS'_f(\underline{m}')[(0, 0, \delta V_S)]$$

$$\underline{\psi} = D\underline{p}(\underline{m}')[(0, 0, \delta V_S)] = D\tilde{S}'_g(\underline{m}')[(0, 0, \delta V_S)]$$

Here, $\underline{w}$ represents the first-order perturbation of the *forward wave-field* $\underline{u}$ induced by δV_S , while $\underline{\psi}$ represents the corresponding first-order perturbation of the *adjoint wave-field* $\underline{p}$.

By formally differentiating the *forward problem* (10.1) with respect to V_S , one obtains the following linearized forward problem for $\underline{w}$:

$$\begin{cases} \rho \frac{\partial^2 \underline{w}}{\partial t^2} - \operatorname{div} \left(2\rho V_S^2 \left(\bar{\varepsilon}(\underline{w}) - \operatorname{div}(\underline{w})\bar{\mathbf{I}} \right) + \rho V_P^2 \operatorname{div}(\underline{w})\bar{\mathbf{I}} \right) = \underline{f}_{V_S}(\underline{u}) & \text{in } I \times \Omega \\ \underline{w} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{w} = \frac{\partial \underline{w}}{\partial t} = \underline{0} & \text{in } \{0\} \times \bar{\Omega} \end{cases} \quad (10.13)$$

where, to lighten the notation, we denoted the source term on the right-hand side as

$$\underline{f}_{V_S}(\underline{u}) = 4 \operatorname{div} \left(\rho V_S \delta V_S \bar{\bar{\varepsilon}}(\underline{u}) \right) - 4 \nabla \left(\rho V_S \delta V_S \operatorname{div}(\underline{u}) \right) \quad (10.14)$$

and we use the same notation when the argument is replaced by any sufficiently regular vector field, such as the *adjoint wave-field* $\underline{p}$.

Similarly, formally differentiating the *adjoint problem* (10.4) with respect to V_S gives the following linearized adjoint problem for $\underline{\psi}$:

$$\begin{cases} \rho \frac{\partial^2 \underline{\psi}}{\partial t^2} - \operatorname{div} \left(2\rho V_S^2 \left(\bar{\bar{\varepsilon}}(\underline{\psi}) - \operatorname{div}(\underline{\psi}) \bar{\bar{\mathbf{I}}} \right) + \rho V_P^2 \operatorname{div}(\underline{\psi}) \bar{\bar{\mathbf{I}}} \right) = \underline{h} + \underline{f}_{V_S}(\underline{p}) & \text{in } I \times \Omega \\ \underline{\psi} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{\psi} = \frac{\partial \underline{\psi}}{\partial t} = \underline{0} & \text{in } \{T\} \times \bar{\Omega} \end{cases} \quad (10.15)$$

where the additional term $\underline{h}$ on the right-hand side comes from the dependence of the adjoint source $\underline{g}$ on the model parameters $\underline{m}'$ through the observation of the *forward wave-field*. Assuming that the observation operator O is model-independent, linear and continuous (i.e. bounded) with respect to suitable norms, the Gâteaux derivative of the *adjoint source* reads

$$\underline{h} = D\underline{g}(\underline{m}')[(0, 0, \delta V_S)] = O^*(O(\underline{w}))$$

Analogously, let us now consider a perturbation of V_P only. Given an increment δV_P , we define the *forward* and *adjoint sensitivity fields*

$$\begin{aligned} \underline{z} &= D\underline{u}(\underline{m}')[(0, \delta V_P, 0)] = DS'_f(\underline{m}')[(0, \delta V_P, 0)] \\ \underline{\theta} &= D\underline{p}(\underline{m}')[(0, \delta V_P, 0)] = D\tilde{S}'_g(\underline{m}')[(0, \delta V_P, 0)] \end{aligned}$$

Here, $\underline{z}$ is the first-order perturbation of the *forward wave-field* induced by δV_P , while $\underline{\theta}$ is the corresponding first-order perturbation of the *adjoint wave-field*.

The linearized forward problem for $\underline{z}$ reads

$$\begin{cases} \rho \frac{\partial^2 \underline{z}}{\partial t^2} - \operatorname{div} \left(2\rho V_S^2 \left(\bar{\bar{\varepsilon}}(\underline{z}) - \operatorname{div}(\underline{z}) \bar{\bar{\mathbf{I}}} \right) + \rho V_P^2 \operatorname{div}(\underline{z}) \bar{\bar{\mathbf{I}}} \right) = \underline{f}_{V_P}(\underline{u}) & \text{in } I \times \Omega \\ \underline{z} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{z} = \frac{\partial \underline{z}}{\partial t} = \underline{0} & \text{in } \{0\} \times \bar{\Omega} \end{cases} \quad (10.16)$$

where we denoted

$$\underline{f}_{V_P}(\underline{u}) = 2\nabla\left(\rho V_P \delta V_P \operatorname{div}(\underline{u})\right) \quad (10.17)$$

and we use the same notation when the argument is replaced by any sufficiently regular vector field, such as the *adjoint wave-field* $\underline{p}$.

Similarly, the linearized adjoint problem for $\underline{\theta}$ is

$$\begin{cases} \rho \frac{\partial^2 \underline{\theta}}{\partial t^2} - \operatorname{div}\left(2\rho V_S^2 \left(\bar{\bar{\varepsilon}}(\underline{\theta}) - \operatorname{div}(\underline{\theta})\bar{\bar{\mathbf{I}}}\right) + \rho V_P^2 \operatorname{div}(\underline{\theta})\bar{\bar{\mathbf{I}}}\right) = \underline{k} + \underline{f}_{V_P}(\underline{p}) & \text{in } I \times \Omega \\ \underline{\theta} = \underline{0} & \text{on } I \times \partial\Omega \\ \underline{\theta} = \frac{\partial \underline{\theta}}{\partial t} = \underline{0} & \text{in } \{T\} \times \bar{\Omega} \end{cases} \quad (10.18)$$

where the additional term $\underline{k}$ comes from the dependence of the adjoint source $\underline{g}$ on the model parameters through the observation of the *forward wave-field*. Under the same assumptions on O , it is given by

$$\underline{k} = D\underline{g}(\underline{m}')[(0, \delta V_P, 0)] = O^*(O(\underline{z}))$$

Cross-parameter sensitivity terms

Let us now introduce the separated *sensitivity fields*. Since the projection operators Π_P and Π_S are linear and model-independent, and assuming that they are continuous (i.e., bounded) with respect to suitable norms, Gâteaux differentiation with respect to $\underline{m}'$ commutes with the action of the projectors. As always, the projection operators are understood to act pointwise in time; the time dependence is omitted in the notation for readability. Therefore, for perturbations of V_S , we obtain

$$\begin{aligned} \underline{w}_P = \Pi_P(\underline{w}) &= D\underline{u}_P(\underline{m}')[(0, 0, \delta V_S)], & \underline{w}_S = \Pi_S(\underline{w}) &= D\underline{u}_S(\underline{m}')[(0, 0, \delta V_S)] \\ \underline{\psi}_P = \Pi_P(\underline{\psi}) &= D\underline{p}_P(\underline{m}')[(0, 0, \delta V_S)], & \underline{\psi}_S = \Pi_S(\underline{\psi}) &= D\underline{p}_S(\underline{m}')[(0, 0, \delta V_S)] \end{aligned}$$

Similarly, for perturbations of V_P , we obtain

$$\begin{aligned} \underline{z}_P = \Pi_P(\underline{z}) &= D\underline{u}_P(\underline{m}')[(0, \delta V_P, 0)], & \underline{z}_S = \Pi_S(\underline{z}) &= D\underline{u}_S(\underline{m}')[(0, \delta V_P, 0)] \\ \underline{\theta}_P = \Pi_P(\underline{\theta}) &= D\underline{p}_P(\underline{m}')[(0, \delta V_P, 0)], & \underline{\theta}_S = \Pi_S(\underline{\theta}) &= D\underline{p}_S(\underline{m}')[(0, \delta V_P, 0)] \end{aligned}$$

We can now use these separated *sensitivity fields* to inspect the cross-parameter sensitivity terms of the modified separation-based gradients. In this heuristic analysis, the residual $V_S \rightarrow V_P$ coupling is the sensitivity of $J_{V_P}^{(PP)}(\underline{m}')$ to perturbations of V_S , i.e., the variation

of the modified V_P gradient induced by an increment δV_S , namely

$$H_{V_P, V_S}^{(\text{PP})}(\underline{m}') = DJ_{V_P}^{(\text{PP})}(\underline{m}')[(0, 0, \delta V_S)]$$

Analogously, the residual $V_P \rightarrow V_S$ coupling is the sensitivity of $J_{V_S}^{(\text{PS,SP,SS})}(\underline{m}')$ to perturbations of V_P , i.e., the variation of the modified V_S gradient induced by an increment δV_P , namely

$$H_{V_S, V_P}^{(\text{PS,SP,SS})}(\underline{m}') = DJ_{V_S}^{(\text{PS,SP,SS})}(\underline{m}')[(0, \delta V_P, 0)]$$

Remark 10.3.

The cross-parameter sensitivity terms introduced above are not entries of the exact Hessian of the original misfit functional. They are sensitivities of the modified gradient components $J_{V_P}^{(\text{PP})}$ and $J_{V_S}^{(\text{PS,SP,SS})}$ with respect to perturbations of the other velocity parameter. We denote them by H in order to distinguish them from second-order derivatives $\partial^2 \chi'$.

Formally differentiating the separated gradient expressions (10.10) and (10.11) with respect to V_S and V_P , respectively, and using the separated *sensitivity fields* introduced above yields the following explicit expression for the cross-parameter sensitivity terms:

$$H_{V_P, V_S}^{(\text{PP})}(\underline{m}') = 2\rho V_P \int_0^T \left(\text{div}(\underline{w}_P) \text{div}(\underline{p}_P) + \text{div}(\underline{u}_P) \text{div}(\underline{\psi}_P) \right) dt \quad (10.19)$$

$$\begin{aligned} H_{V_S, V_P}^{(\text{PS,SP,SS})}(\underline{m}') = 4\rho V_S \int_0^T & \left(\bar{\bar{\varepsilon}}(\underline{z}_P) : \bar{\bar{\varepsilon}}(\underline{p}_S) + \bar{\bar{\varepsilon}}(\underline{u}_P) : \bar{\bar{\varepsilon}}(\underline{\theta}_S) + \bar{\bar{\varepsilon}}(\underline{z}_S) : \bar{\bar{\varepsilon}}(\underline{p}_P) + \right. \\ & \left. + \bar{\bar{\varepsilon}}(\underline{u}_S) : \bar{\bar{\varepsilon}}(\underline{\theta}_P) + \bar{\bar{\varepsilon}}(\underline{z}_S) : \bar{\bar{\varepsilon}}(\underline{p}_S) + \bar{\bar{\varepsilon}}(\underline{u}_S) : \bar{\bar{\varepsilon}}(\underline{\theta}_S) \right) dt \end{aligned} \quad (10.20)$$

Gradient-type forcing terms and qualitative behavior of the *sensitivity fields*

At this point, a useful structural observation concerns the forcing terms $\underline{f}_{V_S}$ and $\underline{f}_{V_P}$ appearing in the linearized forward and adjoint problems introduced above. In particular, from equations (10.14) and (10.17), we observe that they contain the gradient-type contributions

$$-4\nabla(\rho V_S \delta V_S \text{div}(\underline{v})), \quad 2\nabla(\rho V_P \delta V_P \text{div}(\underline{v}))$$

respectively. These terms are relevant because sources in pure gradient form naturally excite compressional perturbations in an ideal homogeneous and infinite setting.

To make this point explicit, let us consider the elastic wave equation in a linear elastic, homogeneous, isotropic and unbounded medium, forced by a source term in pure gradient form. Since the medium is homogeneous, the equation can be formally rewritten in the

Navier form:

$$\begin{cases} \rho \frac{\partial^2 \underline{v}}{\partial t^2} - \mu \Delta \underline{v} - (\mu + \lambda) \nabla \operatorname{div}(\underline{v}) = \nabla s & \text{in } I \times \mathbb{R}^n \\ \underline{v} = \frac{\partial \underline{v}}{\partial t} = \underline{0} & \text{in } \{0\} \times \mathbb{R}^n \end{cases}$$

Let us now apply the curl operator on both sides of the equation. Proceeding formally, we obtain, denoting $\underline{\omega} = \operatorname{curl}(\underline{v})$,

$$\begin{cases} \rho \frac{\partial^2 \underline{\omega}}{\partial t^2} - \mu \Delta \underline{\omega} = \underline{0} & \text{in } I \times \mathbb{R}^n \\ \underline{\omega} = \frac{\partial \underline{\omega}}{\partial t} = \underline{0} & \text{in } \{0\} \times \mathbb{R}^n \end{cases}$$

Since both the forcing term and the initial conditions are identically zero, by uniqueness we get

$$\underline{\omega} = \operatorname{curl}(\underline{v}) = \underline{0} \quad \text{in } I \times \mathbb{R}^n$$

This shows that the resulting wave-field remains irrotational. Hence, in this idealized setting, a source term in gradient form generates, from the point of view of the P–S separation, a purely P-type perturbation of the wave-field.

The argument above has been derived formally in the setting of a homogeneous and infinite medium. However, in the context of this work, the wave propagation problem is set in a bounded and generally heterogeneous medium. Thus, the presence of material heterogeneities may induce P–S conversions. In addition, reflections at boundaries not preceded by absorbing layers (e.g. a free surface) may also generate mode conversions. Nevertheless, the discussion above suggests that a forcing term of pure gradient type primarily generates a compressional perturbation of the wave-field, which may subsequently convert into shear waves due to medium heterogeneities or boundary interactions.

We now attempt to exploit the previous argument to gain insight into the qualitative behavior that it is reasonable to expect from the separated *sensitivity fields*. Recall that the *sensitivity fields* $\underline{w}$ and $\underline{\psi}$ satisfy the linearized forward and adjoint problems (10.13)–(10.15), whose right-hand sides contain the forcing $\underline{f}_{V_S}$, evaluated at $\underline{u}$ and $\underline{p}$, respectively, with the additional term $\underline{h}$ appearing in the adjoint equation. As discussed above, this source includes a contribution in gradient form, which is expected to primarily excite compressional perturbations of the wave-field. Consequently, it is reasonable to expect that $\underline{w}_P$ and $\underline{\psi}_P$ may represent significant contributions to the perturbation. In particular, their divergences may provide non-negligible contributions, since they coincide by construction with those of the complete *sensitivity fields* $\underline{w}$ and $\underline{\psi}$. In view of the ex-

pression of the cross-parameter sensitivity term $H_{V_P, V_S}^{(PP)}(\underline{m}')$, as given by equation (10.19), this heuristic argument suggests that this coupling term may remain significant. In other words, the $V_S \rightarrow V_P$ cross-talk is expected to persist even when the P–S separation is included in the gradient computation. This consideration is consistent with the observation made in (10.12), namely that, in principle, the introduction of the P–S separation does not alter the gradient of the misfit functional with respect to V_P .

Let us now consider the *sensitivity fields* $\underline{z}$ and $\underline{\theta}$, solutions of the linearized forward and adjoint problems (10.16)–(10.18). Although both equations contain the forcing term $\underline{f}_{V_P}$, which is in pure gradient form, and, therefore, primarily generates compressional perturbations of the wave-field, this observation alone does not allow us to conclude that, in general, the S components of the *sensitivity fields* $\underline{z}_S$ and $\underline{\theta}_S$ are negligible. Two main mechanisms prevent such a conclusion. First, during propagation in a bounded and heterogeneous medium, mode conversions may occur and generate significant shear energy. Second, the linearized adjoint problem (10.18) for $\underline{\theta}$ is also forced by the term $\underline{k} = O^*(O(\underline{z}))$, which is not, in general, of pure gradient form. As a consequence, the argument based on irrotational forcing does not provide a sufficiently robust basis for inferring the expected behavior of $\underline{z}_S$ and $\underline{\theta}_S$.

Isotropic-deviatoric structure of the residual $V_P \rightarrow V_S$ coupling

Rather than relying only on heuristic expectations about the modal content of the *sensitivity fields* $\underline{z}$ and $\underline{\theta}$, we now try to gain insight on the residual $V_P \rightarrow V_S$ coupling by inspecting the tensorial structure of the cross-parameter sensitivity term $H_{V_S, V_P}^{(PS, SP, SS)}(\underline{m}')$, as given by equation (10.20).

This term can be analyzed by exploiting the isotropic-deviatoric decomposition of the strain tensor. Namely, for any sufficiently regular vector field $\underline{v}$, we write

$$\bar{\bar{\varepsilon}}(\underline{v}) = \text{iso}(\bar{\bar{\varepsilon}}(\underline{v})) + \text{dev}(\bar{\bar{\varepsilon}}(\underline{v})) = \frac{1}{n} \text{div}(\underline{v}) \bar{\bar{\mathbf{I}}} + \text{dev}(\bar{\bar{\varepsilon}}(\underline{v})) \quad (10.21)$$

The isotropic component is associated with the volumetric part of the deformation, while the deviatoric component is associated with local shape distortions without first-order volume variations.

Two simple properties will be used below. First, by construction, the deviatoric component is traceless:

$$\text{Tr}(\text{dev}(\bar{\bar{\varepsilon}}(\underline{v}))) = 0 \quad (10.22)$$

Second, since the S components are solenoidal, we have

$$\text{iso}(\bar{\bar{\varepsilon}}(\underline{v}_S)) = \frac{1}{n} \text{div}(\underline{v}_S) \bar{\bar{\mathbf{I}}} = \bar{\bar{0}} \quad (10.23)$$

Using decomposition (10.21) inside equation (10.20), together with properties (10.22) and (10.23), all contributions involving an isotropic factor vanish. Therefore, the residual $V_P \rightarrow V_S$ cross-parameter sensitivity term can be rewritten as

$$\begin{aligned} H_{V_S, V_P}^{(\text{PS}, \text{SP}, \text{SS})}(\underline{m}') = 4\rho V_S \int_0^T & \left(\text{dev}(\bar{\bar{\varepsilon}}(\underline{z}_P)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{p}_S)) + \text{dev}(\bar{\bar{\varepsilon}}(\underline{u}_P)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{\theta}_S)) + \right. \\ & + \text{dev}(\bar{\bar{\varepsilon}}(\underline{z}_S)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{p}_P)) + \text{dev}(\bar{\bar{\varepsilon}}(\underline{u}_S)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{\theta}_P)) + \\ & \left. + \text{dev}(\bar{\bar{\varepsilon}}(\underline{z}_S)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{p}_S)) + \text{dev}(\bar{\bar{\varepsilon}}(\underline{u}_S)) : \text{dev}(\bar{\bar{\varepsilon}}(\underline{\theta}_S)) \right) dt \end{aligned}$$

This expression shows that, after the introduction of the P–S separation, the cross-parameter sensitivity term $H_{V_S, V_P}^{(\text{PS}, \text{SP}, \text{SS})}(\underline{m}')$ depends exclusively on the deviatoric components of the strain tensors of the *forward* and *adjoint wave-fields* and of the associated *sensitivity fields*. This should be contrasted with the situation in which the P–P cross-correlation is also included in the computation of the gradient of the misfit functional with respect to V_S . In this case, besides the appearance of the explicit V_P -related contribution identified previously in equation (10.7), the term

$$\bar{\bar{\varepsilon}}(\underline{u}_P) : \bar{\bar{\varepsilon}}(\underline{p}_P)$$

would generate, in the complete cross-parameter sensitivity term $\partial_{V_S, V_P}^2 \chi'(\underline{m}')$, additional volumetric terms of the form

$$\begin{aligned} \text{iso}(\bar{\bar{\varepsilon}}(\underline{z}_P)) : \text{iso}(\bar{\bar{\varepsilon}}(\underline{p}_P)) &= \frac{1}{n} \text{div}(\underline{z}_P) \text{div}(\underline{p}_P) \\ \text{iso}(\bar{\bar{\varepsilon}}(\underline{u}_P)) : \text{iso}(\bar{\bar{\varepsilon}}(\underline{\theta}_P)) &= \frac{1}{n} \text{div}(\underline{u}_P) \text{div}(\underline{\theta}_P) \end{aligned}$$

thereby introducing an additional direct volumetric pathway in the $V_P \rightarrow V_S$ interaction.

The P–S separation therefore suppresses both the explicit volumetric contribution appearing in the original expression of the gradient with respect to V_S and the analogous volumetric terms that would arise inside the complete cross-parameter sensitivity term through the P–P block after the isotropic-deviatoric decomposition. As a consequence, the residual $V_P \rightarrow V_S$ coupling can only persist through deviatoric strain correlations involving at least one S component. In this sense, the separation removes the direct vol-

umetric pathway associated with P–P interactions. However, this does not imply that the residual coupling is negligible in general, since P wave-fields may still have non-zero deviatoric strain components, especially in heterogeneous media and near boundaries or material interfaces, where complex mode interactions may occur.

10.2.2. Connection with Born scattering radiation patterns

The structural analysis carried out in the previous section suggests that the introduction of the P–S separation affects the two cross-talk directions in an asymmetric way. On the one hand, the separation suppresses the direct volumetric pathway for $V_P \rightarrow V_S$ leakage associated to the P–P interactions. On the other hand, the V_P -gradient component, which is, in principle, not affected by the introduction of the separation, remains sensitive to perturbations of V_S through the P component of the corresponding sensitivity fields.

We now provide a complementary physical interpretation of this behavior by relating the *forward sensitivity fields* introduced above to the classical Born scattering radiation patterns for elastic waves. Indeed, the fields

$$\begin{aligned}\underline{w} &= D\underline{u}(\underline{m}')[(0, 0, \delta V_S)] = DS'_f(\underline{m}')[(0, 0, \delta V_S)] \\ \underline{z} &= D\underline{u}(\underline{m}')[(0, \delta V_P, 0)] = DS'_f(\underline{m}')[(0, \delta V_P, 0)]\end{aligned}$$

represent the first variations of the *forward wave-field* with respect to infinitesimal perturbations of the elastic parameters V_S and V_P , respectively. These fields satisfy the linearized forward problems (10.13) and (10.16), whose forcing terms $\underline{f}_{V_S}(\underline{u})$ and $\underline{f}_{V_P}(\underline{u})$, given by equations (10.14) and (10.17), respectively, depend on the background wave-field $\underline{u} = S'_f(\underline{m}')$. From the point of view of the linearized scattering theory, they therefore correspond to the first-order scattered wave-fields arising from the Born linearization of the elastic wave equation.

In order to analyze the modal content of the *forward sensitivity fields* $\underline{w}$ and $\underline{z}$, we consider the classical idealized setting commonly adopted in the study of elastic Born scattering in the so-called *Rayleigh scattering* regime (see, e.g., [42, 43]). More precisely, we assume that:

- The background medium is linear elastic, isotropic, unbounded and homogeneous, with constant elastic parameters $\underline{m}'_0 = (\rho_0, V_{P,0}, V_{S,0}) \in \mathbb{R}^3$.
- The *forward wave-field* is a time-harmonic plane-wave propagating in the back-

ground medium. It can be either a P- or an SV-wave traveling along the x direction:

$$\begin{aligned} \underline{u}(t, \underline{x}) &= \underline{U}^{(P)}(t, \underline{x}), \quad U_x^{(P)}(t, \underline{x}) = \Re \left(e^{-i\omega \left(t - \frac{x}{V_{P,0}} \right)} \right), \quad U_z^{(P)}(t, \underline{x}) \equiv 0 \\ \underline{u}(t, \underline{x}) &= \underline{U}^{(S)}(t, \underline{x}), \quad U_x^{(S)}(t, \underline{x}) \equiv 0, \quad U_z^{(S)}(t, \underline{x}) = \Re \left(e^{-i\omega \left(t - \frac{x}{V_{S,0}} \right)} \right) \end{aligned}$$

- The perturbation of the elastic parameters $\delta \underline{m}' = (\delta \rho, \delta V_P, \delta V_S)$ is localized in a small neighborhood of the point $\underline{x}_0 \in \mathbb{R}^2$, and the characteristic size of the perturbation is much smaller than the wavelength of the incident wave-field $\underline{u}$.
- The magnitude of the perturbation is “infinitesimal”, meaning that it satisfies

$$|\delta \rho(\underline{x})| \ll \rho_0, \quad |\delta V_P(\underline{x})| \ll V_{P,0}, \quad |\delta V_S(\underline{x})| \ll V_{S,0}$$

Under these assumptions, the perturbation can be approximated as a point scatterer localized at $\underline{x}_0$. As the observation distance

$$r = \|\underline{x} - \underline{x}_0\|_{\mathbb{R}^2}$$

tends to infinity, the scattered wave-field generated by the linearized forward problems admits a far-field asymptotic representation. This regime is commonly referred to as *Rayleigh scattering*. In this setting, the amplitude of the far-field scattered wave-field depends on the scattering angle $\alpha \in [0, 2\pi)$, defined as the angle between the incident propagation direction and the observation direction

$$\hat{r} = \frac{\underline{x} - \underline{x}_0}{r} = (\cos \alpha, \sin \alpha)$$

Moreover, the scattered field can be decomposed into the different modal contributions PP, PS, SP and SS. The angular dependence of the amplitude of these scattered modes is described by the corresponding *radiation patterns*.

Let us start by considering a perturbation of V_S only, namely

$$\delta \underline{m}' = (0, 0, \delta V_S)$$

We consider the two cases corresponding to an incident time-harmonic plane P-wave and

SV-wave, respectively. Accordingly, we define

$$\underline{w}^{(P)} = D\underline{U}^{(P)}(\underline{m}'_0)[(0, 0, \delta V_S)], \quad \underline{w}^{(S)} = D\underline{U}^{(S)}(\underline{m}'_0)[(0, 0, \delta V_S)]$$

which are the solutions of the corresponding linearized forward problem (10.13), now considered in the unbounded domain $\Omega = \mathbb{R}^2$ and forced by $\underline{f}_{V_S}(\underline{U}^{(P)})$ and $\underline{f}_{V_S}(\underline{U}^{(S)})$, respectively.

These *sensitivity fields* admit the following asymptotic far-field representations:

$$\underline{w}^{(P)}(t, \underline{x}) \sim f_2(r) \Re \left(A_{PP}^{\delta V_S}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{P,0}} \right)} \hat{r} + A_{PS}^{\delta V_S}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{S,0}} \right)} \hat{r}^\perp \right), \quad r \rightarrow +\infty$$

$$\underline{w}^{(S)}(t, \underline{x}) \sim f_2(r) \Re \left(A_{SP}^{\delta V_S}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{P,0}} \right)} \hat{r} + A_{SS}^{\delta V_S}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{S,0}} \right)} \hat{r}^\perp \right), \quad r \rightarrow +\infty$$

where $f_2(r)$ denotes the far-field radial decay factor in two spatial dimensions. In particular, $f_2(r) \rightarrow 0$ as $r \rightarrow +\infty$, while its precise asymptotic behavior is not relevant for the present discussion.

The *Rayleigh scattering radiation patterns* associated with a perturbation $\delta \underline{m}' = (0, 0, \delta V_S)$ are given by

$$A_{PP}^{\delta V_S}(\alpha) \propto \sin^2(\alpha) \frac{\delta V_S}{V_{S,0}}, \quad A_{PS}^{\delta V_S}(\alpha) \propto \sin(2\alpha) \frac{\delta V_S}{V_{S,0}} \quad (10.24)$$

$$A_{SP}^{\delta V_S}(\alpha) \propto \sin(2\alpha) \frac{\delta V_S}{V_{S,0}}, \quad A_{SS}^{\delta V_S}(\alpha) \propto \cos(2\alpha) \frac{\delta V_S}{V_{S,0}} \quad (10.25)$$

Let us now consider a perturbation of V_P only, namely

$$\delta \underline{m}' = (0, \delta V_P, 0)$$

We again distinguish the two cases corresponding to an incident time-harmonic plane P-wave and SV-wave, respectively. Accordingly, we define

$$\underline{z}^{(P)} = D\underline{U}^{(P)}(\underline{m}'_0)[(0, \delta V_P, 0)], \quad \underline{z}^{(S)} = D\underline{U}^{(S)}(\underline{m}'_0)[(0, \delta V_P, 0)]$$

which are the solutions of the corresponding linearized forward problem (10.16), set in $\Omega = \mathbb{R}^2$ and forced by $\underline{f}_{V_P}(\underline{U}^{(P)})$ and $\underline{f}_{V_P}(\underline{U}^{(S)})$, respectively.

These *sensitivity fields* admit the following asymptotic far-field representations:

$$\underline{z}^{(P)}(t, \underline{x}) \sim f_2(r) \Re \left(A_{PP}^{\delta V_P}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{P,0}} \right)} \hat{r} + A_{PS}^{\delta V_P}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{S,0}} \right)} \hat{r}^\perp \right), \quad r \rightarrow +\infty$$

$$\underline{z}^{(S)}(t, \underline{x}) \sim f_2(r) \Re \left(A_{SP}^{\delta V_P}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{P,0}} \right)} \hat{r} + A_{SS}^{\delta V_P}(\alpha) e^{-i\omega \left(t - \frac{r}{V_{S,0}} \right)} \hat{r}^\perp \right), \quad r \rightarrow +\infty$$

The *Rayleigh scattering radiation patterns* associated with a perturbation $\delta \underline{m}' = (0, \delta V_P, 0)$ are given by

$$A_{PP}^{\delta V_P}(\alpha) \propto \frac{\delta V_P}{V_{P,0}}, \quad A_{PS}^{\delta V_P}(\alpha) \equiv 0 \quad (10.26)$$

$$A_{SP}^{\delta V_P}(\alpha) \equiv 0, \quad A_{SS}^{\delta V_P}(\alpha) \equiv 0 \quad (10.27)$$

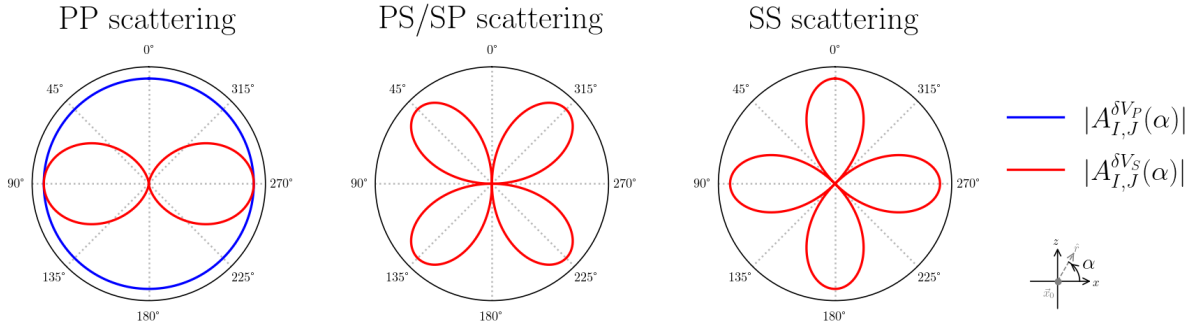


Figure 10.1: Born scattering *radiation patterns* associated with perturbations of the elastic parameters V_P and V_S in the *Rayleigh scattering regime*.

The *radiation patterns* reported in figure 10.1 provide a physical interpretation of the qualitative behavior of the *forward sensitivity fields* introduced in section 10.2.1.

Let us first consider perturbations affecting only V_S . According to equations (10.24) and (10.25), a perturbation of V_S alone generates, in the ideal *Rayleigh scattering regime*, both compressional and shear scattered waves. More precisely, all the scattering modes PP, PS, SP and SS may be activated. In particular, even when the incident wave-field is purely compressional, the scattered field contains both PP and PS contributions. Consequently, the *forward sensitivity fields*

$$\underline{w}^{(P)} = D\underline{U}^{(P)}(\underline{m}'_0)[(0, 0, \delta V_S)], \quad \underline{w}^{(S)} = D\underline{U}^{(S)}(\underline{m}'_0)[(0, 0, \delta V_S)]$$

generally contain a non-vanishing compressional component. In terms of the P–SV sepa-

ration, this can be expressed as

$$\underline{w}_P^{(P)}(t) = \Pi_P(\underline{w}^{(P)}(t)) \neq \underline{0}, \quad \underline{w}_P^{(S)}(t) = \Pi_P(\underline{w}^{(S)}(t)) \neq \underline{0}$$

Although the actual *forward wave-field* $\underline{u} = S'_f(\underline{m}')$ arising in the inversion is not, in general, a time-harmonic plane-wave, the *radiation patterns* suggest that the P component of the *forward sensitivity field*

$$\underline{w} = D\underline{u}(\underline{m}')[(0, 0, \delta V_S)]$$

may represent a significant part of the perturbation. This observation is consistent with the heuristic discussion developed above, where the forcing term $\underline{f}_{V_S}(\underline{u})$ was shown to contain a gradient-type contribution, which provides a direct compressional excitation channel.

Let us now consider perturbations affecting only V_P . According to equations (10.26) and (10.27), a perturbation of V_P produces, in the ideal *Rayleigh scattering regime*, only PP scattering, with isotropic angular dependence. The amplitudes associated with the PS, SP and SS modes vanish identically. Hence, in this idealized setting, the *forward sensitivity fields*

$$\underline{z}^{(P)} = D\underline{U}^{(P)}(\underline{m}_0')[(0, \delta V_P, 0)], \quad \underline{z}^{(S)} = D\underline{U}^{(S)}(\underline{m}_0')[(0, \delta V_P, 0)]$$

are purely compressional, and therefore

$$\underline{z}_S^{(P)}(t) = \Pi_S(\underline{z}^{(P)}(t)) = \underline{0}, \quad \underline{z}_S^{(S)}(t) = \Pi_S(\underline{z}^{(S)}(t)) = \underline{0}$$

Therefore, even if the actual *forward wave-field* is not, in general, a time-harmonic plane-wave, the *radiation patterns* suggest that the SV component of the *forward sensitivity field*

$$\underline{z} = D\underline{u}(\underline{m}')[(0, \delta V_P, 0)]$$

is not primarily generated by the scattering mechanism associated with the V_P only perturbation itself. Rather, in a bounded and heterogeneous medium, the $\underline{z}_S$ component is expected to arise predominantly from secondary mode conversions induced by reflections at the boundaries of the domain or by pre-existing heterogeneities of the background model $\underline{m}'$. Thus, the *radiation patterns* obtained in the *Rayleigh scattering regime* provide a physical confirmation of the mechanism identified above on the basis of the pure gradient form of the forcing term $\underline{f}_{V_P}(\underline{u})$ in the linearized forward problem (10.16).

These observations provide another interpretation of the asymmetric behavior of the

residual coupling terms discussed above. Since a perturbation of V_S is able to generate compressional scattered components already in the ideal *Rayleigh scattering* regime, the P component $\underline{w}_P$ of the corresponding *forward sensitivity field* may be non-negligible. Therefore, the term

$$\text{div}(\underline{w}_P) \text{div}(\underline{p}_P)$$

appearing in $H_{V_P, V_S}^{(\text{PP})}(\underline{m}')$ may remain significant. This explains why the $V_S \rightarrow V_P$ coupling is not expected to be strongly affected by the P–SV separation, consistently with the identity (10.12).

Conversely, a perturbation of V_P generates, in the same idealized regime, only a PP scattered component. Hence, the primary scattering mechanism associated with δV_P feeds precisely the P–P interaction block. Since this block is deliberately removed from the modified V_S -gradient component $J_{V_S}^{(\text{PS}, \text{SP}, \text{SS})}(\underline{m}')$, the direct volumetric PP pathway responsible for the $V_P \rightarrow V_S$ leakage is suppressed at the level of the gradient assembly. The remaining $V_P \rightarrow V_S$ coupling can only arise through secondary mechanisms, such as deviatoric P–S or S–P correlations, mode conversions induced by heterogeneities or boundaries, and the additional forcing term entering the linearized adjoint problem (10.15).

Finally, it is important to remark that the parallelism with the Born scattering theory cannot be applied, strictly speaking, to the *adjoint sensitivity fields*

$$\begin{aligned}\underline{\psi} &= D\underline{p}(\underline{m}')[(0, 0, \delta V_S)] = D\tilde{S}'_g(\underline{m}')[(0, 0, \delta V_S)] \\ \underline{\theta} &= D\underline{p}(\underline{m}')[(0, \delta V_P, 0)] = D\tilde{S}'_g(\underline{m}')[(0, \delta V_P, 0)]\end{aligned}$$

Indeed, the linearized adjoint problems (10.15) and (10.18) contain the additional forcing terms $\underline{h}$ and $\underline{k}$, respectively, which arise from the dependence of the *adjoint source* $\underline{g}$ on the model parameters $\underline{m}'$ through the observation of the *forward wave-field*. As a consequence, the *adjoint sensitivity fields* $\underline{\psi}$ and $\underline{\theta}$ cannot be directly linked with the first-order scattered fields associated with perturbations of the *adjoint wave-field* $\underline{p}$. Therefore, while the *Rayleigh scattering radiation patterns* discussed above provide a useful physical interpretation of the qualitative behavior of the *forward sensitivity fields*, the same argument cannot be straightforwardly extended to the *adjoint sensitivity fields*.

10.3. Numerical inversion experiments

In order to illustrate the theoretical considerations developed in the previous sections, we now present two numerical experiments designed to investigate the cross-talk mechanisms between the parameters V_P and V_S in elastic full waveform inversion. The analysis pre-

sented above suggests that the introduction of the P–SV separation modifies the structure of the adjoint-state gradient in an asymmetric way. In particular, the separation suppresses the direct volumetric pathway contributing to the $V_P \rightarrow V_S$ leakage. By contrast, the opposite $V_S \rightarrow V_P$ coupling is expected to be more persistent, since, at the continuous level, the introduction of the separation does not alter the V_P -gradient component, and perturbations of V_S may still generate compressional components in the associated sensitivity fields.

The purpose of the following numerical experiments is therefore to assess whether this asymmetric behavior is observed in practice. To this end, we compare standard E–FWI with the separation-based strategy introduced in section 10.2, in which the V_P -gradient component is computed from the P–P correlation, whereas the V_S -gradient component is assembled by retaining only the P–S, S–P and S–S interaction blocks. In both cases, the same forward and adjoint wave equations are solved; the difference lies only in the modal selection applied to the wave-field correlations entering the gradient computation.

Two synthetic configurations are considered. The first one is a two-inclusions model, designed as a controlled benchmark in which one anomaly affects only V_P and the other only V_S (see appendix A.3.1). The two inclusions are sufficiently separated to allow the two cross-talk directions to be identified independently, while a full-illumination acquisition geometry is adopted to minimize illumination bias. The second test reproduces the experiment presented in [41]: a sandstone medium with spatially overlapping V_P and V_S perturbations inside a rectangular fluid-saturated reservoir (see appendix A.3.2). This configuration is more representative of realistic subsurface settings, where elastic properties are generally coupled, and of realistic seismic surveys, where sources and receivers are typically placed along surface lines.

Finally, we point out that, since in both experiments all boundaries of the computational domain are equipped with absorbing layers, the P–SV separation is implemented through the Poisson–Dirichlet strategy presented in chapter 6. Indeed, we recall that, according to the results discussed in chapter 7, when absorbing layers surround the whole domain, the choice of boundary conditions to be imposed on the auxiliary Poisson problem has a practically negligible impact on the wave-field decomposition in the bulk of the domain.

In the following, we focus on the interpretation of the inversion results, with particular attention to the reconstructed models, the residual model errors, the quantitative indicators of parameter coupling and the evolution of the misfit functional.

Two inclusions model

We first compare the inversion results obtained on the two-inclusions model, with and without the P–SV separation. As described in appendix A.3.1, the true velocity models consist of two circular anomalies embedded in homogeneous backgrounds: an upper-left anomaly affecting only the P-wave velocity, with $V_{P,1} = 3500 \text{ m s}^{-1}$, and a bottom-right anomaly affecting only the S-wave velocity, with $V_{S,2} = 2330.0 \text{ m s}^{-1}$. The comparison allows us to assess the impact of the separation on the reconstructed models, the residual model errors and the convergence behavior of the inversion.

We begin by inspecting the models obtained at the final iteration of the inversion procedure, namely $k = N_{\text{it}} = 10$. Figure 10.2 shows the reconstructed V_P and V_S fields obtained with and without the P–SV separation.

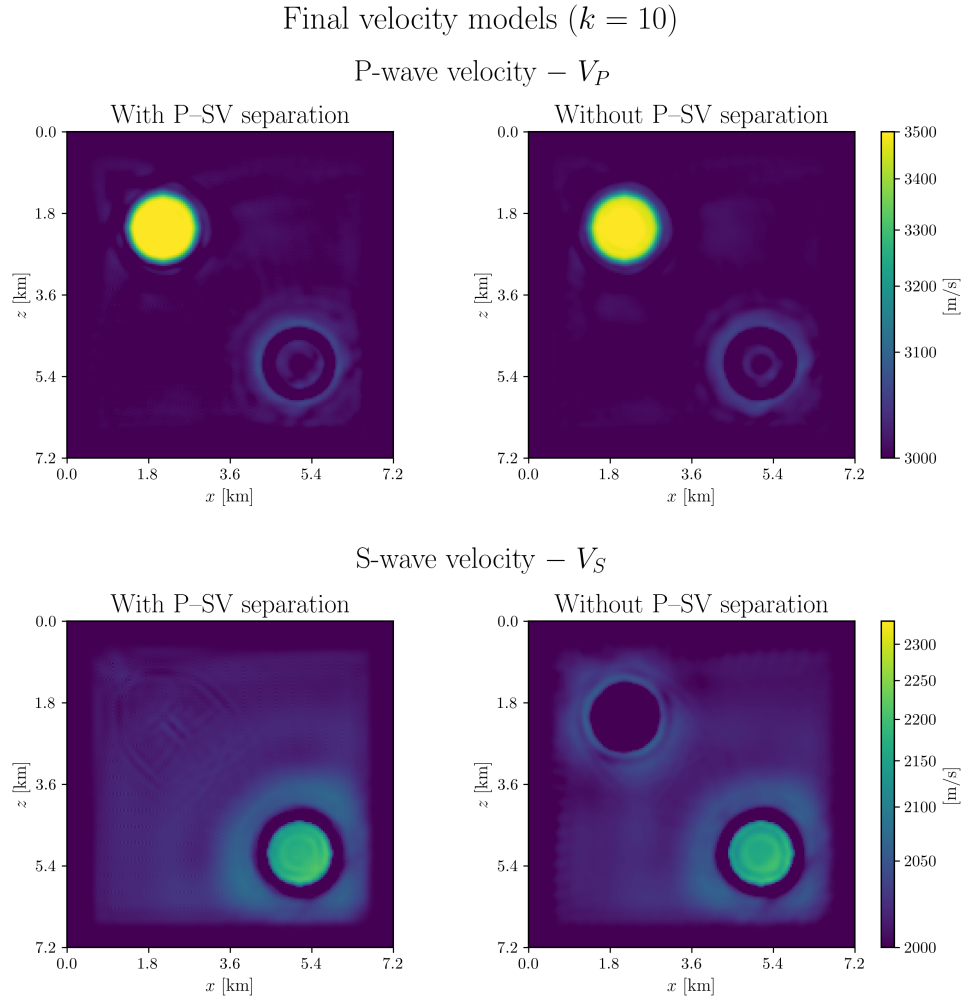


Figure 10.2: Reconstructed V_P (top) and V_S (bottom) models after $N_{\text{it}} = 10$ E-FWI iterations. Left: inversion with P–SV separation. Right: standard inversion without P–SV separation.

Figure 10.2 shows that both inversion strategies are able to correctly recover the two main anomalies of the true model, namely the V_P inclusion located in the upper-left region of the domain and the V_S inclusion located in the lower-right region. At the same time, the reconstructed models already reveal the presence of parameter cross-talk. The $V_S \rightarrow V_P$ leakage appears as a spurious update of V_P in the region of the V_S inclusion, while the $V_P \rightarrow V_S$ leakage appears as a spurious update of V_S in correspondence of the V_P anomaly. Comparing the two inversion strategies, one can notice that the $V_S \rightarrow V_P$ artifact remains of comparable magnitude with and without P–SV separation. By contrast, the opposite $V_P \rightarrow V_S$ artifact is strongly reduced, becoming practically negligible, when the separation-based gradient computation is employed.

In order to further assess both the quality of the correct parameter updates and the structure of the cross-talk between V_P and V_S , we now inspect the residual model errors shown in figure 10.3 and defined as

$$R_P^k(\underline{x}) = V_P^k(\underline{x}) - V_P(\underline{x}), \quad R_S^k(\underline{x}) = V_S^k(\underline{x}) - V_S(\underline{x}), \quad k = 1, \dots, N_{\text{it}}$$

where V_P and V_S denote the true velocity models, while V_P^k and V_S^k denote the reconstructed velocity models at the k -th iteration. In the following, we focus on the residual model errors at the final iteration $k = N_{\text{it}} = 10$.

In order to properly interpret the residual model error maps in figure 10.3, it is useful to stress that small residual values indicate that the corresponding anomaly has been accurately reconstructed, whereas large residuals reveal either incomplete recovery of the true structure or spurious updates caused by parameter cross-talk. In the regions corresponding to the true anomalies, the residual amplitudes are similar with and without P–SV separation. This indicates that the introduction of the separation does not degrade the quality of the correct parameter updates, since the V_P and V_S inclusions are reconstructed with comparable accuracy in the two formulations. The cross-talk mechanisms can be identified by inspecting the residuals away from the correct anomaly locations. In the V_P residual maps, a non-vanishing residual appears in the region of the V_S inclusion, revealing the presence of $V_S \rightarrow V_P$ leakage. This artifact is visible in both formulations and remains of comparable magnitude with and without separation. By contrast, the V_S residual maps show a marked difference between the two strategies. Without separation, a pronounced residual appears in correspondence with the V_P inclusion, indicating a spurious update of V_S induced by the V_P anomaly. When the P–SV separation is employed, this artifact is strongly reduced and becomes practically negligible.

To complement the qualitative analysis provided by the reconstructed models and the residual model error maps, we introduce quantitative error indicators evaluated in local-

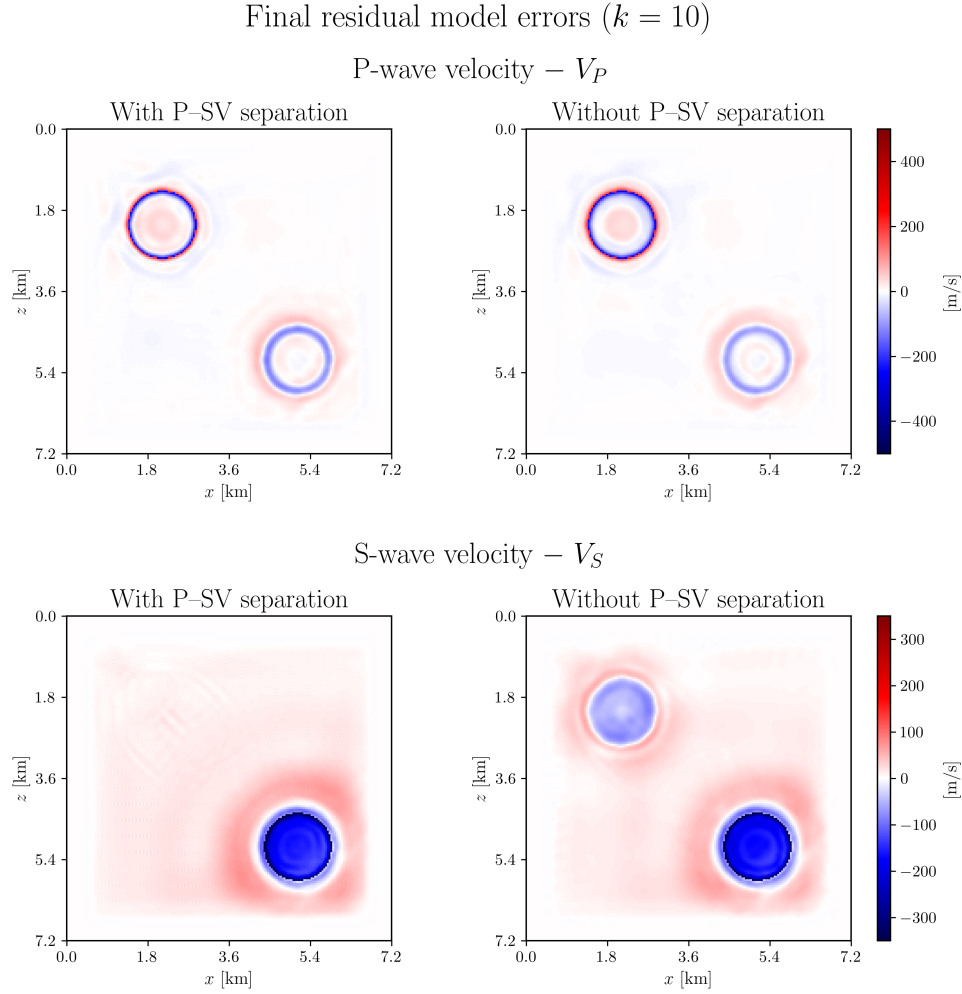


Figure 10.3: Residual V_P (top) and V_S (bottom) model errors after $N_{\text{it}} = 10$ E-FWI iterations. Left: inversion with P–SV separation. Right: standard inversion without P–SV separation.

ized regions surrounding the two inclusions. These metrics allow us to separately assess the quality of the correct parameter updates and the magnitude of the two cross-talk mechanisms. Let D_P and D_S denote two disks centered on the V_P and V_S inclusions, respectively, defined as

$$D_P = B_{R_\gamma}(\underline{x}_1) = \{\underline{x} \in \Omega \mid \|\underline{x} - \underline{x}_1\|_{\mathbb{R}^2} < R_\gamma\}$$

$$D_S = B_{R_\gamma}(\underline{x}_2) = \{\underline{x} \in \Omega \mid \|\underline{x} - \underline{x}_2\|_{\mathbb{R}^2} < R_\gamma\}$$

where $\underline{x}_1$ and $\underline{x}_2$ are the centers of the circular V_P and V_S anomalies (see appendix A.3.1), and we denoted

$$R_\gamma = \gamma R, \quad \gamma > 0$$

Here, R is the radius of both the inclusions (see appendix A.3.1). The quality of the correct parameter updates is measured through the relative L^2 reconstruction errors

$$E_P^k = \frac{\|R_P^k\|_{L^2(D_P)}}{\|V_P - V_{P,0}\|_{L^2(D_P)}}, \quad E_S^k = \frac{\|R_S^k\|_{L^2(D_S)}}{\|V_S - V_{S,0}\|_{L^2(D_S)}}$$

The magnitude of the spurious leakage-induced updates is instead quantified by the relative L^2 coupling errors

$$E_{S \rightarrow P}^k = \frac{\|R_P^k\|_{L^2(D_S)}}{\|V_P - V_{P,0}\|_{L^2(D_P)}}, \quad E_{P \rightarrow S}^k = \frac{\|R_S^k\|_{L^2(D_P)}}{\|V_S - V_{S,0}\|_{L^2(D_S)}}$$

where $V_{P,0}$ and $V_{S,0}$ denote the homogeneous background P-wave and S-wave velocity values, which also define the initial velocity models used in the inversion (see appendix A.3.1). Therefore, the denominators in the definitions above correspond to the L^2 amplitudes of the true velocity contrasts with respect to the homogeneous background. Hence, the indicators measure reconstruction and leakage errors relative to the magnitude of the anomalies to be recovered, rather than relative to the true velocity values.

The following table reports the values of these indicators for the two inversion strategies, computed with $\gamma = 1.1$, at the final iteration $k = N_{\text{it}} = 10$.

Metric	With P–SV separation	Without P–SV separation
E_P	0.209	0.224
E_S	0.611	0.618
$E_{S \rightarrow P}$	0.120	0.103
$E_{P \rightarrow S}$	0.033	0.172

Table 10.1: Quantitative reconstruction and coupling error indicators after $N_{\text{it}} = 10$ E-FWI iterations, computed with $\gamma = 1.1$.

The quantitative indicators gathered in table 10.1 confirm the previous qualitative observations. The errors associated with the correct parameter updates, quantified by E_P and E_S , remain very similar for the two strategies, indicating that the introduction of the P–SV separation in the gradient assembly does not degrade the reconstruction of the true anomalies. In fact, in this experiment, the values obtained with P–SV separation are slightly smaller. Moreover, the $V_S \rightarrow V_P$ coupling error, quantified by $E_{S \rightarrow P}$, remains of comparable magnitude in the two formulations, with a slightly larger value when the P–SV separation is introduced. This confirms that the separation does not significantly affect this cross-talk direction. By contrast, the $V_P \rightarrow V_S$ coupling error, quantified by

$E_{P \rightarrow S}$, is reduced by more than a factor of five when the P–SV separation is employed. This makes the associated artifact practically negligible in the reconstructed V_S model, as already suggested by figures 10.2 and 10.3.

Finally, we examine the evolution of the misfit functional during the inversion, in order to assess whether the introduction of the P–SV separation, associated with a modification of the gradient structure, affects the convergence behavior of the algorithm. Figure 10.4 displays the history of the misfit functional as a function of the iteration number for the two separation strategies.

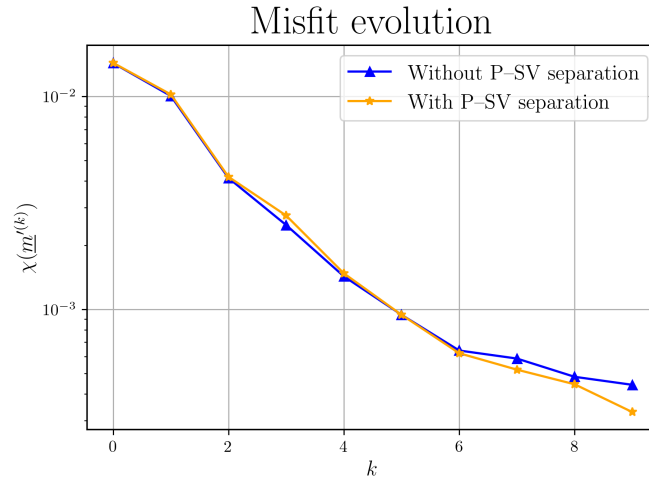


Figure 10.4: Evolution of the misfit functional during the inversion for the two inversion strategies: with P–SV separation (orange) and without P–SV separation (blue). The vertical axis is represented in logarithmic scale.

Figure 10.4 shows that the two curves exhibit a very similar convergence behavior. Despite the modification of the gradient structure associated with the modal selection introduced by the P–SV separation, the misfit decreases at a comparable rate in both cases. This indicates that the separation strategy does not negatively affect the overall convergence of the inversion process.

Taken together, the reconstructed models, the residual model error maps, the quantitative error indicators and the misfit evolution consistently show that the introduction of the P–SV separation into the inversion algorithm, as described in section 10.2, effectively reduces the $V_P \rightarrow V_S$ cross-talk, while preserving both the accuracy of the correct parameter updates and the convergence properties of the inversion.

Fluid-saturated sandstone model

We now compare the inversion results obtained on the fluid-saturated sandstone model, with and without the P–SV separation. As described in appendix A.3.2, the velocity model consists of a rectangular fluid-saturated reservoir embedded in a homogeneous sandstone medium. The anomaly affects both velocity models: the P-wave velocity takes the values $V_{P,1} = 2600.0 \text{ m s}^{-1}$ in the upper part of the reservoir and $V_{P,2} = 3000.0 \text{ m s}^{-1}$ in the lower part, while the S-wave velocity takes the value $V_{S,1} = V_{S,2} = 1660.0 \text{ m s}^{-1}$. As in the previous test, the comparison is carried out in terms of the reconstructed models, the residual model errors and the convergence behavior of the inversion.

We begin by inspecting the models obtained at the final iteration $k = N_{\text{it}} = 10$ of the last frequency stage $s = N_{\text{st}} = 4$ of the inversion procedure. Figure 10.5 shows the reconstructed V_P and V_S fields obtained with and without the P–SV separation.

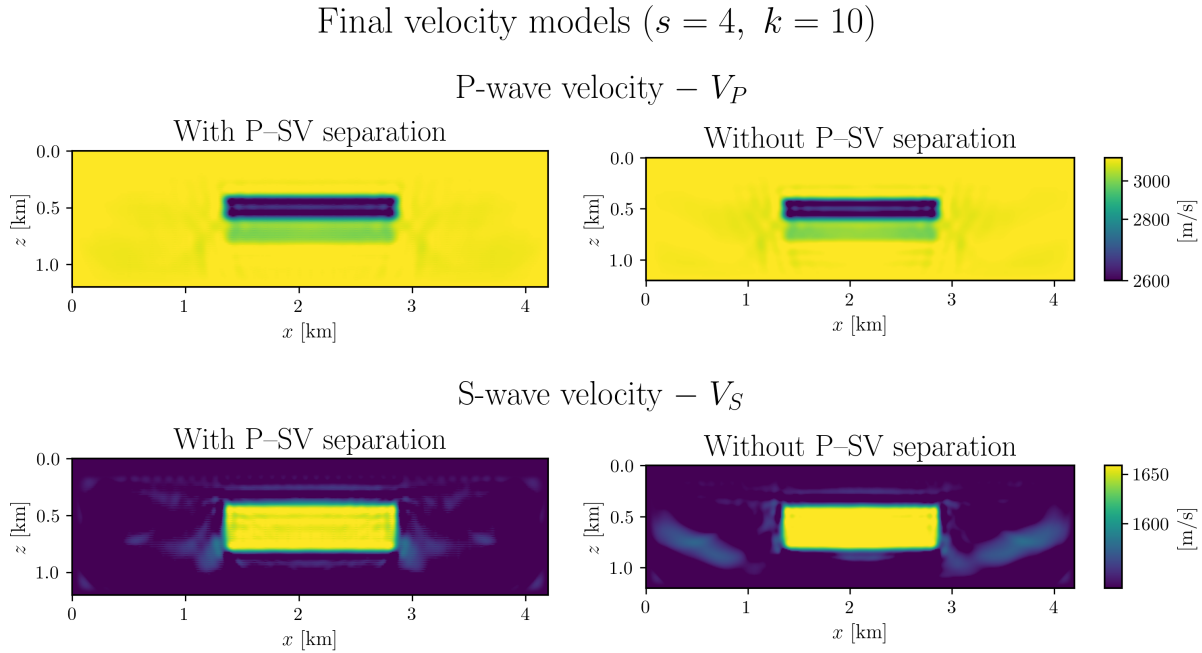


Figure 10.5: Reconstructed V_P (top) and V_S (bottom) models after $N_{\text{it}} = 10$ E–FWI iterations of the final frequency stage, $N_{\text{st}} = 4$. Left: inversion with P–SV separation. Right: standard inversion without P–SV separation.

Because the V_P and V_S anomalies are spatially overlapping in this test, the correct parameter update cannot be clearly distinguished from the spurious update generated by the $V_P - V_S$ coupling, unlike in the previous synthetic example. For this reason, the visual interpretation of the reconstructed models shown in figure 10.5 is less straightforward and must be supported by the residual model error maps discussed below. Nevertheless, both inversion strategies recover the main structure of the true anomalies reasonably well. In

particular, the reconstruction of the V_P anomaly is essentially equivalent in the two cases, showing that the introduction of the P–SV separation in the gradient assembly does not degrade the recovery of the V_P model. Regarding the V_S anomaly, the reconstruction obtained without separation may appear more homogeneous within the target region. This, however, should not be interpreted as a more accurate recovery. Since the same color scale is used in both panels, and is fixed to the extrema of the true V_S model, the apparently more uniform reconstruction obtained without P–SV separation is mainly caused by an overshoot of the reconstructed values, which exceed the extrema of the color scale. Therefore, this visual impression does not necessarily correspond to a better match with the true model. This point will become more evident in the residual model error maps discussed next.

In order to further assess the quality of the reconstructed velocity models, we now examine the residual model error maps at the final iteration $k = N_{\text{it}} = 10$ of the final last frequency stage $s = N_{\text{st}} = 4$ of the inversion procedure.

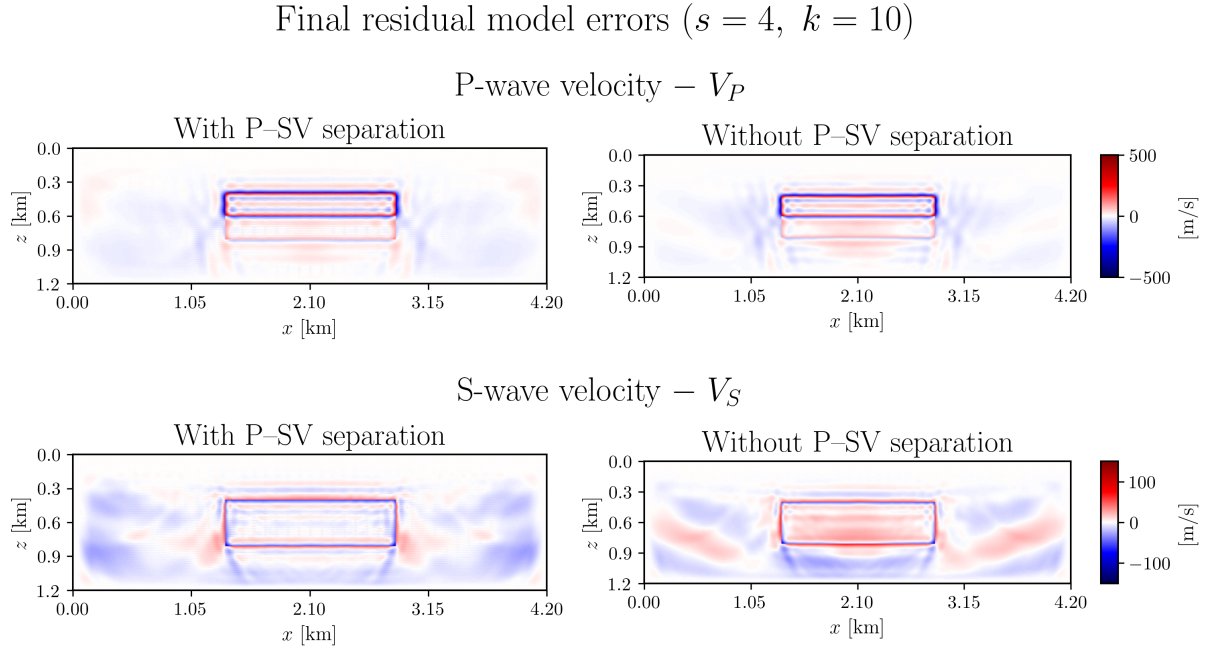


Figure 10.6: Residual V_P (top) and V_S (bottom) model errors after $N_{\text{it}} = 10$ E-FWI iterations of the final frequency stage, $N_{\text{st}} = 4$. Left: inversion with P–SV separation. Right: standard inversion without P–SV separation.

The residual maps shown in figure 10.6 provide a clearer interpretation of the phenomenon briefly addressed above. First, the V_S anomaly is clearly overshoot when the inversion is performed without introducing the P–SV separation. This effect, already suggested by the reconstructed models, becomes particularly evident in the bottom-right residual model

error map, where the interior of the anomaly exhibits significantly larger residual values. By contrast, when the P–SV separation is employed, the residual inside the target region is substantially reduced, as indicated by the much lighter color within the reservoir rectangle. This behavior is consistent with the reduction of the $V_P \rightarrow V_S$ leakage induced by the removal of the P–P contribution from the V_S -gradient component. A similar, although more localized, effect can be observed in the lower part of the V_P anomaly. In absence of the separation, the reconstruction exhibits a slight overshoot in this region, whereas the residuals obtained when using the separation are smaller. A plausible interpretation is that the overshoot of the V_S model generated by the $V_P \rightarrow V_S$ leakage may, in turn, induce a stronger $V_S \rightarrow V_P$ coupling, thereby deteriorating the reconstruction of the lower part of the V_P anomaly. By mitigating the primary $V_P \rightarrow V_S$ cross-talk, the P–SV separation may therefore also reduce this secondary effect. By contrast, the upper part of the V_P anomaly appears to be reconstructed with comparable accuracy by the two inversion strategies.

To complement the qualitative analysis provided by the reconstructed models and the residual model error maps, we rely on the same quantitative error indicators introduced above. However, unlike in the previous test, the V_P and V_S anomalies are spatially overlapping in the present configuration. As a consequence, it is not possible to define localized regions that isolate the correct parameter updates from the spurious ones associated with the $V_P - V_S$ coupling. In particular, the indicators $E_{S \rightarrow P}$ and $E_{P \rightarrow S}$ cannot be evaluated separately in a meaningful way. For this reason, the quantitative analysis in this experiment focuses only on the reconstruction errors E_P and E_S . To this end, we consider a single region surrounding the rectangular anomaly, defined as

$$D = \left\{ \underline{x} \in \Omega \mid |x - x_0| < \frac{l_{x,\delta}}{2}, |z - z_0| < \frac{l_{z,\delta}}{2} \right\}$$

where $\underline{x}_0 = (x_0, z_0)$ is the center of the rectangular anomaly (see appendix A.3.2), and we denoted

$$l_{x,\delta} = l_x + 2\delta, \quad l_{z,\delta} = l_z + 2\delta, \quad |\delta| < \frac{1}{2} \min\{l_x, l_z\} = \frac{l_z}{2}$$

Here, l_x and l_z are the side lengths of the inclusion (see appendix A.3.2).

The following table reports the values of the reconstruction error indicators for the two inversion strategies, computed with $\delta = 40.0$ m, at the final iteration $k = N_{\text{it}} = 10$ of the last frequency stage $s = N_{\text{st}} = 4$.

Metric	With P–SV separation	Without P–SV separation
E_P	0.218	0.218
E_S	0.189	0.220

Table 10.2: Quantitative reconstruction error indicators after $N_{\text{it}} = 10$ E–FWI iterations of the final frequency stage, $N_{\text{st}} = 4$, computed with $\delta = 40.0$ m.

The reconstruction errors reported in table 10.2 show only minor differences between the two inversion strategies. This behavior is consistent with the residual model error maps in figure 10.6, which indicate that the reconstruction error is largely concentrated near the anomaly boundaries. Since the region D , with $\delta = 40.0$ m, includes these interface areas, the indicators are dominated by the boundary residuals and therefore only weakly reflect the differences between the two inversion strategies. Nevertheless, an improvement in the reconstruction of V_S can already be observed when the P–SV separation is employed, as indicated by the smaller value of E_S .

To reduce the influence of the boundary residuals and provide a more representative measure of the reconstruction quality inside the anomaly, we also evaluate the reconstruction error indicators on a smaller region, choosing $\delta = -40.0$ m, always at the final iteration of the last stage. The corresponding values of the indicators are reported in the following table.

Metric	With P–SV separation	Without P–SV separation
E_P	0.142	0.142
E_S	0.058	0.131

Table 10.3: Quantitative reconstruction error indicators after $N_{\text{it}} = 10$ E–FWI iterations of the final frequency stage, $N_{\text{st}} = 4$, computed with $\delta = -40.0$ m.

The reconstruction error indicators gathered in table 10.3 now exhibit a much clearer difference between the two inversion strategies. In particular, the error in the V_S reconstruction, quantified by E_S , is more than halved when the P–SV separation is used. This quantitatively confirms the behavior already suggested by the residual model error maps, where the interior of the V_S anomaly appears significantly cleaner when the separation is introduced. On the other hand, the error in the V_P reconstruction, quantified by E_P , remains essentially unchanged in the two cases. This is consistent with the qualitative observation discussed above: the difference between the two strategies in the V_P model recovery is mainly localized in the lower part of the anomaly, while the upper portion of the inclusion is reconstructed with comparable accuracy. As a consequence, the indicator

E_P , evaluated over the entire region D does not capture this localized improvement.

To better quantify this localized effect, we introduce a region D_{low} focusing on the lower part of the anomaly, defined as

$$D_{\text{low}} = \{\underline{x} \in D \mid z > z_0 - \delta\}$$

The corresponding localized reconstruction error indicator $E_{P,\text{low}}$ allows the improvement observed in this portion of the model to be assessed more directly. The following table displays its value, computed with $\delta = -40.0$ m, at the final iteration of the last frequency stage.

Metric	With P–SV separation	Without P–SV separation
$E_{P,\text{low}}$	0.138	0.180

Table 10.4: Localized V_P reconstruction error indicator after $N_{\text{it}} = 10$ E–FWI iterations of the final frequency stage, $N_{\text{st}} = 4$, computed with $\delta = -40.0$ m.

Thus, table 10.4 confirms that the reconstruction of the lower part of the V_P anomaly is improved when the P–SV separation is employed, with the corresponding reconstruction error indicator, $E_{P,\text{low}}$, decreasing by about 23.3%. As mentioned above, this improvement may be interpreted as an indirect consequence of the reduction of the $V_P \rightarrow V_S$ leakage. A more accurate reconstruction of the V_S model may reduce secondary $V_S \rightarrow V_P$ coupling effects and, therefore, improve the recovery of the lower part of the V_P anomaly.

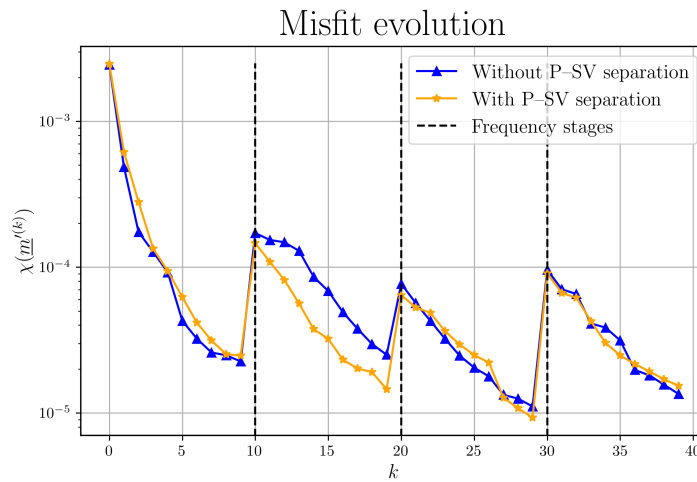


Figure 10.7: Evolution of the misfit functional during the multi-scale inversion for the two inversion strategies: with P–SV separation (orange) and without P–SV separation (blue). The vertical axis is represented in logarithmic scale. The dashed vertical black lines indicate the transitions between consecutive frequency stages.

Finally, figure 10.7 reports the evolution of the misfit functional during the multi-stage inversion. As in the previous test case, the introduction of the P–SV separation does not compromise the convergence of the optimization algorithm. Despite the modification of the gradient structure associated with the use of the P–SV separation, the misfit exhibits a consistent decrease across the inversion stages, with a convergence behavior comparable to that obtained without separation.

Overall, the results of this test confirm, in a more practically relevant setting, that the use of the P–SV separation effectively reduces the $V_P \rightarrow V_S$ cross-talk without compromising the stability of the inversion. While the improvement in the V_P reconstruction remains localized, the recovery of the V_S model is significantly enhanced, confirming the potential of the proposed strategy for mitigating parameter coupling effects in E–FWI.

11 | Conclusions and future developments

11.1. Summary of results

The starting point of this thesis was the classical identification, in linear elastic, homogeneous, isotropic and unbounded media, of P-waves with irrotational displacement fields and S-waves with solenoidal motion. Once this identification is adopted as a working criterion for P–S wave-field separation, the central mathematical question becomes how to isolate the irrotational and solenoidal components of a vector-valued function defined on a bounded computational domain in a mathematically well-posed and physically meaningful way.

Boundary-aware interpretation of Poisson-based P–S separation

The first contribution of this thesis was to reinterpret Poisson-based P–S wave-field separation within the functional framework of the *Helmholtz–Weyl decomposition theorem* in bounded domains. From this point of view, the scalar Poisson equation commonly used to recover the P-wave potential is not merely a numerical tool, but the core equation of an elliptic boundary-value problem. Indeed, in a bounded domain, this equation does not define a complete separation procedure unless it is complemented with suitable boundary conditions.

This observation is essential because the boundary conditions determine how the *harmonic-gradient* contribution of the Helmholtz–Weyl decomposition is assigned between the reconstructed P and S fields. In particular, non-homogeneous Neumann and homogeneous Dirichlet boundary conditions do not represent two interchangeable numerical closures of the same problem, but two different realizations of the decomposition. The former incorporates the *harmonic-gradient* contribution into the irrotational P component, whereas the latter assigns it to the solenoidal S component. Therefore, the choice of boundary conditions is part of the mathematical definition of the separated fields and has a direct impact on their physical interpretation and near-boundary behavior.

Boundary effects and practical equivalence in effectively unbounded media

Beyond their different mathematical meaning, the two boundary closures also lead to dual boundary-induced artifacts. In the Poisson–Neumann formulation, the P component inherits the normal trace of the original wave-field, while the S component has zero normal trace at the boundary. As a consequence, spurious S-to-P leakage may occur when an incoming S wave reaches the boundary with a non-negligible normal component. Conversely, in the Poisson–Dirichlet formulation, the P potential is forced to vanish on the boundary. Under sufficient regularity assumptions, this implies that the reconstructed P field has vanishing tangential component at the boundary. As a consequence, when a P wave reaches the boundary with a non-negligible tangential component, this contribution may be spuriously assigned to the S field, producing P-to-S leakage.

The numerical results in two-dimensional effectively unbounded configurations showed that these effects are essentially boundary-driven. When the separation domain is extended to include the absorbing layers, the wave-field is attenuated before interacting with the artificial boundary on which the auxiliary Poisson problem is closed. In this effectively unbounded setting, the Poisson–Neumann and Poisson–Dirichlet formulations become practically equivalent in the physical bulk, recovering consistent P and SV components also in realistic heterogeneous media. This confirms that, once the artificial boundary interaction is suppressed, the choice of boundary conditions has a negligible impact on the separated wave-fields in the region of interest.

Numerical approximation of the auxiliary Poisson problems

The different boundary closures also led to different strategies for the numerical solution of the auxiliary Poisson problems. The Poisson–Neumann formulation was approximated through a second-order finite-difference discretization, which allowed the non-homogeneous Neumann datum to be incorporated while preserving the consistency between the discrete gradient, divergence and Laplacian operators. At the same time, the resulting linear system retained a structure that could be diagonalized by discrete cosine transforms. The Poisson–Dirichlet formulation was instead approached from a different numerical point of view. Exploiting the explicit spectral representation of the Dirichlet Laplacian on rectangular domains, the algorithm approximates the analytical solution of the continuous boundary-value problem from the information available on the staggered grid, rather than relying on an explicit discretization of the differential operators.

This spectral approach provides a fast alternative to finite-difference Poisson solvers. It retains the same log-linear asymptotic complexity, based on fast trigonometric transforms, but avoids the eigenvalue distortion introduced by an explicit finite-difference approxima-

tion of the Laplacian. As a consequence, it is particularly well suited to wave-fields whose relevant spectral content is resolved by the grid, as suggested by the theoretical analysis and supported by the numerical experiments. The same spectral approach was then extended to the mixed formulation after a divergence-preserving harmonic lifting of the Neumann datum.

Free-surface configurations and mixed formulation

The role of boundary conditions becomes more delicate in free surface configurations, where the wave-field interacts directly with the boundary on which the auxiliary Poisson problem is closed. In the solid free surface case, the Poisson–Neumann and Poisson–Dirichlet formulations exhibited different behaviors, especially in the separation of surface waves. However, the intrinsically coupled physical nature of surface phenomena prevents one from ranking the two strategies.

The fluid free-surface case provides a clearer diagnostic configuration. Since fluids do not support shear wave propagation, any SV field recovered in the fluid region can be interpreted as numerical leakage. In the numerical tests, the Poisson–Neumann formulation performed significantly better than the Poisson–Dirichlet one: it did not generate the boundary-induced spurious P-to-SV conversions observed near the free surface with the homogeneous Dirichlet closure. This is consistent with the fact that the Neumann formulation imposes a vanishing normal trace on the separated SV field, which is compatible with the absence of shear motion in the fluid, whereas the Dirichlet condition on the P potential is not, in general, compatible with such a constraint.

These observations motivated the Poisson–mixed formulation, in which non-homogeneous Neumann boundary conditions are imposed at the free surface, while homogeneous Dirichlet boundary conditions are imposed on the artificial boundaries surrounded by absorbing layers. In the tested fluid free-surface configuration, the mixed formulation retained the favorable near-surface behavior of the Neumann closure, removing the Dirichlet-induced P-to-SV artifact, and reduced the residual SV leakage in the fluid by approximately one order of magnitude with respect to the finite-difference Poisson–Neumann solver.

Application to Elastic Full Waveform Inversion

The last contribution of this thesis concerned the use of P–S separation in Elastic Full Waveform Inversion, with the aim of reducing the coupling between the V_P and V_S updates. In this context, the separated wave-fields were used to perform a modal selection of the time-domain cross-correlations entering the adjoint-state gradients. The modified V_P gradient was assembled by retaining only P–P correlations between forward and ad-

joint wave-fields, whereas the modified V_S gradient was assembled from P–S, S–P and S–S interactions.

The theoretical analysis, although carried out at a formal and heuristic level, provides a structurally and physically informed interpretation of the effect of this strategy. In particular, the separated-gradient formulation is expected to mitigate a specific coupling mechanism from V_P to V_S by removing the direct volumetric cross-talk pathway from the modified V_S gradient. At the same time, the analysis suggests that the coupling in the opposite direction, from V_S to V_P , should remain essentially unaffected, since the modified V_P gradient coincides, at the continuous level, with the original one.

The numerical experiments supported this interpretation. The separated-gradient formulation produced a significantly reduced leakage from V_P to V_S , while the $V_S \rightarrow V_P$ cross-talk remained essentially unchanged. Moreover, the modified gradients preserved the main parameter updates and did not deteriorate the convergence behavior of the inversion, as shown by the stable decrease of the misfit functional. This indicates that the proposed strategy improves the structure of the V_S update without compromising the overall optimization process.

11.2. Limitations and perspectives for future work

Although the results presented in this thesis provide a coherent mathematical and numerical framework for Poisson-based P–S separation in bounded computational domains, several limitations remain and naturally suggest directions for future work. Some of these limitations are intrinsic to the interpretation of P–S separation adopted in this work, whereas others are related to the numerical realization of the proposed algorithms and to their application in more realistic seismic imaging and inversion settings.

Limits of the irrotational/solenoidal criterion

The first limitation concerns the physical interpretation of the separated fields. As standard in the literature, throughout this thesis (see section 2.2), the P component of the wave-field has been identified with the irrotational part of the displacement field, while the S component has been identified with its solenoidal part. This criterion is exact in homogeneous and unbounded linear elastic and isotropic media, where the diagonalization of the *acoustic tensor* provides a clear separation between longitudinal and transverse polarizations. In bounded and heterogeneous media, however, material interfaces and free surfaces generate reflected, converted, interface and surface waves whose P and S contents may be intrinsically coupled.

As a consequence, the Helmholtz–Weyl decomposition used in this work should be understood as a mathematically well-defined and physically meaningful separation criterion, rather than an exact modal diagonalization of the elastic wave-field in every configuration. This distinction is especially important near physical boundaries and interfaces, where the notion of P–S decomposition may itself become ambiguous.

Limits of the numerical approximations

A first numerical limitation concerns the dependence of the proposed algorithms on the staggered grid adopted for the finite-difference solver of the elastic wave equation (see sections 3.1.1 and 5.2.1). The placement of the wave-field components, the discrete gradient, divergence and Laplacian operators, and the quadrature formulas used in the spectral reconstruction were designed to be consistent with this grid arrangement. As a consequence, the extension of the proposed numerical separation procedures to different discretization frameworks is not direct. This is especially relevant for finite element or spectral element solvers on unstructured meshes, since the use of FFT-based fast trigonometric transforms to build efficient Poisson solvers relies on structured grids. Although the continuous Helmholtz–Weyl interpretation remains valid, new discrete Poisson solvers would be required to obtain an efficient boundary-aware separation procedure compatible with those numerical settings.

A second general limitation is that the proposed algorithms were designed, implemented and tested only in two space dimensions. The extension to three-dimensional rectangular domains is conceptually straightforward from the algorithmic point of view, since the same staggered-grid structure and the same fast-transform strategy can be used with three-dimensional trigonometric transforms. The asymptotic complexity therefore remains log-linear in the total number of grid points. However, this observation is restricted to rectangular computational domains. In non-rectangular geometries, either in two or three dimensions, the explicit spectral diagonalization exploited in this work, either at the continuous or discrete level, is not directly available, and the numerical formulation would have to be reconsidered, for instance through coordinate transformations to a rectangular reference domain or through more general efficient Poisson solvers.

A third limitation concerns the accuracy analysis of the spectral Poisson–Dirichlet numerical approximation. In this thesis, the analysis was restricted to the band-limited case, for which the discrete quadrature formulas recover exactly the modal coefficients of strictly sub-Nyquist displacement fields. This result does not provide a complete convergence theory for general, non-band-limited forcing terms. In that case, the accuracy of the approximation depends on the combined effect of spectral truncation, quadrature errors

in the approximation of the displacement expansion coefficients, and the staggered-grid structure of the discrete fields. A rigorous convergence analysis in the full two-dimensional staggered-grid setting remains open. Such an analysis would also help to clarify more precisely the accuracy improvement over the second-order finite-difference Poisson–Neumann solver observed in the numerical experiments.

An additional limitation concerns the Poisson–mixed formulation. In this case, no systematic accuracy analysis was carried out. The expected accuracy of the method was motivated by the structure of the algorithm: after the harmonic lifting of the non-homogeneous Neumann datum, the remaining problem can be treated with a continuous-like spectral approach analogous to that used for the Poisson–Dirichlet formulation. However, this argument remains partly heuristic. The numerical tests confirmed the expected behavior in the specific fluid free surface configuration considered in this thesis, showing a reduced residual SV leakage compared with the second-order finite-difference Poisson–Neumann solver. Nevertheless, a systematic analysis of the mixed spectral solver, including the effect of the harmonic lifting and of the interaction between the different boundary portions, remains to be developed.

Finally, the numerical experiment involving a realistic fluid-solid configuration (see section 9.3) highlighted a difficulty that is not specific to a particular boundary condition or Poisson discretization. Oscillatory artifacts were observed near the fluid-solid interface for all the considered separation strategies, independently of whether Neumann, Dirichlet or mixed boundary conditions were used, and independently of the finite-difference or spectral nature of the Poisson solver. This suggests that these artifacts are not primarily caused by the specific separation strategy, but rather by the interaction between the separation procedure, the sharp material contrast, the vanishing shear modulus in the fluid layer and the staggered-grid treatment of the fluid-solid interface. Future work should therefore investigate more accurate and physically consistent treatments of acoustic-elastic coupling, possibly relying on interface-aware variational formulations better suited to coupled fluid-solid problems.

Perspectives for Elastic Full Waveform Inversion

Another limitation concerns the application of the P–S separation to Elastic Full Waveform Inversion. The analysis carried out in this thesis (see section 10.2) is not a fully rigorous functional-analytic treatment, but should be understood as a formal, structurally and physically motivated investigation of the modified separated adjoint-state gradients. Future work should aim at providing a more solid theoretical background to systematically quantify the reduction of the $V_P \rightarrow V_S$ leakage and to clarify when this reduction

leads to a significant improvement of the final reconstructed model.

Moreover, although the numerical experiments presented in section 10.3 showed promising results for the mitigation of a specific $V_P \rightarrow V_S$ cross-talk mechanism, without compromising the main parameter updates or the convergence of the misfit functional, these tests were carried out in controlled synthetic two-dimensional configurations, with a limited number of models and acquisition settings. A more complete assessment would require more complex geological models, sparse and noisy data, different acquisition geometries, and realistic multi-scale inversion workflows.

Extension to anisotropic media

A major perspective for future work concerns the extension of the present framework to anisotropic media, in particular to Vertical Transversely Isotropic (VTI) media, which are especially relevant in practical and industrial applications. This extension is not straightforward, because the basic irrotational/solenoidal criterion used throughout this thesis is intrinsically tied to isotropic linear elasticity. In homogeneous isotropic media, P and S polarizations are respectively parallel and orthogonal to the wave vector, so that P-waves are naturally associated with curl-free fields and S-waves with divergence-free fields. In VTI anisotropic media, instead, the qP and qS polarization vectors are not aligned with the wave vector and its orthogonal complement. Moreover, they depend on the material parameters and have a non-polynomial angular dependence on the components of the wave vector, making it difficult, if not impossible, to define universal local differential operators able to isolate the qP- and qS-waves.

Future work should therefore consider separation operators based directly on the anisotropic polarization structure. A natural starting point is provided by wavenumber-domain projectors associated with the VTI *acoustic tensor* (see, e.g., [46]). Efficient extensions to heterogeneous media could then be compared with low-rank approximations of separation operators (see, e.g., [7]) and with recent approximate anisotropic wave-mode projectors based on scalar anisotropic pseudo-Poisson formulations (see [11]). The main challenge would be to combine these anisotropic modal projectors with the boundary-aware view-point developed in this thesis. In particular, one should understand how qP and qS projection operators can be defined and approximated in bounded domains, where boundary conditions may again play a non-trivial role in the mathematical and numerical realization of the decomposition.

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A | Appendix A

This appendix collects the definitions of the source wavelet and the numerical models employed throughout the numerical experiments. The material reported here is intended to complement the main text by providing a concise and self-contained reference for the simulation setup.

A.1. Source wavelet used in the tests

In this section, we introduce the temporal profile of the Ricker source wavelet employed in the numerical experiments presented throughout this work, providing its analytical expression.

We denote by t_s , with $[t_s] = \text{s}$, a time shift suitably chosen to ensure that the wavelet is effectively negligible at the initial time, and by f_0 , with $[f_0] = \text{Hz}$, the central frequency of the source wavelet, i.e., the peak frequency of its amplitude spectrum.

The temporal profile of the Ricker wavelet is defined as

$$s : \mathbb{R} \rightarrow \mathbb{R}, \quad s(t) = \left(1 - 2\pi^2 f_0^2 (t - t_s)^2\right) e^{-\pi^2 f_0^2 (t - t_s)^2}$$

The time shift and the maximum frequency content are chosen as

$$t_s = \frac{3}{2f_0}, \quad f_{\max} = \frac{5}{2}f_0$$

A.2. Numerical models used in the separation tests

In this section, we describe the numerical models employed in the separation tests. For each configuration, we specify the physical parameters and the geometric setup used in the simulations.

All the numerical simulations are performed on a uniform grid, i.e., $h_x = h_z = h$. The grid spacing h and the time-step Δt are chosen according to equations (3.15) and (3.16),

using

$$\gamma = 0.7, \quad H = \frac{1}{6}$$

which are below the empirical limits (3.14), thus ensuring a conservative choice.

A.2.1. Homogeneous model

The computational domain is the square

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = L_z = 10.0 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 2.5 \text{ s}$$

The medium is homogeneous. In the solid configuration, it is characterized by the constant elastic parameters

$$\rho = 2590 \text{ kg m}^{-3}, \quad V_P = 5390 \text{ m s}^{-1}, \quad V_S = 2970 \text{ m s}^{-1}$$

These values are taken from the physical model of dolomite rock reported in [26].

In the fluid configuration, the material parameters are

$$\rho = 1000 \text{ kg m}^{-3}, \quad V_P = 1483 \text{ m s}^{-1}, \quad V_S = 0 \text{ m s}^{-1}$$

These values correspond to those of water.

To mimic an unbounded medium, an absorbing frame of thickness and damping factor

$$\ell = 80 h, \quad \alpha_0 = 0.25$$

is added around the computational domain. In free-surface configurations, the upper boundary at $z = 0 \text{ m}$ is not equipped with absorbing layers, while the absorbing frame is retained along the remaining sides of the domain.

A.2.2. Bi-layer model

The computational domain is the square

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = L_z = 10.0 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 2.5 \text{ s}$$

The medium is heterogeneous and consists of two horizontal layers separated by an interface located at

$$\bar{z} = 5.0 \text{ km}$$

The upper layer is characterized by the constant elastic parameters

$$\rho_1 = 2120 \text{ kg m}^{-3}, \quad V_{P,1} = 3800 \text{ m s}^{-1}, \quad V_{S,1} = 2160 \text{ m s}^{-1}$$

while the lower layer is characterized by

$$\rho_2 = 2370 \text{ kg m}^{-3}, \quad V_{P,2} = 4090 \text{ m s}^{-1}, \quad V_{S,2} = 2410 \text{ m s}^{-1}$$

These values are taken from the physical models of consolidated sediment and sandstone rocks reported in [26].

To mimic an unbounded medium, an absorbing frame of thickness and damping factor

$$\ell = 120 h, \quad \alpha_0 = 0.30$$

is added around the computational domain.

A.2.3. Marmousi–II model

We consider two distinct configurations extracted from the Marmousi–II model. The land section is characterized by the density, P-wave and S-wave velocity fields shown in figure A.1. The marine configuration includes an upper fluid layer and is characterized by the density, P-wave and S-wave velocity fields shown in figure A.2.

In both cases, the computational domain is the square

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = L_z = 2.5 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 1.5 \text{ s}$$

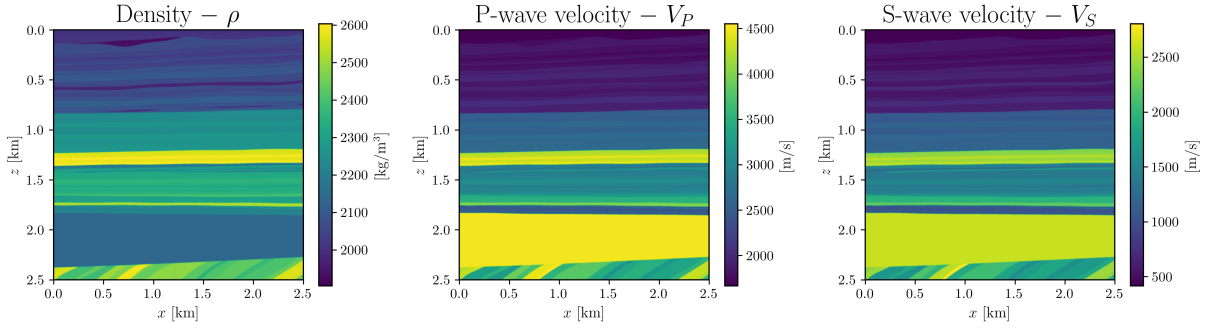


Figure A.1: Processed land Marmousi-II model used in the simulations. From left to right: density ρ , P-wave velocity V_P , and S-wave velocity V_S .

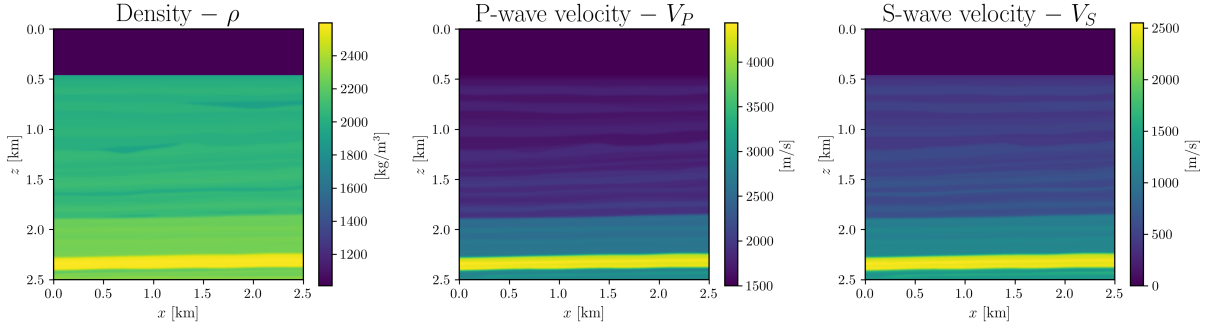


Figure A.2: Processed marine Marmousi-II model used in the simulations. From left to right: density ρ , P-wave velocity V_P , and S-wave velocity V_S .

To mimic an unbounded medium, an absorbing frame of thickness and damping factor

$$\ell = 100 h, \quad \alpha_0 = 0.30$$

is added around the computational domain. In free-surface configurations (considered only in the marine case), the upper boundary at $z = 0$ m is not equipped with absorbing layers, while the absorbing frame is retained along the remaining sides of the domain.

The Marmousi-II model was obtained from publicly available repositories (see [18]). The original dataset provides spatially varying elastic parameters on a particularly fine grid ($h = 1.25$ m), which is significantly finer than the numerical dispersion limit imposed by the maximum source frequency considered in the simulations. In order to construct a computationally efficient representation, the model was resampled onto a coarser grid consistent with the dispersion constraints of the numerical scheme. An anti-aliasing Gaussian low-pass filter was first applied to ensure compatibility with the spectral resolution of the target grid, and the model was subsequently downsampled using block arithmetic averaging.

A.2.4. Sigsbee-salt model

The model is characterized by the density, P-wave and S-wave velocity fields shown in figure A.3.

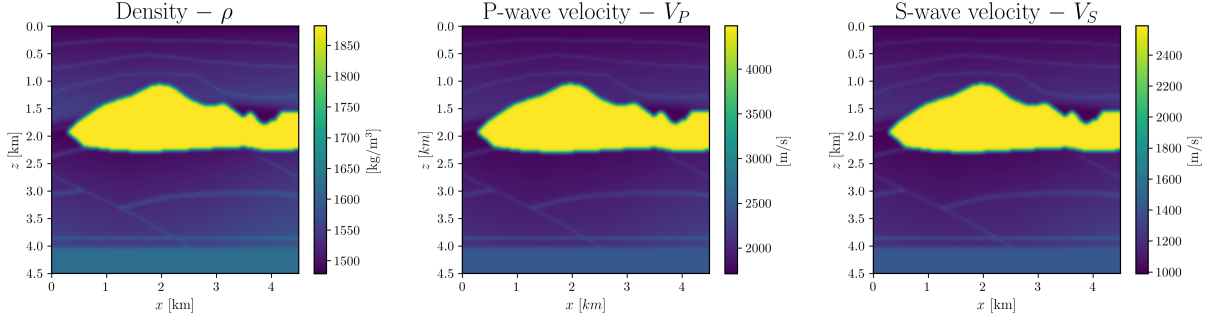


Figure A.3: Processed Sigsbee–Salt model used in the simulations. From left to right: density ρ , P-wave velocity V_P , and S-wave velocity V_S .

The computational domain is the square

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = L_z = 4.2 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 3.0 \text{ s}$$

To mimic an unbounded medium, an absorbing frame of thickness and damping factor

$$\ell = 80 h, \quad \alpha_0 = 0.30$$

is added around the computational domain.

The Sigsbee–Salt model was obtained from publicly available repositories (see [18]). The original dataset provides the P-wave velocity field on a relatively coarse grid ($h = 20 \text{ m}$), which is larger than the numerical dispersion limit imposed by the maximum source frequency considered in the simulations. Therefore, the model was refined up to a compatible resolution. The refinement was performed using spectral interpolation (see [45]). Due to the presence of sharp material discontinuities, the interpolation step introduces spurious oscillations in the vicinity of interfaces. To mitigate this effect, a Gaussian smoothing filter was subsequently applied. Since only the V_P field was available in the original dataset, the corresponding V_S and ρ fields were derived through simplified empirical relations,

namely

$$V_S = \frac{V_P}{\sqrt{3}}, \quad \rho = 230 V_P^{1/4}$$

A.3. Numerical models used in the inversion tests

In this section, we describe the numerical models employed in the elastic full waveform inversion tests. For each configuration, we specify the physical parameters and the geometric and inversion setups used in the simulations.

In the inversion tests, spurious reflections from the artificial boundaries of the computational domain are attenuated by means of convolutional perfectly matched layers (CPMLs), rather than by the sponge absorbing layers employed in the separation tests (see section 3.3.1). This choice follows the implementation adopted in the inversion code used for the numerical experiments. CPMLs are an absorbing boundary treatment based on a coordinate stretching of the wave equation in the frequency domain and are commonly used in finite-difference simulations of seismic wave propagation (see, e.g., [20]). The CPMLs are characterized by the thickness of the absorbing frame in number of grid points, denoted by N_{PML} , by a reference damping velocity V_{PML} , a characteristic frequency f_{PML} used in the PML construction, and the polynomial degree n_{PML} of the damping function.

A.3.1. Two inclusions model

The true model consists of a homogeneous background medium containing two circular anomalies, one affecting only the P-wave velocity and the other affecting only the S-wave velocity. The associated density, P-wave and S-wave velocity fields are shown in figure A.4.

The computational domain is the square

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = L_z = 7.2 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 5.0 \text{ s}$$

The background medium is homogeneous and characterized by the constant elastic parameters

$$\rho_0 = 4000.0 \text{ kg m}^{-3}, \quad V_{P,0} = 3000.0 \text{ m s}^{-1}, \quad V_{S,0} = 2000.0 \text{ m s}^{-1}.$$

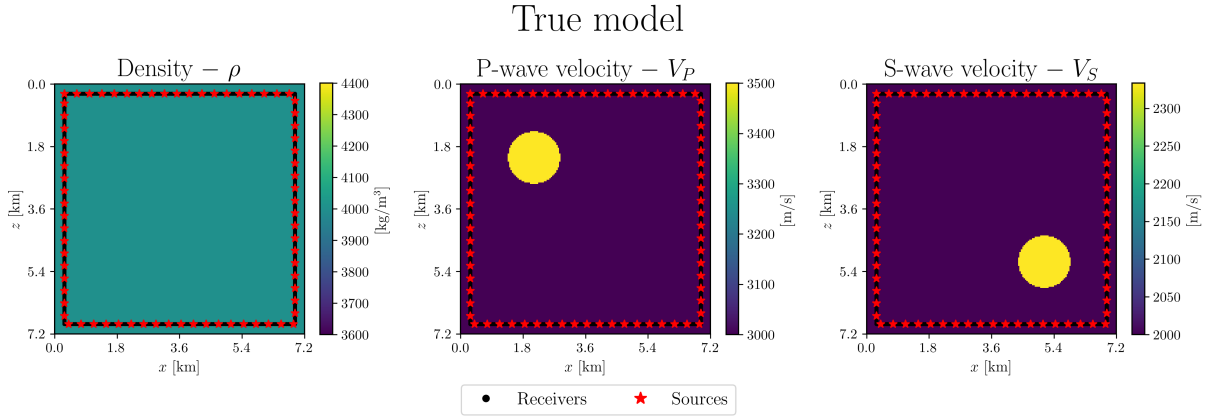


Figure A.4: Two inclusions model used in the inversions. From left to right: density ρ , P-wave velocity V_P , and S-wave velocity V_S . The acquisition geometry is also shown.

The same homogeneous medium is used as initial guess for the inversion. In particular, the initial density model coincides with the true one and is kept fixed throughout the inversion, while only the parameters V_P and V_S are updated.

Two circular inclusions of radius

$$R = 750.0 \text{ m}$$

are embedded in the background medium. The first anomaly affects only the parameter V_P and is centered at

$$\underline{x}_1 = (x_1, z_1) = (2.1 \text{ km}, 2.1 \text{ km})$$

Inside this inclusion, the P-wave velocity is

$$V_{P,1} = 3500.0 \text{ m s}^{-1}$$

while the density and the S-wave velocity remain equal to their background values. The second anomaly affects only the parameter V_S and is centered at

$$\underline{x}_2 = (x_2, z_2) = (5.1 \text{ km}, 5.1 \text{ km})$$

Inside this inclusion, the S-wave velocity is

$$V_{S,2} = 2330.0 \text{ m s}^{-1}$$

while the density and the P-wave velocity remain equal to their background values.

To mimic an unbounded medium, a CPML absorbing frame characterized by

$$N_{\text{PML}} = 10, \quad V_{\text{PML}} = 3000.0 \text{ m s}^{-1}, \quad f_{\text{PML}} = 15.0 \text{ Hz}, \quad n_{\text{PML}} = 2$$

is added around the computational domain.

Sources and receivers are distributed along a square acquisition frame located inside the computational domain. The acquisition frame is placed at an offset

$$d_{\text{acq}} = 280.0 \text{ m}$$

from the boundaries of the computational domain. Along this acquisition frame, we deploy

$$N_r = 664, \quad h_r = 40.0 \text{ m}, \quad N_s = 74, \quad h_s = 360.0 \text{ m}$$

receivers and sources, where N_r and N_s denote the number of receivers and sources, respectively, while h_r and h_s denote the corresponding spatial spacings. The sources are modeled as explosive sources with a Ricker wavelet temporal profile (see appendix A.1), with a central frequency

$$f_0 = 10.0 \text{ Hz}$$

During the solution of the *adjoint problem*, the *adjoint source* is injected as a multi-component vector field. Moreover, a low-pass filter with cut-off frequency

$$f_c = 5.0 \text{ Hz}$$

is applied to the adjoint source. During the inversion, a taper is applied to the gradient near the artificial boundaries of the computational domain. This operation confines the model updates to the physical bulk of the domain and mitigates the imprint of the acquisition geometry, especially near the source locations.

Finally, the inversion is carried out for a total of

$$N_{\text{it}} = 10$$

iterations, using a preconditioned conjugate gradient optimization scheme.

A.3.2. Fluid-saturated sandstone model

The true model consists of a homogeneous sandstone background containing a rectangular fluid-saturated reservoir. The associated density, P-wave and S-wave velocity fields are shown in figure A.5.

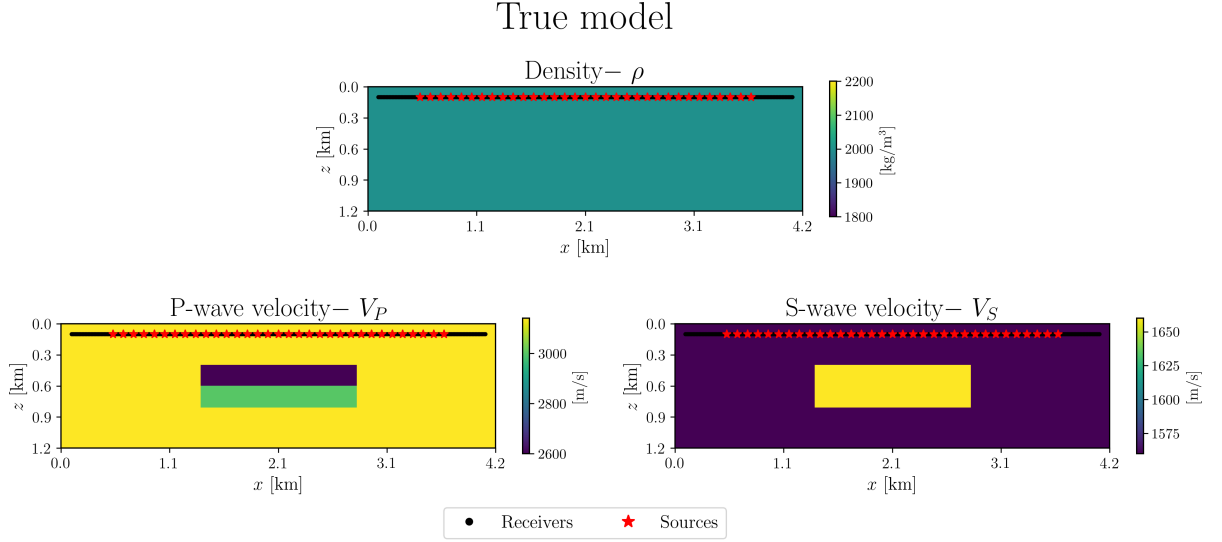


Figure A.5: Fluid-saturated sandstone model used in the inversions. From left to right: density ρ , P-wave velocity V_P , and S-wave velocity V_S . The acquisition geometry is also shown.

The computational domain is the rectangle

$$\Omega = (0, L_x) \times (0, L_z), \quad L_x = 4.2 \text{ km}, \quad L_z = 1.2 \text{ km}$$

and the simulations are performed over the time interval

$$I = (0, T), \quad T = 2.0 \text{ s}$$

The background sandstone medium is homogeneous and characterized by the constant elastic parameters

$$\rho_0 = 2000.0 \text{ kg m}^{-3}, \quad V_{P,0} = 3140.0 \text{ m s}^{-1}, \quad V_{S,0} = 1560.0 \text{ m s}^{-1}$$

The same homogeneous medium is used as initial guess for the inversion. In particular, the initial density model coincides with the true one and is kept fixed throughout the inversion, while only the parameters V_P and V_S are updated.

A rectangular inclusion with side lengths

$$l_x = 1500.0 \text{ m}, \quad l_z = 400.0 \text{ m}$$

is embedded in the background medium and its center is located at

$$\underline{x}_0 = (x_0, z_0) = (2.1 \text{ km}, 0.6 \text{ km})$$

This inclusion represents a fluid-saturated reservoir. Its upper part is gas-saturated and characterized by

$$V_{P,1} = 2600.0 \text{ m s}^{-1}, \quad V_{S,1} = 1660.0 \text{ m s}^{-1}$$

whereas its lower part is water-saturated and characterized by

$$V_{P,2} = 3000.0 \text{ m s}^{-1}, \quad V_{S,2} = 1660.0 \text{ m s}^{-1}$$

The density remains equal to its background value throughout the whole model. The reservoir velocity values are taken from the physical sandstone model proposed in [26].

To mimic an unbounded medium, a CPML absorbing frame characterized by

$$N_{\text{PML}} = 20, \quad V_{\text{PML}} = 3000.0 \text{ m s}^{-1}, \quad f_{\text{PML}} = 10.0 \text{ Hz}, \quad n_{\text{PML}} = 2$$

is added around the computational domain.

Sources and receivers are distributed along a horizontal acquisition line located inside the computational domain. The acquisition line is placed at a vertical offset

$$d_{\text{acq}} = 100.0 \text{ m}$$

from the upper boundary of the computational domain. The receivers are deployed along the segment

$$x \in [100.0 \text{ m}, 4100.0 \text{ m}]$$

with

$$N_r = 401, \quad h_r = 10.0 \text{ m}$$

The sources are deployed along the segment

$$x \in [500.0 \text{ m}, 3700.0 \text{ m}]$$

with

$$N_s = 33, \quad h_s = 100.0 \text{ m}$$

Here, N_r and N_s denote the number of receivers and sources, respectively, while h_r and h_s denote the corresponding spatial spacings. The sources are modeled as explosive sources with a Ricker wavelet temporal profile (see appendix A.1), with a central frequency

$$f_0 = 10.0 \text{ Hz}$$

During the solution of the *adjoint problem*, the *adjoint source* is injected as a single-component vertical force.

To mitigate the risk of convergence to local minima, the inversion is performed through a multi-scale strategy from low to high frequencies. More precisely, a low-pass filter is applied to the *adjoint source* in order to progressively introduce higher frequencies during the inversion. The inversion is divided into

$$N_{\text{st}} = 4$$

stages, associated with cut-off frequencies

$$f_c = 2.0 \text{ Hz}, \quad f_c = 4.0 \text{ Hz}, \quad f_c = 6.0 \text{ Hz}, \quad f_c = 10.0 \text{ Hz}$$

For each stage, the inversion is carried out for a maximum number of

$$N_{\text{it}} = 10$$

iterations, using a preconditioned conjugate gradient optimization scheme. During the inversion, a taper is applied to the gradient near the artificial boundaries of the computational domain. This operation confines the model updates to the physical bulk of the domain and mitigates the imprint of the acquisition geometry, especially near the source locations.

B | Appendix B

This appendix collects some classical results from linear algebra and functional analysis used throughout the thesis, providing a concise reference for statements that are not recalled in the main text in order to preserve readability.

Theorem B.1 (Spectral theorem for symmetric matrices).

Let $\bar{M} \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then,

- All its eigenvalues are real;
- It is orthogonally diagonalizable, or, equivalently, there exists an orthonormal basis of $\mathbb{R}^n$ made of eigenvectors of $\bar{M}$.

See, e.g., chapter 9 in [32].

Theorem B.2 (Orthogonal decomposition theorem).

Let $(H, (\cdot, \cdot)_H)$ be a Hilbert space and let $V \subset H$ be a closed vector subspace. Then,

$$H = V \oplus V^\perp$$

where $V^\perp$ denotes the orthogonal complement of V . More precisely, this means:

- $\forall x \in H, \exists! v \in V, w \in V^\perp \mid x = v + w$;
- $x \in V \Leftrightarrow w = 0$ and $x \in V^\perp \Leftrightarrow v = 0$;
- $\forall x \in H, \|x\|_H^2 = \|v\|_H^2 + \|w\|_H^2$.

Moreover, the mappings

$$\Pi_V : H \rightarrow V, \quad \Pi_V(x) = v$$

$$\Pi_{V^\perp} : H \rightarrow V^\perp, \quad \Pi_{V^\perp}(x) = w$$

are called projection operators onto V and $V^\perp$, respectively, and are both linear and continuous (bounded).

See, e.g., chapter 5 in [4].

Theorem B.3 (Riesz representation theorem for Hilbert spaces).

Let $(H, (\cdot, \cdot)_H)$ be a Hilbert space and let H^* be the dual space of H . Then

$$\forall L \in H^*, \exists! h \in H \mid \langle L, v \rangle = (h, v)_H, \quad \forall v \in H$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between H^* and H .

Moreover, $\|L\|_{H^*} = \|h\|_H$. Equivalently, the map

$$I : H \rightarrow H^*, \quad (I(h))(v) = (h, v)_H$$

is an isometric isomorphism between H and H^* , allowing the identification

$$H \cong H^*$$

See, e.g., chapter 5.2 in [4].

Theorem B.4 (Korn's inequality in $[H_{\Gamma_D}^1(\Omega)]^n$).

Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, open, bounded and connected, such that $\partial\Omega \in \text{Lip}$. Let $\Gamma_D \subset \partial\Omega$, such that $|\Gamma_D| > 0$. Then there exists a constant $C_K > 0$, depending on Ω , such that

$$\|\bar{\varepsilon}(\underline{v})\|_{[L^2(\Omega)]^{n \times n}} \geq C_K \|\underline{v}\|_{[H^1(\Omega)]^n}, \quad \forall \underline{v} \in [H_{\Gamma_D}^1(\Omega)]^n$$

where

$$[H_{\Gamma_D}^1(\Omega)]^n = \{\underline{v} \in [H^1(\Omega)]^n \mid \gamma_0(\underline{v})|_{\Gamma_D} = \underline{0}\}$$

and $\gamma_0 : [H^1(\Omega)]^n \rightarrow [H^{1/2}(\partial\Omega)]^n$ denotes the trace operator.

See, e.g., chapter 6.3 in [8].

Theorem B.5 (Generalized Gauss–Green formula).

Let $\Omega \subset \mathbb{R}^n$, open and bounded, such that $\partial\Omega \in \text{Lip}$. Then

$$\int_{\Omega} \underline{u} \cdot \nabla v \, d\Omega + \int_{\Omega} v \, \text{div}(\underline{u}) \, d\Omega = \langle \gamma_{\nu}(\underline{u}), \gamma_0(v) \rangle, \quad \forall \underline{u} \in H_{\text{div}}(\Omega), \quad \forall v \in H^1(\Omega)$$

where $\gamma_0 : H^1(\Omega) \rightarrow H^{1/2}(\partial\Omega)$ and $\gamma_{\nu} : H_{\text{div}}(\Omega) \rightarrow H^{-1/2}(\partial\Omega)$ denote the trace operator and the normal trace operator, respectively, and $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$.

See, e.g., chapter 6.7 in [12].

Theorem B.6 (Lax–Milgram lemma).

Let $(V, (\cdot, \cdot)_V)$ be a Hilbert space. Moreover, let $a : V \times V \rightarrow \mathbb{R}$ be a bilinear form and $F : V \rightarrow \mathbb{R}$ be a linear functional such that:

- a is continuous (i.e. bounded), namely, there exists $M > 0$ such that

$$|a(u, v)| \leq M \|u\|_V \|v\|_V, \quad \forall u, v \in V$$

- a is coercive, namely, there exists $\alpha > 0$ such that

$$a(u, u) \geq \alpha \|u\|_V^2, \quad \forall u \in V$$

- F is continuous (i.e. bounded), namely, there exists $C > 0$ such that

$$|\langle F, v \rangle| \leq C \|v\|_V, \quad \forall v \in V$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between V^* and V .

Then the problem

$$a(u, v) = \langle F, v \rangle \quad \forall v \in V$$

admits a unique solution $u \in V$.

See, e.g., chapter 5.3 in [4].

Theorem B.7 (Poincaré–Wirtinger inequality).

Let $\Omega \subset \mathbb{R}^n$ be open, bounded and connected, such that $\partial\Omega \in \text{Lip}$. Then there exists a constant $C_P > 0$, depending on Ω , such that

$$\|u - u_\Omega\|_{L^2(\Omega)} \leq C_P \|\nabla u\|_{L^2(\Omega)}, \quad \forall u \in H^1(\Omega)$$

where

$$u_\Omega = \frac{1}{|\Omega|} \int_\Omega u \, d\Omega$$

See, e.g., chapter 12.2 in [22].

Theorem B.8 (Parseval identity).

Let $(H, (\cdot, \cdot)_H)$ be a Hilbert space, and let $\{e_n\}_{n \in \mathbb{N}} \subset H$ be an orthonormal base of H . Then,

$$\|v\|_H^2 = \sum_{n=1}^{+\infty} |(v, e_n)_H|^2, \quad \forall v \in H$$

See, e.g., chapter 5.4 in [4].

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List of Symbols

Geometric and time notation

Variable	Description	SI unit
n	spatial dimension	—
Ω	spatial domain	—
$\partial\Omega$	boundary of the spatial domain	—
Ω_{int}	interior physical domain	—
Ω_{ext}	absorbing frame surrounding Ω_{int}	—
Γ_D	Dirichlet boundary portion	—
Γ_N	Neumann boundary portion	—
$\hat{\nu}$	outward unit normal vector to $\partial\Omega$	—
$\hat{\tau}$	unit tangent vector to $\partial\Omega$	—
I	time interval	—
T	final time	s

Continuous elastic fields and material parameters

Variable	Description	SI unit
$\underline{u}$	displacement field	m
$\underline{v}$	velocity field	m s ⁻¹
$\underline{f}$	body force	N m ⁻³

Variable	Description	SI unit
$\bar{\sigma}$	Cauchy stress tensor	Pa
$\bar{\varepsilon}$	infinitesimal strain tensor	—
ρ	mass density	kg m^{-3}
λ	first Lamé modulus	Pa
μ	second Lamé modulus	Pa
κ	bulk modulus	Pa
ν	Poisson's ratio	—
$\mathbf{C}$	fourth-order elasticity tensor	Pa
$\bar{\mathbf{I}}$	identity tensor	—

Time-harmonic plane-wave analysis and acoustic tensor

Variable	Description	SI unit
$\underline{k}$	wave vector	m^{-1}
k	wavenumber	m^{-1}
ω	angular frequency	s^{-1}
c	wave velocity	m s^{-1}
$\underline{a}$	polarization vector	m
$\hat{e}$	unit propagation vector	—
$\hat{s}$	unit transverse polarization vector in 2D	—
$\bar{A}$	acoustic tensor	Pa
V_P	P-wave velocity	m s^{-1}
V_S	S-wave velocity	m s^{-1}
$V_{\parallel}$	longitudinal polarization subspace	—
$V_{\perp}$	transverse polarization subspace	—

Variable	Description	SI unit
$\bar{\Pi}_{\parallel}$	orthogonal projector onto $V_{\parallel}$	–
$\bar{\Pi}_{\perp}$	orthogonal projector onto $V_{\perp}$	–

Helmholtz–Weyl decomposition and P/S subspaces

Variable	Description	SI unit
$G_1(\Omega)$	solenoidal subspace with zero normal trace	–
$G_2(\Omega)$	harmonic-gradient subspace	–
$G_3(\Omega)$	irrotational subspace with zero-trace potential	–
$\mathcal{U}_P$	P-wave subspace	–
$\mathcal{U}_S$	S-wave subspace	–
Π_P	orthogonal projector onto $\mathcal{U}_P$	–
Π_S	orthogonal projector onto $\mathcal{U}_S$	–
Id	identity operator	–
h	harmonic potential in G_2	m ²
g	zero-trace potential in G_3	m ²
$f = g + h$	scalar P-potential	m ²
$\underline{u}_1$	solenoidal component in $G_1(\Omega)$	m
$\underline{u}_2$	harmonic-gradient component in $G_2(\Omega)$	m
$\underline{u}_3$	irrotational component in $G_3(\Omega)$	m

Computational domain, grid and index sets

Variable	Description	SI unit
L_x	domain length in the x -direction	m

Variable	Description	SI unit
L_z	domain length in the z -direction	m
N_x	number of cells in the x -direction	—
N_z	number of cells in the z -direction	—
N_t	number of time steps	—
h_x	grid spacing in the x -direction	m
h_z	grid spacing in the z -direction	m
h	uniform grid spacing	m
Δt	time-step size	s
$\Sigma^{(c)}$	index set for cell centers	—
$\Sigma^{(v)}$	index set for centers of vertical cell edges	—
$\Sigma^{(h)}$	index set for centers of horizontal cell edges	—
$\Sigma^{(n)}$	index set for cell vertices	—
$\Theta^{(i)}$	index set for integer time levels	—
$\Theta^{(h)}$	index set for half time levels	—
$\Sigma^{(s)}, \tilde{\Sigma}^{(s)}$	index set of admissible wavenumbers	—
x_i	grid point in the x -direction	m
z_j	grid point in the z -direction	m
t^k	integer time level	s
$t^{k+1/2}$	half time level	s

Discrete differential operators

Variable	Description	SI unit
$D_x^{(4)}$	fourth-order finite-difference x -derivative	m^{-1}
$D_z^{(4)}$	fourth-order finite-difference z -derivative	m^{-1}

Variable	Description	SI unit
∇_h	second-order finite-difference gradient operator	m^{-1}
div_h	second-order finite-difference divergence operator	m^{-1}
Δ_h	second-order finite-difference Laplacian operator	m^{-2}

Stability, dispersion and spectral-resolution quantities

Variable	Description	SI unit
γ	normalized Courant number	–
$\gamma_{\max}$	maximum admissible value of γ	–
θ	propagation angle with respect to the x -axis	rad
H	inverse number of grid points per wavelength	–
$H_{\max}$	maximum admissible value of H	–
Q_P	normalized numerical P-wave velocity	–
Q_S	normalized numerical S-wave velocity	–
$f_{\max}$	maximum relevant source frequency	Hz
$V_{\min}$	minimum non-zero propagation velocity	m s^{-1}
$V_{P,\max}$	maximum P-wave velocity	m s^{-1}
$k_{x,\max}, k_{z,\max}$	maximum resolvable wavenumbers	m^{-1}
k_M	physical cutoff wavenumber	m^{-1}

Absorbing layers and averaged material parameters

Variable	Description	SI unit
d	distance from the nearest absorbing boundary	m
ℓ	thickness of the absorbing layer	m

Variable	Description	SI unit
s	normalized distance inside the absorbing layer	—
α	one-dimensional sponge damping profile	—
α_0	sponge damping strength parameter	—
d_x	x -distance to absorbing boundary	m
d_z	z -distance to absorbing boundary	m
G	two-dimensional sponge mask	—
R	averaged ρ on the staggered grid	kg m ⁻³
M	averaged μ on the staggered grid	Pa
K	averaged κ on the staggered grid	Pa
L	averaged λ on the staggered grid	Pa

Poisson right-hand sides and spectral bases

Variable	Description	SI unit
b	Dirichlet/mixed Poisson RHS	—
$\phi^{(n,m)}$	discrete Neumann Laplacian eigenfunction	—
$\lambda^{(n,m)}$	discrete Neumann Laplacian eigenvalue	m ⁻²
$\alpha^{(n,m)}$	discrete Neumann eigenfunction normalization coefficient	—
$\hat{q}^{(n,m)}$	spectral coefficient of q in a discrete basis	case-dependent
$\varphi_{n,m}$	continuous Dirichlet/mixed Laplacian eigenfunction	m ⁻¹
$\lambda_{n,m}$	continuous Dirichlet/mixed Laplacian eigenvalue	m ⁻²
$\hat{q}_{n,m}$	spectral coefficient of q in a continuous basis	case-dependent
$\xi_{n,m}$	cosine–sine basis function for u_x	m ⁻¹
$\eta_{n,m}$	sine–cosine basis function for u_z	m ⁻¹
V_x, V_z	finite-dimensional spaces for band-limited u_x, u_z	—

Mixed formulation potentials and auxiliary fields

Variable	Description	SI unit
f_1	harmonic lifting of the Neumann datum	m^2
f_0	lifted scalar P-potential	m^2
$\underline{u}_0$	auxiliary displacement field, gradient of f_0	m
$\underline{u}_1$	auxiliary displacement field, gradient of f_1	m
$\tilde{\underline{u}}$	auxiliary displacement field with zero normal trace	m

Quadrature weights and spectral-energy indicators

Variable	Description	SI unit
$w_i^{(x)}, w_j^{(z)}$	quadrature weights	—
$e_{n,m}$	modal energy of the displacement field	m^4
E_{tot}	total spectral energy	m^4
ρ_M	fraction of modal energy below k_M	—
η_{crit}	fraction of energy associated with Nyquist modes	—

Elastic Full Waveform Inversion quantities and notation

Variable	Description	SI unit
$\mathcal{M}$	admissible model space in (ρ, λ, μ) parametrization	—
$\mathcal{M}'$	admissible model space in (ρ, V_P, V_S) parametrization	—
$\underline{m}$	elastic model in (ρ, λ, μ) parametrization	—
$\underline{m}'$	elastic model in (ρ, V_P, V_S) parametrization	—
$\delta \underline{m}$	generic model perturbation in (ρ, λ, μ) parametrization	—

Variable	Description	SI unit
$\delta \underline{m}'$	generic model perturbation in (ρ, V_P, V_S) parametrization	—
Φ	change-of-parametrization map	—
$\mathcal{U}$	space of forward wave-fields	—
$\tilde{\mathcal{U}}$	space of adjoint wave-fields	—
$\mathcal{Y}$	data space	—
N_r	number of receivers	—
S_f	forward solution operator in (ρ, λ, μ) parametrization	—
S'_f	forward solution operator in (ρ, V_P, V_S) parametrization	—
$\tilde{S}_g$	adjoint solution operator in (ρ, λ, μ) parametrization	—
$\tilde{S}'_g$	adjoint solution operator in (ρ, V_P, V_S) parametrization	—
O	observation operator	—
O^*	adjoint observation operator	—
F	reduced forward operator	—
$\underline{d}$	observed data	m
$\underline{r}$	data residual	m
χ	misfit functional in (ρ, λ, μ) parametrization	—
χ'	misfit functional in (ρ, V_P, V_S) parametrization	—
$DA(m)[\delta m]$	Gâteaux derivative of the map A at m along δm	—
g	adjoint source	N m ⁻³
$\underline{p}$	adjoint wave-field	m
$\underline{p}_P$	P component of the adjoint wave-field	m
$\underline{p}_S$	S/SV component of the adjoint wave-field	m
$J_{V_P}^{(PP)}$	separation-based V_P gradient component	—
$J_{V_S}^{(PS,SP,SS)}$	separation-based V_S gradient component	—
$H_{V_P, V_S}^{(PP)}$	cross-parameter sensitivity of $J_{V_P}^{(PP)}$ to δV_S	—

Variable	Description	SI unit
$H_{V_S, V_P}^{(PS, SP, SS)}$	cross-parameter sensitivity of $J_{V_S}^{(PS, SP, SS)}$ to δV_P	–
$\underline{w}$	forward sensitivity field associated with δV_S	m
$\underline{\psi}$	adjoint sensitivity field associated with δV_S	m
$\underline{z}$	forward sensitivity field associated with δV_P	m
$\underline{\theta}$	adjoint sensitivity field associated with δV_P	m
$\underline{f}_{V_P}$	linearized source term associated with δV_P	N m ^{−3}
$\underline{h}$	additional adjoint source term associated with δV_S	N m ^{−3}
$\underline{k}$	additional adjoint source term associated with δV_P	N m ^{−3}

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