

Chapter 2

Introduction

In this chapter we present the basic elements for the numerical modelling of seismic wave propagation. Following a summary of notational conventions, we introduce the elastic wave equation in its different formulations (Sect. 2.2). The acoustic wave equation is treated as a special case in Sect. 2.3. While numerical methods differ in the details of the spatio-temporal discretisation, they can still be treated within a unifying framework. The approximation of the spatial derivatives generally leads to a system of ordinary differential equations in time that is commonly referred to as the semi-discrete form of the wave equation. The semi-discrete form can be written in terms of mass and stiffness matrices (Sect. 2.4). Depending on the specifics of an application, the remaining time derivatives can then be approximated using either the Fourier transform or time-stepping algorithms such as the Newmark or leapfrog methods (Sect. 2.5).

2.1 Notational Conventions

Throughout this book we have tried to stay close to notations commonly found in the seismological literature. While the meaning of the different symbols is mostly clear from the context, we start with a small collection of conventions that we shall use consistently.

The Fourier transform of a function f is defined as

$$\tilde{f}(\omega) := F[f](\omega) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(t) e^{-i\omega t} dt, \quad \mathbf{i} := \sqrt{-1}, \quad (2.1)$$

where the symbol $:=$ means that the expression to the left is defined by the expression to the right. The boldface \mathbf{i} is intended to distinguish the imaginary unit from the frequently occurring index variable i . The inverse Fourier transform corresponding to (2.1) is

$$f(t) = F^{-1}[\tilde{f}](t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \tilde{f}(\omega) e^{i\omega t} d\omega. \quad (2.2)$$

With the exception of \mathbf{i} , we use bold-faced symbols for vectors and tensors. The scalar product of two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$ is denoted by

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i . \quad (2.3)$$

We more generally use the dot to signify contraction over adjacent indices. Using this notation, the i -component of a matrix–vector product is written as

$$(\mathbf{A} \cdot \mathbf{a})_i = \sum_{j=1}^n A_{ij} a_j , \quad \mathbf{A} \in \mathbb{R}^{n \times n} , \quad (2.4)$$

and the ij -component of a matrix–matrix product is

$$(\mathbf{A} \cdot \mathbf{B})_{ij} = \sum_{k=1}^n A_{ik} B_{kj} . \quad (2.5)$$

Following this scheme, a double dot denotes a contraction over two adjacent indices, for instance

$$\mathbf{A} : \mathbf{B} = \sum_{i,j=1}^n A_{ij} B_{ij} , \quad \mathbf{B} \in \mathbb{R}^{n \times n} \quad (2.6)$$

and

$$(\mathbf{B} : \mathbf{C})_{kl} = \sum_{i,j=1}^n B_{ij} C_{ijkl} , \quad \mathbf{C} \in \mathbb{R}^{n \times n \times n \times n} . \quad (2.7)$$

For the real part of a complex-valued variable $z = x + \mathbf{i}y$, we use the fraktur symbol \Re , i.e.

$$\Re z = x = \frac{1}{2}(z + z^*) , \quad (2.8)$$

where $z^* = x - \mathbf{i}y$ denotes the complex conjugate of z . The symbol \Im denotes the imaginary part of z :

$$\Im z = y = \frac{1}{2i}(z - z^*) . \quad (2.9)$$

Of outstanding importance in any deterministic inverse problem is the definition of a misfit functional χ that quantifies the difference between observed and synthetic data. The misfit functional depends on an Earth model $\mathbf{m} \in \mathfrak{M}$, where \mathfrak{M} is the

model space. The functional or the Fréchet derivative of χ with respect to \mathbf{m} in a direction $\delta\mathbf{m} \in \mathfrak{M}$ is defined by

$$\nabla_m \chi(\mathbf{m}) \delta\mathbf{m} := \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [\chi(\mathbf{m} + \varepsilon \delta\mathbf{m}) - \chi(\mathbf{m})]. \quad (2.10)$$

The derivative $\nabla_m \chi(\mathbf{m})$ is a linear operator acting on the differentiation direction $\delta\mathbf{m}$. In the special case where \mathbf{m} is a vector, the Fréchet derivative $\nabla_m \chi(\mathbf{m}) \delta\mathbf{m}$ coincides with the directional derivative $\delta\mathbf{m} \cdot \nabla_m \chi(\mathbf{m})$. For convenience, we will mostly use the term ‘derivative’ instead of ‘Fréchet derivative’. The symbol ∇ , without subscript, signifies the regular gradient with respect to the position vector \mathbf{x} .

2.2 The Elastic Wave Equation

2.2.1 Governing Equations

Full waveform inversion is founded on the solution of the *forward problem*, which consists in the simulation of seismic wave propagation through an Earth model \mathbf{m} and the computation of synthetic seismograms. The propagation of seismic waves in the Earth can be modelled with the *elastic wave equation*

$$\rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}, t) - \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t) = \mathbf{f}(\mathbf{x}, t), \quad \mathbf{x} \in G \subset \mathbb{R}^3, \quad t \in [t_0, t_1] \subset \mathbb{R} \quad (2.11)$$

that relates the displacement field \mathbf{u} in the Earth $G \subset \mathbb{R}^3$ to its mass density ρ , the stress tensor $\boldsymbol{\sigma}$ and an external force density \mathbf{f} . A truly marvellous matter of fact! Equation (2.11) is the linearised version of Newton’s second law that balances the momentum of particle displacement $\rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}, t)$, forces resulting from internal stresses $\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t)$ and external forces $\mathbf{f}(\mathbf{x}, t)$ that represent the sources of seismic wave motion. For detailed derivations of Eq. (2.11) the reader is referred to Dahlen & Tromp (1998), Kennett (2001) or Aki & Richards (2002). At the surface ∂G of the Earth, the normal components of the stress tensor $\boldsymbol{\sigma}$ vanish, i.e.

$$\boldsymbol{\sigma} \cdot \mathbf{n}|_{\mathbf{x} \in \partial G} = \mathbf{0}, \quad (2.12)$$

where \mathbf{n} is the unit normal on ∂G . Equation (2.12) is the *free surface boundary condition*. Both the displacement field \mathbf{u} and the velocity field $\mathbf{v} = \dot{\mathbf{u}}$ are required to satisfy the *initial condition* of being equal to zero prior to $t = t_0$ when the external force \mathbf{f} starts to act:

$$\mathbf{u}|_{t \leq t_0} = \mathbf{v}|_{t \leq t_0} = \mathbf{0}. \quad (2.13)$$

For convenience we will mostly choose $t_0 = 0$. To obtain a complete set of equations, the stress tensor $\boldsymbol{\sigma}$ must be related to the displacement field \mathbf{u} . For this we assume that $\boldsymbol{\sigma}$ depends linearly on the history of the strain tensor $\boldsymbol{\varepsilon} := \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \int_{-\infty}^{\infty} \dot{\mathbf{C}}(\mathbf{x}, t - t') : \boldsymbol{\varepsilon}(\mathbf{x}, t') dt' . \quad (2.14)$$

Equation (2.14) defines a *linear visco-elastic rheology*. The 4th-order tensor \mathbf{C} is the *elastic tensor*. Since the current stress cannot depend on future strain, we require the elastic tensor to be causal:

$$\mathbf{C}(t)|_{t < t_0} = \mathbf{0} . \quad (2.15)$$

The symmetry of $\boldsymbol{\varepsilon}$, the conservation of angular momentum and the relation of \mathbf{C} to the internal energy (e.g. Aki & Richards, 2002) require that the components of \mathbf{C} satisfy the following symmetry relations:

$$C_{ijkl} = C_{klij} = C_{jikl} . \quad (2.16)$$

The symmetries of the elastic tensor reduce the number of its independent components to 21, and they allow us to write (2.14) directly in terms of the displacement gradient $\nabla \mathbf{u}$:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \int_{-\infty}^{\infty} \dot{\mathbf{C}}(\mathbf{x}, t - t') : \nabla \mathbf{u}(\mathbf{x}, t') dt' . \quad (2.17)$$

The number of non-zero independent elastic tensor components – also referred to as elastic parameters or elastic moduli – determines the *anisotropic properties* of the medium. For instance, a triclinic crystal such as plagioclase requires all 21 independent parameters for its complete description and 3 elastic parameters are needed to describe crystals with cubic symmetry such as garnet (Babuska & Cara, 1991). On a macroscopic scale the Earth can often be described sufficiently well as an isotropic body where the elastic tensor components are linear combinations of only two elastic moduli: the *Lamé parameters* λ and μ :

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \delta_{ik} \delta_{jl} + \mu \delta_{il} \delta_{jk} . \quad (2.18)$$

The parameter μ relates strain to shear stresses and is therefore called *shear modulus*. Since λ has no intuitive physical meaning, it is commonly replaced by the *bulk modulus* $\kappa = \lambda + \frac{2}{3}\mu$ that relates strain to the scalar pressure, defined as $p =: -\kappa \nabla \cdot \mathbf{u}$.

The time dependence of the elastic tensor is responsible for visco-elastic dissipation, that is the process of transforming elastic energy into heat. In the case of a non-dissipative medium, the time dependence of \mathbf{C} takes the form of a unit step or Heaviside function $H(t)$:

$$\mathbf{C}(\mathbf{x}, t) = \mathbf{C}(\mathbf{x}) H(t) . \quad (2.19)$$

The constitutive relation (2.17) then takes the form

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \mathbf{C}(\mathbf{x}) : \nabla \mathbf{u}(\mathbf{x}, t) . \quad (2.20)$$

For simplicity we will assume a non-dissipative medium throughout most of this book. This is also justified because dissipation can be incorporated easily with the help of memory variables, as we shall see in Chap. 5. Memory variables allow us to circumvent the numerically inconvenient convolution in Eq. (2.17).

2.2.2 Formulations of the Elastic Wave Equation

Equations (2.11) and (2.20) constitute the *displacement–stress formulation* of the elastic wave equation in the absence of dissipation. Together with the initial and boundary conditions they uniquely specify the displacement field $\mathbf{u}(\mathbf{x}, t)$.

Different but fully equivalent formulations are possible and sometimes required by a specific numerical method. We may, for instance, eliminate the stress tensor $\boldsymbol{\sigma}$ by combining Eqs.(2.11) and (2.20). This results in the *displacement formulation* of the elastic wave equation:

$$\rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}, t) - \nabla \cdot [\mathbf{C}(\mathbf{x}) : \nabla \mathbf{u}(\mathbf{x}, t)] = \mathbf{f}(\mathbf{x}, t) . \quad (2.21)$$

Of particular relevance in numerical modelling is the *velocity–stress formulation* where the wave equation is written as a first-order system in both time and space. We find the velocity–stress formulation by simply differentiating Eq. (2.20) with respect to time and then substituting \mathbf{v} for $\dot{\mathbf{u}}$:

$$\rho(\mathbf{x}) \dot{\mathbf{v}}(\mathbf{x}, t) - \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t) = \mathbf{f}(\mathbf{x}, t) , \quad (2.22a)$$

$$\dot{\boldsymbol{\sigma}}(\mathbf{x}, t) - \mathbf{C}(\mathbf{x}) : \nabla \mathbf{v}(\mathbf{x}, t) = \mathbf{0} . \quad (2.22b)$$

The elastic wave equation in its different formulations has been studied extensively. Analytical solutions exist for numerous classes of models including, for instance, the isotropic and homogeneous half space (e.g. Lamb, 1904; de Hoop, 1958; Aki & Richards, 2002), stratified media (e.g. Kennett, 1979, 1980, 1981) and spherically symmetric globes with radial anisotropy (e.g. Takeuchi & Saito, 1978; Woodhouse, 1988; Friederich & Dalkolmo, 1995). Ray theory (e.g. Červený, 2001) and perturbation methods (e.g. Woodhouse & Dahlen, 1978; Maupin, 2001) can be used to approximate solutions to the elastic wave equation for mildly heterogeneous media. In full waveform inversion, the focus is on strongly heterogeneous regions of the Earth where analytical or perturbation methods are not applicable. This is the domain of numerical methods that are the subject of the first part of this book.

2.3 The Acoustic Wave Equation

The equations of motion simplify significantly in the fluid regions of the Earth (e.g. the outer core, oceans, and melt bodies), where the shear modulus μ is effectively zero. Inserting $\mu = 0$ into the isotropic constitutive relation (2.18), yields

$$\sigma_{ij} = \kappa \delta_{ij} \nabla \cdot \mathbf{u} = -p \delta_{ij}, \quad (2.23)$$

where we introduced the scalar pressure $p := -\kappa \nabla \cdot \mathbf{u}$. With the help of Eq. (2.23) the momentum balance law (2.11) reduces to

$$\rho \ddot{\mathbf{u}} + \nabla p = \mathbf{f}. \quad (2.24)$$

Dividing (2.24) by the density ρ and taking the divergence gives

$$\nabla \cdot \ddot{\mathbf{u}} + \nabla \cdot (\rho^{-1} \nabla p) = \nabla \cdot (\rho^{-1} \mathbf{f}). \quad (2.25)$$

Using the definition of the pressure p , we can eliminate the displacement field \mathbf{u} from Eq. (2.25):

$$\kappa^{-1} \ddot{p} - \nabla \cdot (\rho^{-1} \nabla p) = -\nabla \cdot (\rho^{-1} \mathbf{f}). \quad (2.26)$$

When density varies much more slowly than the pressure field p and the source \mathbf{f} , we can simplify (2.26) to a scalar partial differential equation, known as the *acoustic wave equation*:

$$\ddot{p} - v_a^2 \Delta p = -v_a^2 \nabla \cdot \mathbf{f}, \quad (2.27)$$

with the *acoustic wave speed* $v_a := \sqrt{\frac{\kappa}{\rho}}$. It follows from (2.27) that wave motion in fluid media can be fully described with a single scalar field (the pressure, p), the properties of which depend only on the source term and the spatial distribution of the acoustic wave speed.

While being strictly valid only in fluid and gaseous media, the acoustic wave equation is frequently used in active-source full waveform inversion (see for example Chap. 14), because its numerical solution is computationally inexpensive compared to the solution of the elastic wave equation. The consequences of this *acoustic approximation* include the restriction to isotropic source radiation patterns and the absence of Rayleigh waves and P-to-S conversions. The acoustic approximation is, nevertheless, justifiable when the data analysis is restricted to the first-arriving P waves and when the seismic sources radiate little S wave energy (e.g. explosions).

With the exception of Chap. 14, the focus of this book will be on elastic wave propagation. The transition to the acoustic case is mostly straightforward.

2.4 Discretisation in Space

Analytical solutions to the elastic wave equation exist only for comparatively simple models that often do not reflect the structural complexities of the Earth. This deficiency motivates the development of numerical methods for the simulation of seismic wave propagation through almost arbitrarily heterogeneous Earth models. While being different in the technical details, all numerical methods have one point in common: the discrete spatial approximation of the continuously defined wave field $\mathbf{u}(\mathbf{x}, t)$. This means that $\mathbf{u}(\mathbf{x}, t)$ is approximated by a finite number of time-dependent coefficients $\bar{u}_1(t), \dots, \bar{u}_N(t)$ that can be summarised in an N -dimensional vector $\bar{\mathbf{u}}(t)$. Depending on the specifics of the numerical method used, the coefficients $\bar{u}_i(t)$ ($i = 1, \dots, N$) may represent, for instance, discrete values of $\mathbf{u}(\mathbf{x}, t)$ sampled at a finite number of points, or polynomial coefficients when $\mathbf{u}(\mathbf{x}, t)$ is approximated by a polynomial.

Following spatial discretisation, the displacement formulation of the elastic wave equation, given in (2.21), turns into an algebro-differential equation that can always be written in the following canonical form:

$$\mathbf{M} \cdot \ddot{\bar{\mathbf{u}}}(t) + \mathbf{K} \cdot \bar{\mathbf{u}}(t) = \bar{\mathbf{f}}(t). \quad (2.28)$$

The matrices \mathbf{M} and \mathbf{K} are referred to as the *mass matrix* and the *stiffness matrix*, respectively. The vector $\bar{\mathbf{f}}$ represents a discrete version of the force density \mathbf{f} . Both \mathbf{M} and \mathbf{K} tend to be sparse. In practice, the mass and the stiffness matrices are rarely computed explicitly because only the vector–matrix products are needed in actual computations. They are, nevertheless, useful tools in theoretical developments, as we will soon discover.

Depending on the numerical method, it may be more advantageous to discretise the displacement–stress formulation Eqs. (2.11) and (2.20) or the velocity–stress formulation (Eq. 2.22) of the elastic wave equation. The corresponding space-discrete systems are then

$$\mathbf{M} \cdot \ddot{\bar{\mathbf{u}}}(t) + \mathbf{K}_1 \cdot \bar{\mathbf{s}}(t) = \bar{\mathbf{f}}(t), \quad (2.29a)$$

$$\bar{\mathbf{s}}(t) = \mathbf{K}_2 \cdot \bar{\mathbf{u}}(t) \quad (2.29b)$$

for the displacement–stress formulation and

$$\mathbf{M} \cdot \dot{\bar{\mathbf{v}}}(t) + \mathbf{K}_1 \cdot \bar{\mathbf{s}}(t) = \bar{\mathbf{f}}(t), \quad (2.30a)$$

$$\dot{\bar{\mathbf{s}}}(t) - \mathbf{K}_2 \cdot \bar{\mathbf{v}}(t) = \mathbf{0} \quad (2.30b)$$

for the velocity–stress formulation. The matrices \mathbf{K}_1 and \mathbf{K}_2 are stiffness matrices in a broader sense and $\bar{\mathbf{s}}$ represents a discrete approximation to the stress tensor $\boldsymbol{\sigma}$. The transition from the continuous wave equation in its various formulations to one of the space-discrete systems (2.28), (2.29) or (2.30) reduces the forward problem to the solution of a large algebraic system and an ordinary differential equation in time.

2.5 Discretisation in Time or Frequency

The ordinary differential equations in time that arise from the spatial discretisation of the equations of motion can be solved either in the time domain or in the frequency domain. Both approaches have advantages and disadvantages that must be weighted depending on the particular application and the available computational resources.

2.5.1 Time-Domain Modelling

The time-domain modelling of wave propagation is mostly based on the replacement of the time derivatives in the space-discrete equations of motion by suitable finite-difference approximations. These allow us to advance the wave field in discrete time steps Δt . The choice of a particular finite-difference scheme depends on the formulation of the wave equation.

Throughout the following paragraphs we assume that the mass matrix \mathbf{M} can be inverted, noting, however, that the inversion of \mathbf{M} may present a formidable numerical challenge.

2.5.1.1 Displacement and Displacement–Stress Formulation

The space-discrete version of the displacement formulation (2.28) involves the second time derivative of the discrete displacement field $\ddot{\mathbf{u}}$, which is explicitly given by

$$\ddot{\mathbf{u}}(t) = \mathbf{M}^{-1} \cdot [\bar{\mathbf{f}}(t) - \mathbf{K} \cdot \bar{\mathbf{u}}(t)]. \quad (2.31)$$

Approximating $\ddot{\mathbf{u}}(t)$ by the second-order finite difference

$$\ddot{\mathbf{u}}(t) \approx \frac{1}{\Delta t^2} [\bar{\mathbf{u}}(t + \Delta t) - 2\bar{\mathbf{u}}(t) + \bar{\mathbf{u}}(t - \Delta t)] \quad (2.32)$$

leads to an explicit time-stepping scheme that allows us to compute the displacement at time $t + \Delta t$ from the displacement at times t and $t - \Delta t$:

$$\bar{\mathbf{u}}(t + \Delta t) = 2\bar{\mathbf{u}}(t) - \bar{\mathbf{u}}(t - \Delta t) + \Delta t^2 \mathbf{M}^{-1} \cdot [\bar{\mathbf{f}}(t) - \mathbf{K} \cdot \bar{\mathbf{u}}(t)]. \quad (2.33)$$

For notational clarity we replaced \approx by $=$ in Eq. (2.33), keeping in mind that this is an approximation.

A frequently used alternative to (2.33) is the *Newmark scheme* (Newmark, 1959; Chaljub et al., 2007), defined by

$$\bar{\mathbf{u}}(t + \Delta t) = \bar{\mathbf{u}}(t) + \Delta t \bar{\mathbf{v}}(t) + \Delta t^2 \left[\left(\frac{1}{2} - \beta \right) \ddot{\mathbf{u}}(t) + \beta \ddot{\mathbf{u}}(t + \Delta t) \right], \quad (2.34a)$$

$$\bar{\mathbf{v}}(t + \Delta t) = \bar{\mathbf{v}}(t) + \Delta t [(1 - \gamma) \ddot{\mathbf{u}}(t) + \gamma \ddot{\mathbf{u}}(t + \Delta t)], \quad (2.34b)$$

with the parameters $\gamma \in [0, 1]$ and $\beta \in [0, \frac{1}{2}]$. Second-order accuracy instead of first-order accuracy is achieved if and only if $\gamma = \frac{1}{2}$. In the special case $\gamma = \frac{1}{2}$ and $\beta = 0$, we obtain an explicit central-difference scheme:

$$\bar{\mathbf{u}}(t + \Delta t) = \bar{\mathbf{u}}(t) + \Delta t \bar{\mathbf{v}}(t) + \frac{1}{2} \Delta t^2 \ddot{\mathbf{u}}(t), \quad (2.35a)$$

$$\bar{\mathbf{v}}(t + \Delta t) = \bar{\mathbf{v}}(t) + \frac{1}{2} \Delta t [\ddot{\mathbf{u}}(t) + \ddot{\mathbf{u}}(t + \Delta t)]. \quad (2.35b)$$

The order of operations in the iterative advancement of $\bar{\mathbf{u}}$ is then as follows. (1) Compute $\bar{\mathbf{u}}$ at time $t + \Delta t$ from the discrete field variables at time t , using Eq. (2.35a). (2) With the help of Eq. (2.31), compute the acceleration $\ddot{\mathbf{u}}(t + \Delta t)$ from $\bar{\mathbf{u}}(t + \Delta t)$. (3) Advance the velocity $\bar{\mathbf{v}}$ from time t to $t + \Delta t$, using Eq. (2.35b). (4) Go back to (1) and repeat as often as needed. While being more complicated than (2.33), the Newmark scheme has the advantageous property of conserving linear and angular momentum (e.g. Kane et al., 2003).

We note that the time discretisation schemes for the displacement formulation are immediately applicable to the displacement–stress formulation from Eq. (2.29).

2.5.1.2 Velocity–Stress Formulation

The most commonly used time discretisation scheme for the velocity–stress formulation (2.30) is the *leapfrog method*. This is based on alternating updates of the discrete velocity and stress fields. Starting from $\bar{\mathbf{s}}(t - \Delta t/2)$ and $\bar{\mathbf{v}}(t)$, we obtain $\bar{\mathbf{s}}(t + \Delta t/2)$ via a second-order finite-difference approximation of Eq. (2.30b):

$$\bar{\mathbf{s}}(t + \Delta t/2) = \bar{\mathbf{s}}(t - \Delta t/2) + \Delta t \mathbf{K}_2 \cdot \bar{\mathbf{v}}(t). \quad (2.36a)$$

With the help of the discrete stress field $\bar{\mathbf{s}}(t + \Delta t/2)$ we can then advance the velocity field from time t to time $t + \Delta t$, using the same second-order approximation applied to Eq. (2.30a):

$$\bar{\mathbf{v}}(t + \Delta t) = \bar{\mathbf{v}}(t) + \Delta t \mathbf{M}^{-1} \cdot [\bar{\mathbf{f}}(t + \Delta t/2) - \mathbf{K}_1 \cdot \bar{\mathbf{s}}(t + \Delta t/2)]. \quad (2.36b)$$

Again, for notational convenience, we replaced \approx by $=$ in Eq. (2.36a) and (2.36b).

2.5.1.3 Stability

All of the above time-stepping algorithms are explicit in the sense that the dynamic fields at time $t + \Delta t$ depend only on the dynamic fields at times *prior* to $t + \Delta t$. This implies that the algorithms are only conditionally stable. The stability criterion, named *CFL condition* in honour of R. Courant, K. Friedrichs and H. Lewy (R. Courant, K. Friedrichs and H. Lewy, Courant et al. 1928), typically takes the form

$$\Delta t \leq \text{const.} \frac{\min h}{\max v}, \quad (2.37)$$

where h is the width of the numerical grid and v is the propagation speed of the fastest wave, that is the P wave. The constant on the right-hand side of Eq. (2.37) depends on the methods used for the space and time discretisation. Its order of magnitude is 1. The CFL condition limits the maximum possible time increment and therefore the efficiency of any explicit time stepping. In Sect. 3.1 we derive the CFL condition for a finite-difference approximation of the 1D scalar wave equation.

2.5.1.4 Alternative Methods

The Newmark and the leapfrog schemes are by far the most frequently used methods for the time discretisation of the space-discrete equations of motion. This may appear surprising given the availability of numerous alternatives such as predictor–corrector variants of implicit multi-step methods or higher order Runge–Kutta methods (e.g. Quarteroni et al., 2000).

The restriction to conditionally stable methods of comparatively low order can be explained not only by the larger computational requirements of implicit and higher order methods but also by the good performance of the explicit second-order schemes. Empirical studies show that the numerical error is often dominated by the inaccuracies of the *spatial* discretisation. This is true even when the number of time steps is large, that is on the order of several thousands. Whether the conventional Newmark and leapfrog schemes are sufficient for future applications, such as global-scale wave propagation at periods around 2 s, is still an open question.

2.5.2 Frequency-Domain Modelling

Frequency-domain modelling is based on the Fourier-transformed version of the space-discrete displacement formulation (2.28):

$$-\omega^2 \mathbf{M} \cdot \bar{\mathbf{u}}(\omega) + \mathbf{K} \cdot \bar{\mathbf{u}}(\omega) = \bar{\mathbf{f}}(\omega). \quad (2.38)$$

Upon defining the *impedance matrix* \mathbf{L}

$$\mathbf{L}(\omega) := -\omega^2 \mathbf{M} + \mathbf{K}, \quad (2.39)$$

Eq. (2.38) simplifies to the linear system

$$\mathbf{L}(\omega) \cdot \bar{\mathbf{u}}(\omega) = \bar{\mathbf{f}}(\omega). \quad (2.40)$$

The solution of (2.40) is the discrete wave field $\bar{\mathbf{u}}$ at one frequency ω .

It is particularly attractive to solve the system (2.40) using direct matrix factorisation methods, such as LU decomposition (e.g. Press et al., 2007). Once the

matrix factors are known, they can be reused to solve the forward problem for any new source $\bar{\mathbf{f}}$ at very low computational cost (e.g. Pratt et al., 1998; Pratt, 1999). However, in realistic 3D applications, the memory requirements of direct methods can become prohibitive so that iterative solvers must be used (e.g. Quarteroni et al., 2000).

Frequency-domain modelling is the method of choice when solutions for a few dominant or well-chosen frequencies are needed or when the problem is 2D thus permitting the application of direct linear system solvers.

One of the outstanding advantages of this approach is the easy implementation of visco-elastic dissipation. This is because the convolution in Eq. (2.14) translates to a simple product in the frequency domain. Additional memory variables as in time-domain modelling are therefore not needed (see Chap. 5). In Chap. 14 we present an application of frequency-domain modelling in the context of full waveform tomography with active-source data.

2.6 Summary of Numerical Methods

In the course of the past decades a large number of numerical methods for the solution of the seismic wave equation have been developed – often for the purposes of ground motion prediction or waveform inversion. Each method comes with advantages and disadvantages that need to be weighted carefully in the light of a specific application.

The most significant distinction between different approaches concerns the spatial discretisation, that is, the transformation of the exact spatial derivatives in the wave equation into an algebraic system. The following is a list of some methods that try to highlight their major similarities and differences.

Finite-difference methods: Numerical modelling in nearly all physical sciences started with the finite-difference method, and seismology is no exception. Early applications can be found in Alterman & Karal (1968), Boore (1970, 1972), Alford et al. (1974) and Kelly et al. (1976). To illustrate the finite-difference concept, we consider a generic function $f(x)$ that represents the dynamic fields that appear in the wave equation (e.g. stress, strain, and displacement). The fundamental idea is to consider only a finite number of evenly spaced grid points x_i ($i=1, \dots, N$) and to replace the derivative $\partial_x f(x_i)$ at grid point x_i by a *finite-difference approximation* that involves f evaluated at neighbouring grid points. The best-known example is the second-order central finite-difference approximation

$$\partial_x f(x_i) = \frac{1}{2\Delta x} [f(x_i + \Delta x) - f(x_i - \Delta x)] + \mathcal{O}(\Delta x^2), \quad (2.41)$$

where Δx is the grid spacing. The feasibility of finite-difference modelling in three dimensions rests on the definition of a *staggered grid* where the dynamic fields are defined at different grid positions (e.g. Madariaga, 1976; Virieux, 1984, 1986, Igel et al., 1995). This is in contrast to the *conventional grid* where all field variables

are defined at coincident grid positions. The staggered grid results in a reduced average grid spacing that greatly reduces the *numerical dispersion*, i.e. the artificial dispersion introduced by the discretisation of the original equations of motion.

The popularity of finite-difference modelling is largely due to the comparatively low computational costs and the accuracy especially in the modelling of body wave propagation. In Chap. 3 we treat the finite-difference method in detail.

Optimal operators: The discretisation of the equations of motion introduces numerical errors that are particularly prominent near the eigenfrequencies of the elastic medium. This observation led Geller & Takeuchi (1995) to the construction of optimal operators that are designed to minimise the discretisation error first of all in the vicinity of the eigenfrequencies.

The very general criterion for an operator to be optimal is that the inner product of an exact eigenfunction with the net error of the discrete equations of motion at the corresponding eigenfrequency is approximately 0. This criterion is independent of the actual space discretisation scheme. In the particular framework of finite-difference methods, optimality means that the lowest order errors of the time and the space discretisations cancel, thus leading to highly accurate numerical schemes (Geller & Takeuchi, 1998; Takeuchi & Geller, 2000).

Since time-domain optimal operators are inherently implicit, predictor–corrector algorithms must be used to avoid the solution of large algebraic systems in the time stepping. The increased solution accuracy clearly compensates the additional computational costs of the predictor–corrector scheme (Mizutani et al., 2000; Kristek & Moczo, 2006).

Pseudospectral methods: Like finite-difference methods, pseudospectral methods directly discretise the spatial derivatives in the equations of motion (e.g. Kosloff & Baysal, 1982; Furumura et al., 1998). The discretisation proceeds in three steps. Firstly, the wave field sampled at a finite number of grid points is transformed to the wave number domain using the fast Fourier transform. The transformed wave field is then multiplied by ik , where k is the wave number. This multiplication corresponds to a space derivative. Finally, using the inverse fast Fourier transform, the wave field is transformed back to the space domain. Since the derivative is exact up to the Nyquist wave number, as few as two grid points per wavelength are theoretically sufficient for the spatial sampling of the wave field.

Kosloff et al. (1990) proposed a variant of the Fourier pseudospectral method where a Chebyshev transform is used in the vertical direction in order to account more accurately for the free surface condition. An extension to the 3D case with surface topography can be found in Tessmer & Kosloff (1994). The application of the Chebyshev pseudospectral method to wave propagation on the scale of the mantle is presented in Igel (1999).

Pseudospectral methods outperform finite-difference methods regarding the very small amount of numerical dispersion. However, due to the global nature of the derivative approximation, they are restricted to comparatively smooth media (Mizutani et al., 2000). Furthermore, pseudospectral methods face issues of parallelisation because global memory access is required for the computation of the Fourier and Chebyshev transforms.

Finite-element methods: Finite-element methods are based on the *weak* or the *variational form* of the wave equation that we describe in Sect. 4.1.1. The computational domain is decomposed into disjoint subdomains, called the elements. Within each element the dynamic fields are approximated by polynomials of low order (e.g. piecewise linear functions Bao et al., 1998), and continuity between the elements is imposed explicitly. The elastic wave equation then reduces to a space-discrete system for the polynomial coefficients.

Despite its capability to correctly account for irregular geometries and the free surface, applications of the pure finite-element method to elastic wave propagation are comparatively rare (e.g. Lysmer & Drake, 1972; Toshinawa & Ohmachi, 1992; Bao et al., 1998). This is mostly due to the comparatively large numerical dispersion that results from the low-order polynomial approximations. Moreover, the mass matrix in finite-element methods is not diagonal, which renders its inversion computationally expensive.

While the pure finite-element method does not appear to be well suited for wave propagation, hybrid schemes have been used very successfully. Moczo et al. (1997, 2007), for instance, combined the finite-element and finite-difference methods for the simulation of wave propagation along irregular surface topography. They discretised the equations of motion in the interior of the computational domain using finite differences. A rim of finite elements was then used to mesh the topography.

Spectral-element methods: Spectral-element methods are half way between finite-element and pseudospectral methods, combining the advantages of both approaches while avoiding many of their drawbacks. Like in finite-element methods, the computational domain is subdivided into non-overlapping elements that can be adapted to irregular geometries. Inside the elements a high-order spectral approximation is used for the dynamic fields. The spectral-element method as originally developed for fluid mechanics (Patera, 1984) and seismic wave modelling (Priolo et al., 1994; Seriani et al., 1995; Seriani, 1998) indeed uses Chebyshev polynomials as basis functions, thus establishing a direct link to the Chebyshev pseudospectral methods.

In a widely used spectral-element variant the Chebyshev polynomials are replaced by Lagrange polynomials collocated at the Gauss–Lobatto–Legendre (GLL) points. The combination with GLL quadrature leads to a diagonal mass matrix that can be trivially inverted. In Chap. 4 and Appendix A we provide a detailed introduction to the spectral-element method. Applications on a variety of scales can be found in Faccioli et al. (1997), Komatitsch (1997), Komatitsch & Vilotte (1998), Komatitsch & Tromp (2002), Chaljub et al. (2003), Chaljub & Valette (2004) and Nissen-Meyer et al. (2007, 2008)

Direct solution method: The direct solution method was introduced in a series of papers by Geller & Ohminato (1994) and Cummins et al. (1994a,b). As finite-element and spectral-element methods, it is founded on the weak form of the equations of motion. What distinguishes the direct solution method is the choice of basis functions: linear splines in the radial direction and spherical harmonics in the horizontal directions. The space-discrete equations are then solved in the frequency domain.

Takeuchi (2000) applied the optimal operator formalism of Geller & Takeuchi (1995) to the direct solution method and investigated its applicability to waveform inversion. The method was extended to radially anisotropic media by Kawai et al. (2006) and then applied to waveform inversion for localised heterogeneities by Konishi et al. (2009) and Kawai & Geller (2010).

Discontinuous Galerkin methods: Discontinuous Galerkin methods for seismic wave propagation have been developed only recently (e.g. Dumbser & Käser, 2006; Käser et al., 2007; de la Puente et al., 2007, 2008). They represent a class of finite-element methods where neighbouring elements are linked by numerical fluxes and not by continuity constraints. This allows for solutions that are discontinuous across element boundaries. Discontinuous Galerkin methods are therefore particularly well suited for the modelling of earthquake rupture processes (de la Puente et al., 2009). An application of a discontinuous Galerkin method in the context of full waveform inversion can be found in Brossier et al. (2009).

In Chaps. 3 and 4 two of the above-mentioned discretisation approaches are described in more detail: the finite-element and the spectral-element method.

Choosing two out of many possible methods was a difficult but inevitable decision. Since this book is intended to cover both the forward and the inverse problems, I gave preference to the methods that are currently employed most frequently in the context of waveform tomography. The finite-difference and spectral-element methods also offer the opportunity to introduce a large number of concepts that are of general importance in numerical seismology.

A comprehensive treatise on all the different approaches to the numerical solution of the seismic wave equation is still to be written, and I offer my apologies to colleagues whose work I was not able to present here.



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