

A review of the spectral, pseudo-spectral, finite-difference and finite-element modelling techniques for geophysical imaging

Jean Virieux¹, Henri Calandra², and René-Édouard Plessix³

¹*LGIT, Université Joseph Fourier, Grenoble I, BP 53, 38041 Grenoble CEDEX 9, France;*
email: Jean.Virieux@obs.ujf-grenoble.fr.

²*TOTAL Pau, France;*
email: Henri.CALANDRA@total.com

³*Shell Global Solutions International, Kesslerpark 1, 2288 AB Rijswijk, The Netherlands;*
email: ReneEdouard.Plessix@shell.com.

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SUMMARY

Modelling methods are nowadays at the heart of any geophysical interpretation approach. These are heavily relied upon by imaging techniques in elastodynamics and electromagnetism, where they are crucial for the extraction of subsurface characteristics from ever larger and denser datasets. While high-frequency or one-way approximations are very powerful and efficient, they reach their limits when complex geological settings and solutions of full equations are required at finite frequencies. A review of three important formulations is carried out here: the spectral method, which is very efficient and accurate but generally restricted to simple earth structures, and often layered earth structures; the pseudo-spectral, finite-difference and finite-volume methods based on strong formulation of the partial differential equations, which are easy to implement and currently represent a good compromise between accuracy, efficiency and flexibility; and the continuous or discontinuous Galerkin finite-element methods that are based on the weak formulation, which lead to more accurate earth representations and therefore to more accurate solutions, although with higher computational costs and more complex use. The choice between these different approaches is still difficult and depends on the applications. Guidelines are given here through discussion of the requirements for imaging/ inversion.

Key words: Modelling, Imaging, Seismic, Electromagnetism

1 INTRODUCTION

Interpreting geophysical data in complex geological terrains requires solutions of the partial differential equations (PDEs) governing the physics of the related field experiments. In seismology and exploration geophysics, modelling in various realistic media for various purposes, ranging from risk analysis to crustal imaging, has promoted studies across a wide range of analytical, semi-analytical and numerical methods. This is particularly true in diffusive electromagnetic and seismic scanning methods, as we consider in this review. Numerical methods can be based on an approximation of the PDE, e.g., the high-frequency approximation (see Virieux and Lambaré (2007) for references), or the one-way propagation approximation (Claerbout 1985). However, handling these approximations for forward modelling can bias image construction when the waves observed are not included in the approximation we consider.

The need for solutions of the full/ complete differential equations (or the corresponding integral equations) was quickly recognised. Numerical methods with their discretisation for geophysical applications were discussed as soon as computers became powerful enough for numerical simulations in heterogeneous media; e.g. in propagative elastodynamics Alterman and Karal (1968); Bolt and Smith (1976); Kelly *et al.* (1976); Marfurt (1984); Virieux (1984); Dablain (1986); Levander (1988), and in diffusive electromagnetism Cognon (1971); Kuo and Cho (1980); Goldman and Stover (1983); Oristaglio and Hohmann (1984); Hohmann (1988); Druskin and Knizhnerman (1988). These methods have their own limitations that are related to time and space discretisation. Although these numerical methods have rarely been used on large-scale imaging problems because of their computational cost, their applications have been intensively discussed in the context of seismic reverse-time migration

(RTM) and seismic full-waveform inversion (FWI) (Baysal *et al.* 1983; Lailly 1983; Whitmore 1983; Gauthier *et al.* 1986; Tarantola 1987), as well as for diffusive electromagnetic inversion (Constable *et al.* 1987; Hohmann 1988; Ramm and Somersalo 1989). These studies form the basis of the current developments in both seismic and diffusive electromagnetic imaging.

The diversity of the numerical methods in geophysics questions the relevance and the pertinence of each approach. Some scientific disciplines appear to have a more focussed approach. For instance, in meteorology and in physical chemistry, the pseudo-spectral method (which is often referenced as a spectral method in the literature) represents the main approach used to address the challenging problems of weather prediction and climate change (Haltiner and Williams 1980; Jarraud and Baede 1985; Fornberg 1998). The complex physical processes are put into sub-grid phenomenological evolution, such as the chemical interactions inside clouds. In structural mechanics, the finite-element method is the method of choice (Zienkiewicz and K. Morgan 1983). Extensions to complex non-linear rheological behaviours has been preformed with the distinct/discrete element methods (Toomey and Beans 2000; Mariotti 2007). The diversity involved in solving geophysical modelling might, however, reflect the different challenges in geophysics. These challenges can require different practical solutions. For instance, to be economically valuable, the migration of hundreds of thousands of shots of a marine dataset are needed to obtain a structural image from compressional waves, which demands a different way of implementation of the wave propagation problem than the precise modelling of surface waves generated by a superficial earthquake.

Methodological efforts over the years have produced sophisticated tools that are well tuned for specific purposes. This intensive exploration of various simulation techniques comes from our difficulties in trying to understand the Earth interior from propagation, diffusion, or even potential fields. The challenges here come from

- the different types of data we handle: such as seismic compressional waves in exploration geophysics for structural images, trapped and surface waves in seismology, electric and/or magnetic diffusive fields for crustal and lithosphere modelling and imaging;
- the various types of media we have to consider: such as marine environments with a liquid/ solid interface, sedimentary basins with shallow, very low velocity structures, foothill complex zones with velocity inversion, complex topography, and resistivity variations of several orders of magnitude;
- the lack of precise knowledge of the geological structures;
- the modelling scale: in seismics, a wave can be recorded after having propagated over hundreds of wavelengths; in controlled source electromagnetics, the electric and magnetic fields are recorded over at least five orders of magnitude and after having diffused over several skin depths; in exploration, the depth of investigation is several kilometres with a resolution of tens to hundreds of metres; and in global seismology, the investigation zone is in hundreds of kilometres and the resolution is in kilometres;

- the computational cost, especially when the modelling represents just the kernel of a parameter inversion scheme.

In this review, we provide an overview of some of the important numerical methods for solving PDEs in the context of continuum mechanics. For complex heterogeneous media imaging, these local equations are better suited than integral equation methods (Hohmann 1983). Whatever the approach, we need spatial and time/ frequency discretisation for numerical computation. Decomposition of the unknown fields with curvelets, beamlets or other similar wavelets, can lead to some mixed representations; however, we do not discuss these here. We specifically consider three different ways of finding the numerical solution:

- **The spectral formulation:** the PDEs are first formulated in dual spaces, as for example the space Fourier domain, where partial derivatives are translated into algebraic forms. The difficult (and not always possible) step is the expression of the boundary conditions when necessary, as well as the excitation conditions, in this new space. However, sometimes it can ease the expression of source excitation; e.g., plane-wave excitation in magnetotellurics.
- **The strong formulation:** the PDEs should be verified specifically on discrete points on which the continuum is interpolated, or their integral forms should be satisfied. We will discuss spatial discretisation with spatial global and local supports, each of which has specific advantages.
- **The weak formulation:** the PDEs should be verified globally over elements that use a discrete norm for the solution. While this method might be quite general and can include the strong formulation by using a specific norm through a Dirac comb (using operators as distributions), we will restrict ourselves to the standard Galerkin approach, where the test functions are identical to the basis functions on which the expected solution is expanded. We will consider continuous as well as discontinuous formulations (Zienkiewicz and K. Morgan 1983).

In section 2, we introduce the main equations and make some preliminary comments. Spectral methods are presented in section 3, and these have been the methods of choice for waveform imaging of the global Earth (Woodhouse and Dziewonski 1984). Section 4 is devoted to the strong formulation with pseudo-spectral methods, finite-difference methods, and finite-volume methods; all of these are widely used in seismic and electromagnetic FWI, without forgetting seismic RTM. Section 5 then introduces the popular finite-element methods in the framework of the weak formulation. Although these are heavier than the previous methods from the point of view of computer resources, they start to be used at different scales for FWI (Askan *et al.* 2007; Tape *et al.* 2009). The advantages and disadvantages of continuous and discontinuous approaches are discussed. In section 6, some of the current applications are listed, in section 7, the imaging requirements that can influence our modelling choices are presented, and finally, in section 8, we summarise our conclusions.

2 THE EQUATIONS AND SOME EARLY COMMENTS

The equations used in elastodynamic and electromagnetic modelling can be written either as first-order systems or as second-order systems. The second-order systems contain fewer unknowns, which provides a numerical advantage despite the more complex structure of the numerical system. Also, a parsimonious approach can be used after discretisation of a first-order system, to reduce the number of unknowns (Luo and Schuster 1990), which leads to a system that is equivalent to a discrete second-order system.

2.1 The time-domain approach

In this review, we assume the earth parameters independent of time.

The velocity-stress first-order elastodynamic equations are

$$\begin{cases} \rho \partial_t v_i = \partial_{x_j} \sigma_{ij} + f_i^v; \\ \partial_t \sigma_{ij} = c_{ijkl} \partial_{x_l} v_k + f_{ij}^\sigma. \end{cases} \quad (1)$$

Here, v_i are the components of the velocity vector, σ_{ij} the components of the stress tensor, c_{ijkl} the components of the stiffness tensor, ρ the density, and f_i^v and f_{ij}^σ the components of the force source vector and the moment rate source tensor, respectively. (The Einstein convention on repetitive indexes is used.)

The first-order electromagnetic wave equations are

$$\begin{cases} \mu \partial_t \mathbf{h} = -\nabla \times \mathbf{e} + \mathbf{f}^h; \\ \varepsilon \partial_t \mathbf{e} - \sigma = \nabla \times \mathbf{h} + \mathbf{f}^e. \end{cases} \quad (2)$$

Here, \mathbf{e} is the electric vector, \mathbf{h} is the magnetic vector, σ the conductivity, μ the magnetic permeability, ε the dielectric permittivity, and \mathbf{f}^h and \mathbf{f}^e the magnetic and electric source vectors, respectively.

The displacement second-order elastodynamic equation is

$$\rho \partial_{tt} u_i = \partial_{x_j} c_{ijkl} \partial_{x_l} u_k + f_i, \quad (3)$$

where the components of the displacement vector are denoted by u_i .

The second-order electromagnetic equation for the electric field is

$$\varepsilon \partial_{tt} \mathbf{e} + \sigma \partial_t \mathbf{e} + \nabla \frac{1}{\mu} \times \nabla \mathbf{e} = \mathbf{f}, \quad (4)$$

with an equivalent equation for the magnetic field.

Both the first-order and the second-order equations should be complemented with their initial conditions. We generally assume that the fields and their time derivatives are zero at negative times. Boundary conditions also need to be added, as we are modelling inside a finite computational domain. In elastodynamics, at the free surface the traction is zero, so

$$\sigma_{ij} n_j = 0, \quad (5)$$

where n_i are the components of the vector normal to the free surface.

In electromagnetism, perfectly electrically conducting boundary conditions are currently implemented, such that

$$\mathbf{e} \times \mathbf{n} = 0 \quad \text{and} \quad \mathbf{h} \cdot \mathbf{n} = 0, \quad (6)$$

where \mathbf{n} is the vector normal to the boundary.

Other boundary conditions come from the limited numerical domain: absorbing boundary conditions need to be implemented as surface conditions (Clayton and Engquist 1977) in relation to the radiation conditions or layer conditions, as the now popular perfectly matched layer (PML) technique (Bérenger 1994; Chew and Weedon 1994) for electromagnetism and for elastodynamics (Chew and Liu 1996; Drossaert and Giannopoulos 2007; Komatitsch and Martin 2007). Due to the discretisation, the PML conditions are not perfect, although they are relatively efficient, and they limit the size of the PML zone while maintaining its efficiency, and long-term stabilities still need to be better understood (Collino and Tsogka 2001; Bécache *et al.* 2004)

The time and spatial discretisations are often treated separately. Before discussing the spatial discretisation scheme, let us formulate the PDEs in a general framework. The systems to be solved can be cast in a matrix form. For the first-order system with the unknown vector \mathbf{p} , we have

$$\mathbf{M} \partial_t \mathbf{p} + \mathbf{K} \mathbf{p} = \mathbf{S} \mathbf{p} + \mathbf{f}, \quad (7)$$

and for the second-order system with the unknown vector \mathbf{p}' , we end up with

$$\mathbf{M}' \partial_{tt} \mathbf{p}' + \mathbf{K}' \partial_t \mathbf{p}' = \mathbf{S}' \mathbf{p}' + \mathbf{f}', \quad (8)$$

where the vectors \mathbf{f} and \mathbf{f}' represent the excitation. Usually, the matrices \mathbf{M} and \mathbf{M}' , which are often called the mass matrices, describe the inertial terms and the matrices \mathbf{K} and \mathbf{K}' describe the viscous terms. The matrices \mathbf{S} and \mathbf{S}' are often called the stiffness matrices, and they correspond to the discretisation of the spatial derivatives and contain the material properties of the wave equations and Maxwell equations. Let us consider first-order systems.

The behaviour of the system greatly depends on the relative importance of \mathbf{M} and \mathbf{K} . If \mathbf{K} is 'small', the inertial terms are dominant and the system is principally a propagation system. With $\mathbf{K} = 0$, the system is a hyperbolic system. This is the case with elastodynamic systems or with electromagnetic systems in the air or at high frequencies. If \mathbf{M} is 'small', the viscous terms are dominant and the system is principally a diffusive system; e.g., electromagnetic systems at low frequencies. We can proceed through a time marching approach for solving these PDEs iteratively. With a propagation system, the Courant-Friedrickson-Lewy (CFL) stability condition (Courant *et al.* 1967) leads to time discretisation that is proportional to the space discretisation, making the explicit time-marching method relatively attractive. With a diffusive system, the CFL condition provides time discretisation that is proportional to the square of the space discretisation, here making the explicit time-marching method less attractive. DuFort and Frankel (1953) proposed a scheme that allows us to improve the CFL condition by effectively adding a propagative term in the discrete schemes. However, the implicit schemes, such as the simple backward Euler scheme, constitute the logical approach. This means solving a linear system at each time step. At early times, the time stepping should still be small enough to represent the solution correctly. Fortunately, the diffusive nature of the system allows us to increase the time stepping during the computation.

With first-order systems, and especially with propagation systems, leapfrog time integration is often implemented to obtain a conditionally stable scheme; a first-order forward

time derivation directly applied to the equation (7) leads to an unstable scheme (LeVeque 2002). The leapfrog time derivation approach updates the stress and displacement, or the electric and magnetic fields, sequentially. Sometimes, instabilities are encountered when dealing with dissipation terms and there is the need to use implicit time schemes. With second-order systems, a central second-order time derivative is generally used, and this allows explicit marching with two previously estimated fields for the computation of the next one. Higher-order time integration, such as the Lax-Wendroff scheme (Dablain 1986), the higher-order scheme known as the arbitrary accuracy derivative Riemann problem (ADER) scheme (Toro 2009), and the Runge-Kutta schemes (Cockburn 2003), have been proposed for hyperbolic systems. In certain cases, spectral integration with an arbitrary precision can even be adopted (Tal-Ezer *et al.* 1990; Mikhailenko *et al.* 2003).

2.2 The frequency-domain approach

Systems (7) and (8) can be written in the frequency domain as

$$(-i\omega\mathbf{M} + \mathbf{K} - \mathbf{S})\mathbf{p} = \mathbf{f}; \quad (9)$$

and

$$(-\omega^2\mathbf{M}' - i\omega\mathbf{K}' - \mathbf{S}')\mathbf{p}' = \mathbf{f}', \quad (10)$$

where ω is the angular frequency, and i the pure imaginary number with $i^2 = -1$. (For simplicity, we use the same symbols for the fields in the time and in the frequency domains.) The structure of the linear system is different for the propagation equations and the diffusive equations. Indeed, the propagation system leads to an indefinite system, namely a system with (large) negative and positive (real part of the) eigenvalues, limiting the efficiency of the iterative approach for solving it. A preconditioner based on a damped wave equation and a multi-grid cycle has been proposed, to speed up the convergence of the iterative approach (Erlangga *et al.* 2006; Plessix 2007). Direct solvers based on LU decomposition are an alternative (Marfurt 1984; Operto *et al.* 2007). The sparse matrix of a linear system has, however, a large bandwidth, meaning that direct solvers in 3D require an extremely large amount of memory. On the contrary, a linear system associated with the diffusion equations can be efficiently solved with an iterative method (Mackie *et al.* 1993; Newman and Alumbaugh 1999; Haber *et al.* 2000; Aruliah and Ascher 2003; Mulder 2006).

In the following sections, we principally discuss the spatial discretisation that generally applies to both time-domain and frequency-domain formulations. However, our presentation of the spectral formulation mainly concerns the frequency-domain formulation.

3 SPECTRAL FORMULATION

By moving to a dual domain such as the space Fourier/wavenumber domain, we can efficiently transform partial spatial derivatives into products. We can even go to the time Fourier domain, which gives us the algebraic dispersion relation. Analytical or semi-analytical solutions can be worked out using the Cagniard-De Hoop path in the

frequency-wavenumber domain if it is possible to construct it (Cagniard 1962; de Hoop 1960; Aki and Richards 2002). When the media variations become too complex, we can expand the solution on special functions, which forms a complete basis as a relatively compact description when the medium is smooth. When boundaries exist, simple geometries such as spherical/ ellipsoidal shapes can still lead to semi-analytical solutions, while more complex shapes are handled by numerical techniques. The medium is decomposed into simple domains where the fundamental solution is obtained through a linear combination of elementary solutions that form a complete basis, which is often expressed in a transformed domain. When the boundary conditions are satisfied by each elementary solution, they will be automatically satisfied by the solution wanted, due to the linearity of the problem. These methods are often expressed in the frequency-wavenumber space, although some of them are in the time domain (Wheeler and Sternberg 1968).

The restriction to laterally invariant 3D media provides a dramatically efficient and accurate method, as only a few nodes are required in the discretisation of boundaries in the vertical direction (one point per layer). The solution is decomposed in plane waves with a constant wavenumber vector \mathbf{k}_h . After the Fourier transform over the time and the horizontal coordinates, the first-order equation is

$$\frac{d\tilde{\mathbf{p}}}{dz} = i\omega\mathbf{A}\tilde{\mathbf{p}} + \tilde{\mathbf{f}}\delta(z - z_s), \quad (11)$$

where \mathbf{A} is the propagator matrix that depends on the earth parameters and the horizontal wavenumber, $\tilde{\mathbf{p}}$ the field vector, $\tilde{\mathbf{f}}$ the source vector, and z_s the source depth. The variables with tilde depend on the angular frequency, ω , the horizontal wavenumber, \mathbf{k}_h , and the depth, z . With the acoustic-wave equation, for instance, $\tilde{\mathbf{p}}$ is formed by the vertical displacement and the pressure, and the propagator matrix is equal to

$$\mathbf{A}(z) = \begin{bmatrix} 0 & \frac{k_h^2(z)}{\rho(z)\omega^2} - \frac{1}{\kappa(z)} \\ -\rho(z) & 0 \end{bmatrix}, \quad (12)$$

where the density is denoted by ρ and the bulk modulus by κ .

This linear system can be diagonalised in each layer by finding the eigenvalues and eigenvectors of the matrix \mathbf{A} , which leads to two independent upwards and downwards plane-wave solutions. The solution can then be propagated by generalised reflection/ transmission coefficients from the source to the free surface, where free-surface boundary conditions are applied. Then, the solution is moved back down to the bottom half-space, where the radiation condition is applied, which builds up the final solution. When considering sources at various depths, the method is as efficient as a substitution technique. This technique was developed in elastodynamics (Spencer 1960; Kennett 1983), as well as in diffusive electromagnetism (Cagniard 1953; Wannamaker *et al.* 1984). To model the magnetotelluric response, the source terms are introduced as plane-wave boundary conditions on the top of the model (Wannamaker *et al.* 1984).

There are similar procedures for laterally varying media, although these are more computer intensive. Potentialities for imaging can be considered with the fast moment method (FMM), which dramatically reduces the memory requirements. The solution is efficiently found iteratively for

each source (see Chaillat *et al.* (2008) for applications to elastodynamics). Therefore, we can foresee that the FMM (which requires few computer resources for modelling) could be a tool for imaging techniques that has not been explored yet, as far as we know, with open questions remaining as to the reliability of the method for complex structures.

4 STRONG FORMULATION

Nowadays, scientific challenges concern complex zones of the earth with rapid spatial variabilities in the medium properties. Spectral methods are often inadequate. When considering PDEs, we can consider volumetric discretisation of the medium properties, and the fields wanted should be similarly discretised. We can consider global spatial discretisation (which is often presented as a modal approach), such as pseudo-spectral methods where the partial derivatives are estimated by going back and forth in the dual domain (e.g., Fourier, Legendre or Chebychev domains), which leads to specific regular/ non-regular sampling (Kosloff and Baysal 1982; Druskin and Knizhnerman 1988; Seriani and Priolo 1994; Priolo *et al.* 1994). We can also consider spatial discretisation with local support, and more specifically, the finite-difference method that is widely used in many fields (Levander 1988; Mackie *et al.* 1993; Robertsson *et al.* 1994; Newman and Alumbaugh 1999; Pitarka 1999; Taflove and Hagness 2000; Moczo *et al.* 2007). The finite-volume methods go one step further, which allows a more accurate description of the medium while keeping the simple geometrical construction of the finite-difference method (LeVeque 2002). However, this often leads to a low-order scheme. In the strong formulation, the PDEs need to be exactly satisfied at collocation points or at elementary domains of the volumetric mesh that describes the model space.

4.1 The pseudo-spectral and finite-difference methods

Volumetric discretisation of the PDEs has been considered in many studies for the solving of efficiently linear propagation or diffusion. Differences come from the geometry of the mesh associated with the selected spatial interpolation functions.

The solution vector $\mathbf{p}(\mathbf{x})$ where we ignore the time or frequency variation can be approximated through an expansion using basis functions, ψ_j , as

$$\mathbf{p}(\mathbf{x}) = \sum_{j=1}^N \mathbf{p}(\mathbf{x}_j) \psi_j(\mathbf{x}), \quad (13)$$

where the nodes \mathbf{x}_j define the collocation points at which the PDE has to be satisfied. The total number of these nodes is denoted by N . Multi-dimensional elementary functions $\psi_j(\mathbf{x})$ are selected according to the spatial support we consider. Often, we rely on tensorial descriptions over dimensions. Global support for Fourier polynomials with regularly spaced collocation points or Chebyshev polynomials with irregularly spaced collocation points (Kosloff and Baysal 1982; Kosloff *et al.* 1990; Tessmer and Kosloff 1994) provide the pseudo spectral methods (PSMs). These lead to a dramatic reduction in the unknowns at the expense of interactions between nodes, which can be a critical issue for imaging;

any misestimation of properties and/or fields has an impact everywhere. Local support with Lagrange polynomials leads to the finite-difference method (FDM), which is popular because of its simplicity and its efficiency.

The approximate derivative along one direction x_i is obtained through the application of a matrix \mathbf{D} to the discrete field values $\mathbf{p}(\mathbf{x}_j)$ at collocation points \mathbf{x}_j :

$$\frac{\partial \mathbf{p}}{\partial x_i}(\mathbf{x}_l) = \sum_{j=1}^N \mathbf{p}(\mathbf{x}_j) \psi'_j(\mathbf{x}_l), \quad (14)$$

where the components of the matrix are $\mathbf{D}_{lj} = \psi'_j(\mathbf{x}_l)$. This transformation is sometimes called a stencil. Higher derivatives can be constructed by repetitively applying \mathbf{D} . With global support (PSM), the cost of computing the derivatives is $O(N^2)$ operations from matrix multiplication, or $O(N \log N)$ by spectral estimation through direct and inverse FFT. With local support (FDM), this leads to the following stencil:

for the first-order derivative with regular spacing Δ

$$\partial_x \mathbf{p} = \sum_{n=1}^{K/2} \frac{a_n}{2\Delta} (\mathbf{p}(x + n\Delta) - \mathbf{p}(x - n\Delta)); \quad (15)$$

and for the second-order derivative

$$\partial_{xx} \mathbf{p} = \sum_{k=0}^{K/2} \frac{a_k}{\Delta^2} (\mathbf{p}(x + k\Delta) + \mathbf{p}(x - k\Delta)), \quad (16)$$

where K is the order of the scheme, and a_k are coefficients to determine.

For FDM, the cost of computing the derivative is reduced at the expense of the precision, and therefore of the accuracy of the solution, as the order K is often much smaller than the number of nodes N . The collocation density or the mesh discretisation must be increased when considering short spatial support. A fourth-order stencil is considered to be optimal for a second-order time integration. Higher-order stencils (e.g., tenth-order) can, however, provide drastic computational time and core memory reductions that are crucial for 3D simulations, although at the expense of accuracy in non-smooth media (Dablain 1986). Optimal design of the matrix \mathbf{D} (i.e. optimal choice of the coefficients a_k), in association with the definition of the collocation points, has been an endless investigation with this strong formulation. The main purpose has been the reduction of the numerical dispersion (Marfurt 1984; Holberg 1987; Operto *et al.* 2007), through looking at the spatial shape of the stencil (Saenger *et al.* 2000), the spectral shape of the derivative operator (Jo *et al.* 1996; Hustedt *et al.* 2004), or the minimisation of the residual energy through the Rayleigh-Ritz variational investigation (Takeuchi and Geller 2000). These efforts are relatively specific to acoustic and elastic propagation modelling. In diffusive electromagnetism, second-order spatial derivatives are generally sufficient, as they already lead to large grid spacing compared to the desired earth discretisation.

Regular cartesian grids are often associated with the FDM because of its efficiency. Stretching the collocation points in relation to strong gradients of the medium properties might drastically reduce solution errors for both global and local supports at the expense of computer resources; e.g., FDM approaches have been extended to irregular grids for seismic

propagation (Moczo 1989; Jastram and Tessmer 1994; Aoi and Fujiwara 2001; Wang *et al.* 2001). In diffusive electromagnetics, stretched grids are very common, especially in the depth direction, because of the strong field attenuation. We can consider that the FDM generally performs better on smooth media, especially when we consider high-order stencils and coarse grids, for speeding up the forward modelling. Reductions in modelling costs have been achieved through the introduction of the staggered grid approach. The components of the solution vector \mathbf{p} are not defined at all of the nodes of the grid, which reduces the size of the field vector without damaging the dispersion of the scheme (Yee 1966; Virieux 1986). Some difficulties can appear with free boundary conditions and anisotropy, which require interpolation of some fields. This approach turns out to be stable at boundaries between solids and liquids. An alternative partial grid approach, as proposed by Saenger *et al.* (2000), mitigates the difficulties related to free boundary conditions and anisotropy, while the full grid approach (Tam and Webb 1993) will still be required for long-term stability conditions at the free surface (Lombard and Piraux 2004; Lombard *et al.* 2008). An approach based on Lebedev's grid has been proposed, to handle anisotropy (Davydycheva and Druskin 1999; Lisitsa and Vishnevsky 2010).

Whatever method we choose for the spatial discretisation, we end up with an evolution system in the time domain (systems (7) or (8)), or a linear system in the frequency domain (systems (9) or (10)). In the frequency domain, the efficiency of a direct solver depends on the bandwidth of the matrix of the linear solver. High-order stencils along one dimension considerably increase this bandwidth. The compactness of the stencil is a critical issue. With acoustic-pressure second-order wave equations, almost fourth-order compact schemes have been proposed through the optimal reduction of the dispersion of the scheme in the frequency band of the forward modelling (Marfurt 1984; Stekl and Pratt 1998; Operto *et al.* 2007), which leads to this very compact system,

$$\frac{-\omega^2}{v^2} a_0 p(x, y, z) + \sum_{k=-1}^1 \sum_{l=-1}^1 \sum_{m=-1}^1 \frac{a_{k,l,m}}{\Delta} p(x+k\Delta, y+l\Delta, z+m\Delta), \quad (17)$$

where a_0 , $a_{k,l,m}$ are the coefficients to be determined following rules mentioned above. This scheme involves only neighbouring points, and does not increase the bandwidth of the linear system, as compared to the standard second-order scheme, and it leads to an 'optimal' tool for acoustic forward modelling for seismic imaging when a frequency-domain direct solver is used.

4.2 The finite-volume methods

One of the limitations of standard finite-difference methods comes from the earth discretisation on rectangular regular or irregular grids, which prevents efficient representation of non-flat interfaces. This limitation can be eliminated when we work with the integral form of the PDEs. This idea consists of writing the PDEs in a first-order (pseudo) conservative form, and taking the integral over the computational domain. In certain cases, this integral form of the PDEs can be obtained directly from the physical conservation laws. The local lower-order interpolation of the fields allows an

intuitive construction, which leads to the success of this formulation. We proceed through a geometrical interpretation, rather than through a variational approach. This technique appears to have the flexibility to describe the medium using complex meshing, while retaining the simple approach of the FDM. The so-called grid method, which was introduced by Zhang and Tielin (1999) and is based on local integration of elastodynamics, and the finite-integration technique, which is based on local integration of Maxwell's equations (Clemens and Weiland 2001), follow similar strategies and can be considered as finite-volume methods. As Clemens and Weiland (2001) considered regular rectangular grids, the technique collapses into a FDM approach, although arbitrary grids might have been considered. The equivalence of a finite-volume approach over a regular rectangular grid and a FDM was noted by Brossier *et al.* (2008) in the frequency domain.

The finite-volume method starts with the decomposition of the computation domain, Ω , into a set of subdomains, Ω_e , here called finite volumes: $\Omega = \cup_e \Omega_e$. Let us consider the equation

$$\mathbf{M} \partial_t \mathbf{p} = \mathbf{A}^k \partial_{x_k} \mathbf{p} + \mathbf{f}, \quad (18)$$

where $k = 1, 2, 3$ is an index over the spatial directions, and \mathbf{A}^k the matrices containing the earth parameters. Equation [code for equation 18 please] corresponds to equation 7 before spatial discretisation and with the viscous term $\mathbf{K} = 0$. Assuming \mathbf{A}^k is constant, the integral form of equation [code for equation 18 please] over a volume Ω_e is simply:

$$\int_{\Omega_e} d\mathbf{x} \mathbf{M}_e \partial_t \mathbf{p}_e = \int_{\Omega_e} d\mathbf{x} \partial_{x_k} (\mathbf{A}_e^k \mathbf{p}_e) + \int_{\Omega_e} d\mathbf{x} \mathbf{f}_e, \quad (19)$$

where \mathbf{M}_e and \mathbf{A}_e^k are the matrices associated with the volume e , \mathbf{f}_e the source, and \mathbf{p}_e the fields.

We transform the volume integral containing the spatial derivatives to a surface integral through the divergence (Gauss) theorem. This gives the following equation,

$$\int_{\Omega_e} d\mathbf{x} \mathbf{M}_e \partial_t \mathbf{p}_e = \int_{\partial\Omega_e} d\mathbf{x} \mathbf{A}_e^k \mathbf{p}_e n_k^e + \int_{\Omega_e} d\mathbf{x} \mathbf{f}_e, \quad (20)$$

where n_k^e are the components of the normal to the boundary $\partial\Omega_e$.

In the finite-volume approach, we work with the field volume averages per volume; these are discontinuous at the boundary $\partial\Omega_e$. Indeed, the surface integral relates to (numerical) fluxes, $\mathbf{A}^k \mathbf{p}$, between the adjacent volumes. With $\partial\Omega_e = \cup_{e' \in V_e} \Gamma_{e,e'}$ and V_e the set of the adjacent volumes to the volume e , we can write the equation [code for equation 20 please] as (LeVeque 2002)

$$\mathbf{M}_e \partial_t \mathbf{p}_e = \sum_{e' \in V_e} \int_{\Gamma_{e,e'}} d\mathbf{x} \phi_{e,e'}^k(\mathbf{p}_e, \mathbf{p}_{e'}) n_k^{e,e'} + \mathbf{f}_e, \quad (21)$$

where \mathbf{p}_e and \mathbf{f}_e are now volume averages and $\phi_{e,e'}^k$ the flux through the boundary $\Gamma_{e,e'}$ between the volumes e and e' that depend on \mathbf{p}_e and $\mathbf{p}_{e'}$, and $\mathbf{n}^{e,e'}$ the normal to $\Gamma_{e,e'}$, with $\mathbf{n}^{e,e'} = -\mathbf{n}^{e',e}$. As only the fluxes are shared on the boundary of each finite volume, material and field discontinuities can be handled. Finite-volume approaches differ in the flux approximations and the time-integration schemes. Note that we can develop a similar approach in

the frequency domain. On the boundary of the computation domain, Ω , specific fluxes need to be defined to take into account the boundary conditions (LeVeque 2002).

There are two main strategies to define the fluxes: the centred flux between two adjacent elements; or the disymmetrical flux based on physics. The centred flux is simply obtained by averaging the flux components between two adjacent elements, which gives a symmetrical estimation. On rectangular regular grids, this returns to the scheme obtained by centred finite differences. This strategy has useful conservative properties and can be applied to non-hyperbolic systems. However, it can induce numerical errors when sharp variations or discontinuities are expected in the field.

With a hyperbolic system, we can use its propagative nature to define the disymmetrical fluxes. This is obtained by solving the Riemann problems using Godunov's approach and upwind fluxes (LeVeque 2002). The fluxes are then determined according to the local propagation directions of the waves. While sharp variations and discontinuities are well handled, this approach leads to a dissipative scheme. Important improvements have been performed since the study of Roe (1981), with the propagation of discontinuities: the initial approach is only first-order and has large numerical dispersion. Higher-order schemes can be obtained with the Lax-Wendroff approach, or with its extensions, that are associated with generalised (derivative) Riemann solvers that give the ADER method (Toro 2009). Some of these high-order schemes create oscillations around discontinuities. Slope limiters or (weighted) essential non-oscillatory schemes have been proposed. These approaches are generally not applied in seismic or electromagnetic modellings in geophysics.

The quality of the solution depends on the meshing. Small meshes and meshes with poor aspect ratios can significantly affect the numerical solution. The time evolution is controlled by the smallest element of the medium. The resolution of the linear system in the frequency domain can provide difficulties with respect to the different sizes of the elements. The meshing strategy is in fact shared by both the finite-volume and the finite-element methods, and it is the common bottle-neck of forward modelling.

5 WEAK FORMULATION

Despite their advantages, the discretisation methods discussed so far reach their limits in complex geological settings when the geometry of the interfaces have predominant roles in the recorded data: very fine discretisation is required for accuracy, which can lead to relatively expensive and inefficient simulations, as this fine discretisation impacts upon the whole domain. High-order differential stencils based on overlapping elements/ meshes and high-order finite-volume methods are questionable. The finite-element method based on the weak formulation of the PDEs appears to give us more freedom to adapt the discretisation to particular geometries.

The weak formulation is obtained by multiplying the PDEs by test functions (unlike the finite-volume methods), by integrating over a given domain, and by carrying out an integration that in part reduces the derivation order of the fields wanted (which weakens the derivability conditions by

transferring them to the test functions) (Zienkiewicz and K. Morgan 1983; Brenner and Ridgway Scott 2008; Hesthaven and Warburton 2008). As the weak formulation has an integral form like the finite-volume methods, we can decompose the total integration volume into small domains, which are also called elements, of a-priori arbitrary shapes; the integral over the total domain is the sum of the integrals over the small domains. The introduction of test functions gives us the extra freedom to develop high-order schemes without overlap between the elements. However, it has a numerical cost, since the mass matrix often becomes non-diagonal; this is a drawback when comparing this with the strong formulation with an explicit time scheme. The choice of the test functions together with the representation of the field inside the domains determine the type of finite-element methods. Classically, the fields and the test functions are functions of the same space: this corresponds to the Galerkin formulation. When the test functions are defined through the values on a given set of nodes, we speak about the nodal approach. In practice, in the nodal approach, the test functions are the product of Lagrange polynomials. When test functions are global polynomials in the element, we speak about the modal approach. The (maximum) degree of the polynomials gives the order of the element. In this review, we consider two approaches: the continuous Galerkin finite-element method (CGFEM); and the discontinuous Galerkin finite-element method (DGFEM). The purpose is not to describe here all of the developments in finite-element methods, as the literature has become too numerous over the last 50 years, but to give some highlights that can help the reader.

5.1 The continuous Galerkin finite elements

With the (classic) CGFEM approach, the fields involved in the differential equations are assumed to be continuous in the entire computation domain. They are decomposed on a local piece-wise functional basis, which is also used for the test functions. To highlight the main features of the CGFEM, we consider the displacement second-order wave equations (3). The weak form is obtained by multiplying these equations by the test functions, \mathbf{w} , and by integrating over the computation domain Ω (w_i are the components of \mathbf{w} and Einstein's convention on repetitive indices), as

$$\int_{\Omega} d\mathbf{x} \rho \partial_{tt} u_i w_i = \int_{\Omega} d\mathbf{x} \partial_{x_j} \sigma_{ij} w_i + \int_{\Omega} d\mathbf{x} f_i w_i \quad (22)$$

and integrating by parts, assuming continuous test functions and fields,

$$\int_{\Omega} d\mathbf{x} \rho \partial_{tt} u_i w_i = - \int_{\Omega} d\mathbf{x} \sigma_{ij} \partial_{x_j} w_i + \int_{\partial\Omega} d\mathbf{x} \sigma_{ij} w_i n_j + \int_{\Omega} d\mathbf{x} f_i w_i \quad (23)$$

where n_j are the components of the vector normal to the boundary $\partial\Omega$.

At the free-surface boundaries, the surface integral on the righthand side is zero. This integral is also zero when the test functions can be chosen as null on the boundary conditions (Dirichlet conditions). This is one of the advantages of the CGFEM: the free-surface boundary condition is intrinsically satisfied, which allows precise modelling of the surface waves. More complicated boundary conditions can also be handled explicitly through the boundary integral. From here

on, this surface contribution is taken as zero.

In the discrete formulation, the test function space is of finite dimension; it can be represented by P basis functions. We call w_i^p the components of the p basis function. In this CGFEM approach, as the fields and test functions are part of the same function space, we have

$$u_i(\mathbf{x}, t) = \hat{u}_i^p(t) w_i^p(\mathbf{x}); \quad (24)$$

and

$$\sigma_{ij} = \sum_k c_{ijkl} \hat{u}_k^p(t) \partial_{x_l} w_k^p(\mathbf{x}). \quad (25)$$

We can then rewrite equation (23) as

$$\int_{\Omega} \sum_i d\mathbf{x} \rho w_i^p w_i^q \partial_{tt} \hat{u}_i^p = - \int_{\Omega} \sum_i d\mathbf{x} c_{ijkl} \hat{u}_i^p \partial_{x_l} w_k^p \partial_{x_j} w_i^q + \int_{\Omega} \sum_i d\mathbf{x} \rho w_i^p \partial_{tt} \hat{u}_i^p. \quad (26)$$

The computational domain is decomposed into elements, ($\Omega = \cup_e \Omega_e$). For each element, we obtain the semi-discrete system from equation 26:

$$\mathbf{M}_e \partial_{tt} \hat{\mathbf{u}}_e = \mathbf{S}_e \hat{\mathbf{u}}_e + \mathbf{f}_e, \quad (27)$$

where \mathbf{M}_e , \mathbf{S}_e are the mass and stiffness matrices of the element e , respectively, and $\hat{\mathbf{u}}_e$ and \mathbf{f}_e the field and source vectors, respectively.

The total unknown vector, $\hat{\mathbf{u}}$, is formed with all of the components \hat{u}_k^p , which are sorted according to a given numbering procedure. In the CGFEM, the elements share the field values at the faces, edges and corners of the elements. Therefore, the field vector of the element e shares component elements with the field vectors of the neighbouring elements, forcing the continuity of the fields at the edges of the elements. The system satisfied by $\hat{\mathbf{u}}$ has the form of system (8). Assembly of the matrices \mathbf{M}_e and \mathbf{S}_e gives the (total) mass and stiffness matrices, \mathbf{M} and \mathbf{S} , respectively. The mass matrix is not diagonal in the general case, because \mathbf{M}_e is a priori not diagonal and because of the assembling. It can have a large bandwidth. It is, however, a sparse matrix. In the frequency domain, the CGFEM leads to system (10). Similar results are obtained with the electromagnetic wave equations. In this formulation, the earth parameters can vary in each element. This variability of the earth parameters in each element has to be taken into account in the computation of the integrals that define the mass and stiffness matrices. With the nodal approach and a Gaussian quadrature technique, this can be achieved easily by defining the earth parameters at the nodes of the test functions.

We have considered only one test function space here. To more accurately represent the derivatives of the fields, we can use a different test function space per equation of the system. This leads to the so-called mixed-element methods (Nédélec 1980; Stenberg 1988). This idea resembles the staggered-grid idea of the FDM. This is used, for instance, with the first-order elastodynamic wave equation to more accurately compute displacement and stress (Bécache *et al.* 2002), or with the electromagnetic equations to handle the divergence operator and the possible discontinuity of the normal components via the so-called edge elements, and then to avoid some spurious numerical modes that arise from medium discretisation (Hiptmair 2002; Monk 2003).

The conditioning of the mass matrix, \mathbf{M} , depends on the shapes of the elements. Badly shaped elements, e.g., very

elongated elements, lead to a poorly conditioned system and can create numerical instability. This is one of the difficulties of the meshing, which needs to avoid elements with too large an aspect ratio. The condition number of \mathbf{M} also depends on the choice of the test functions; in the nodal approach, this is seen as the choice of the location of the nodes in the element. For high-order elements, equidistant nodes lead to poor condition numbers, and in practice only non-equidistant nodes are used, and especially nodes based on the Gauss-Lobato points with quadrant or hexagonal elements (Cohen 2002). While it is not a real drawback with frequency-domain formulation or with an implicit time scheme (as in diffusive electromagnetics), with an explicit time scheme, the solving of a non-diagonal system at each time step can limit the usefulness of the approach. The remedy here is to apply a mass-lumping technique: namely, to replace the mass matrix with a diagonal matrix built by summing all of the elements of a line onto the diagonal (Cohen 2002). This simplification is not always accurate, and therefore careful choice of the quadrature and the nodes is required. This approach is often adequate with Gauss-Lobato points and a Gaussian quadrature. The spectral element method, which is often used in seismology, is developed in Komatitsch and Vilotte (1998); Chaljub *et al.* (2007), and used the Gauss-Lobato-Legendre integration technique to obtain a diagonal mass matrix with a high-order quadrant in 2D and a hexagonal in 3D elements. Aside from the property of a diagonal mass matrix, this leads to spectral convergence behaviour in space.

For practical applications, the meshing needs to be adapted to the earth structure, with generally fine meshes in complex zones or in zones with low velocity or low resistivity, in order to speed up the computation. With the CGFEM, grid adaptation (also called h-refinement) is regularly used. However, because elements share information through the nodes that are on the boundaries, it is complicated to use different types of elements, and especially different element orders (the so-called p-refinement). This sometimes limits the flexibility of the method, especially when high-order elements would be needed in most of the domain to gain efficiency.

5.2 The discontinuous Galerkin finite elements

Some of the limitations of the CGFEM approach can be addressed by the DGFEM, including, as already mentioned, when some of the field components need to be discontinuous across interfaces. In CGFEM, forcing the continuity of the test functions can introduce some spurious artificial modes. Relaxing the continuity of the test functions helps to better represent the fields. The p-refinement can also be easily handled with DGFEM. DGFEM approaches are, however, not a replacement for the classic Galerkin approaches, because they also suffer from numerical complications.

To discuss the main features of DGFEM, let us consider the hyperbolic first-order wave equation as for the finite volume. We also decompose the computational domain Ω into elements, Ω_e as previously. The weak form is obtained by multiplying the equations by the test functions \mathbf{w}^q . These test functions, together with the fields, are a priori not continuous at the boundaries of the element. Therefore, after integration in parts, the weak form in the element Ω_e is

(Hesthaven and Warburton 2008):

$$\int_{\Omega_e} d\mathbf{x} \mathbf{M}_{ij} \partial_t p_{ej} w_i^q = - \int_{\Omega_e} d\mathbf{x} p_{ej} \partial_{x_k} (\mathbf{A}_{ij}^k w_i^q) + \int_{\partial\Omega_e} d\mathbf{x} \phi_{ei}^k n_k^e w_i^q \quad (28)$$

with the numerical flux

$$\phi_{ei}^k = \mathbf{A}_{ij}^k p_{ej}. \quad (29)$$

On the boundary $\partial\Omega_e$, the numerical flux is not known because the fields are discontinuous. As with finite-volume methods, the main difference between the different DGFEMs is in the numerical estimation of this flux. The fluxes are shared by the adjacent elements. We assume that the fluxes depend on the values of the fields in the element and on its adjacent elements. With $\partial\Omega_e = \cup_{e' \in V_e} \Gamma_{e,e'}$ and V_e as the set of the neighbour elements of the element e , we can write the flux on $\Gamma_{e,e'}$ as

$$\phi_{ei}^k = \hat{\phi}_i^k(\mathbf{p}_e, \mathbf{p}_{e'}). \quad (30)$$

Here, $\hat{\phi}$ remains to be determined. As previously, we consider the Galerkin approach for the discretisation:

$$p_{ei} = \hat{p}_{ei}^p w_i^p. \quad (31)$$

The weak formulation becomes

$$\int_{\Omega_e} d\mathbf{x} \sum_j \mathbf{M}_{ij} \partial_t (\hat{p}_{ej}^p w_j^p) w_i^q = - \int_{\Omega_e} d\mathbf{x} \sum_j \hat{p}_{ej}^p w_j^p \partial_{x_k} (\mathbf{A}_{ij}^k w_i^q) + \sum_{e' \in V_e} \int_{\Gamma_{e,e'}} d\mathbf{x} \hat{\phi}_i^k(\hat{\mathbf{p}}_e, \hat{\mathbf{p}}_{e'}) n_k^{e,e'} w_i^q \quad (32)$$

With constant test functions per element (and constant matrices \mathbf{A}^k), the first volume integral on the righthand side is null and we retrieve the equation (21) of the finite-volume methods. The lower-order finite-volume method is equivalent to the lower-order DGFEM, showing that the DGFEM generalises the finite-volume method in one way, while alternative higher-order formulations of the finite-volume method are also possible.

With a linear flux $\hat{\phi}$, we obtain the linear system

$$\mathbf{M}_e \partial_t \hat{\mathbf{p}}_e = \mathbf{S}_e \hat{\mathbf{p}}_e + \sum_{e' \in V_e} \mathbf{S}'_{e,e'} \hat{\mathbf{p}}_{e'} + \mathbf{f}_e, \quad (33)$$

which has the form of system (7).

Before assembling the matrices, we need to take care of the conditions at the boundaries of the computation domain, and notably at the free surface. Contrary to the continuous case, the free-surface condition is not naturally accounted for with this method; specific numerical fluxes need to be defined as with the finite-volume method.

The total unknown vector, $\hat{\mathbf{p}}$, is built from the vectors $\hat{\mathbf{p}}_e$. The vectors $\hat{\mathbf{p}}_e$ do not share elements, and therefore the vector $\hat{\mathbf{p}}$ is just the concatenation of all of the vectors $\hat{\mathbf{p}}_e$. This means that the global mass matrix \mathbf{M} is block-diagonal. The linear system associated with the DGFEM is then often easier to solve than that associated with standard finite-element methods. We must however note that the size of the vector $\hat{\mathbf{p}}$ can be much larger with DGFEM than with CGFEM, especially with low-order elements, because the nodes on the element boundaries are duplicated, which represents an effect of the flux approach balancing the advantages of the p adaptivity.

The flux strategies described for finite-volumes methods can be adopted here. An upwind approach has been tested by Dumbser *et al.* (2007); Käser *et al.* (2007), and centred

fluxes by Etienne *et al.* (2010). With DGFEM, high-order schemes can also be obtained using high-order polynomials for the test functions, which is a great advantage. With the centred fluxes, the earth parameters can be gathered in the matrix \mathbf{M} , in front of the time derivatives (e.g., by using the compliance matrix -the inverse of the stiffness matrix- in the elastodynamic equation). Consequently, the numerical fluxes are independent of the earth parameters, and for imaging/ inversion, where we need to compute the gradient of the misfit function with respect to the earth parameters, the derivatives of the flux terms disappear, which makes the implementation simpler. However, it can complicate the implementation when we have large earth parameter discontinuities, e.g., at the acoustic-elastic interface.

DGFEM has also been proposed for the second-order wave equation (Rivière and Wheeler 2003; Grote *et al.* 2006; de Basabe *et al.* 2008). The use of the second-order wave equation is interesting because it reduces the number of unknowns. The schemes differ according to the penalty applied in the numerical flux estimation.

Although the mass matrix is block-diagonal for the DGFEM, the blocks can be relatively large in 3D for high-order elements. The quadratures discussed in the CGFEM section can be applied, to obtain a diagonal matrix (de Basabe *et al.* 2008). The use of an orthogonal basis, e.g., with the Legendre polynomials, in a modal approach, automatically leads to a diagonal mass matrix, assuming constant material properties per element (Cockburn 2003).

In practical applications, grid refinement and order refinement can be easily implemented, leading to the so-called hp-adaptivity, because the elements share flux values and not field values, as in CGFEM (Cockburn 2003). In most of the geophysical modelling applications of DGFEM, the elements used in the meshing are triangular in 2D and tetrahedral in 3D, which leads to simpler meshing than with the quadrant or hexahedral elements classically used with the spectral finite-elements method. However, to our knowledge, DGFEM has been mainly used with low-order elements in an imaging approach.

In the presence of complex geometry and complex geological models, adaptivity and the mesh refinement are the key features for efficient numerical solutions of the elastodynamic and electromagnetic equations. Refining meshes impose severe stability constraints on explicit time-stepping schemes to respect the CFL condition and to ensure stability of the numerical scheme. When the mesh refinement is restricted to a small region, the smallest time step will be used in the entire computational domain. Overcoming this limitation is essential to achieve high performance and high numerical accuracy. If there is only a limited number of small cells, then decreasing the interpolation order is a practical approach (p-adaptivity) (Dumbser *et al.* 2007; Etienne *et al.* 2010), while local time-stepping schemes with local stability conditions will be the method of choice Collino *et al.* (2006); Dumbser *et al.* (2007); Diaz and Grote (2009). The methods of local time steps have not yet achieved the maturity level for efficient load balancing between processors in a high-performance computer environment, as the computational complexity varies dramatically between processors with the local time stepping: an optimal domain decomposition strategy remains to be found, as far as we know.

6 SOME APPLICATIONS

Without being exhaustive, we now give some of the geophysical applications of the modelling methods described above.

As discretisation is different from other formulations, spectral methods are often used to validate the solutions of the volumetric methods, especially when an interface phenomenon has an important role. A well-known application is for global earth modelling where both material properties and fields are developed on spherical harmonic functions for latitude/ longitude coordinates, and simple polynomial interpolation for the radial coordinate (Woodhouse and Dziewonski 1984; Geller and Ohminato 1994; Woodhouse 2007). These spectral approaches (at least for horizontal distances) have a low number of parameters (Takeuchi *et al.* 2000; Kawai *et al.* 2006), which allows efficient computations of seismograms for relatively smooth media. For global earth imaging, spectral methods have been the methods of choice as the earth is a closed medium. Since the seminal study of Woodhouse and Dziewonski (1984), FWI has been performed up to 0.05 Hz from recorded seismograms with earthquakes of magnitudes greater than 6.5, due to the closed-form estimations of the Fréchet derivatives and the relatively compact form of the Hessian matrix (Geller and Hara 1993): various local targets have been investigated as the database has increased (see references provided by Thurber and Ritsema (2007)).

Due of the efficiency and accuracy with layered 3D media, spectral methods have also been used for FWI, often with a stochastic approach (Sen and Stoffa 1995; Pica *et al.* 1990; Kormendi and Dietrich 1991; Hoversten *et al.* 2006; De Barros and Dietrich 2008).

Spectral methods also have an important role when the state equations are reformulated with the introduction of Green functions. We can cite the primary/ secondary formulation that is often used in diffusive electromagnetism (Hohmann 1988; Zhdanov 2002). In this formulation, the primary solution in a layered background is often computed with a spectral method, allowing analytical discretisations of the source; the secondary field is computed by a volumetric (FDM or finite-element) formulation. We should also mention the integral equations formulation. These might be of interest when the sought properties of the medium are confined in a more limited domain than the one where we must solve the forward problem, or when weak perturbations in the variations of properties are expected (Zhdanov 2002). Here, volumetric methods, such as the FDM, are also used to compute the Green functions. These approximations could be similarly applied using the partial differential equations (Robertsson and Chapman 2000; Abubakar *et al.* 2009). It is worth noting that the integral equation methods can be collapsed into the boundary integral methods where discretisation is only along the boundaries between domains, as long as solutions are available inside each domain. We often consider domains with homogeneous properties leading to local analytical solutions (Kausel 2006), although numerical local solutions can be constructed at the expense of computer resources (Wolf 2003).

A lot of large-scale geophysical inversion/ imaging uses

the FDM or the finite-volume method. In 3D electromagnetic imaging, applications can be found in magnetotelluric data imaging (Mackie *et al.* 1993) and in marine-controlled source electromagnetic data imaging (Newman and Alumbaugh 1999; Carazzone *et al.* 2005; Plessix and Mulder 2008). In these applications, most of the time, the inversion is carried out in the frequency domain and second-order spatial schemes are used. In seismic imaging, 3D acoustic RTM of P-waves is nowadays a commodity, especially in the Gulf of Mexico. In 3D, only time-domain implementations with time marching are competitive, because a sufficiently large band-frequency window has to be taken into account to obtain sufficient depth localisation. To improve the efficiency, large optimal stencils are implemented (Etgen and O'Brien 2007). The use of large stencils is not only crucial from a computational time point of view, but also from a memory and I/O point of view. In exploration geophysics and geodynamic lithospheric interpretations, 3D acoustic FWI also principally relies on FDM techniques. However, contrary to the RTM, only a sparse set of frequencies can be used. Here, computation of the gradient of the misfit function is required, making the implementation somewhat more challenging than for the RTM application. Processing frequency per frequency allows the I/O requirements to be reduced. Indeed, the time-harmonic incident field can generally be stored in the memory while computing the data back-propagated field, as the finite-volume method currently uses only the low frequency part of the data spectrum. Therefore, both 3D time-domain and frequency-domain implementations are now used (Ben-Hadj-Ali *et al.* 2008; Vigh and Starr 2008; Warner *et al.* 2008; Plessix 2009; Sirgue *et al.* 2010). Despite some attempts (Brossier *et al.* 2009), finite-volume methods are not routinely used in seismic imaging. While attractive for the representation of sharp interfaces, as we can use triangle or tetrahedral meshes, these low-order methods remain too expensive and less flexible than finite-element methods. We can also question the relevance for imaging of the high-order finite-volume methods based on high-order time integration, such as the ADER technique, because of their complexity. FDMs represent a good compromise. These are less accurate than other numerical methods, but they are efficient, notably with the high-order stencils in seismic imaging, and easy to implement even with gradient computation. While the model representation can be crude (for instance with rough topography), model discretisation through a grid is easy and generally does not lead to numerical difficulties. In exploration geophysics, we often do not have precise knowledge of the geological interfaces (except at the air-earth and water-earth interfaces). Therefore, working with relatively smooth earth parameters at a wavelength scale is often sufficient, at least in the first stages of velocity model building with P-waves or resistivity imaging in a marine environment.

In the oil and gas industries, finite-element methods have rarely been used so far in large-scaled applications. In contrast, they have been applied in seismology. Various implementations have been studied, from standard finite-element approaches (Marfurt 1984) to octree-based finite-element methods (Bielak *et al.* 2003) in active and passive seismology, and with classic and mixed continuous finite-

element methods, sometimes with edge elements, in electromagnetism; e.g., see Cognon (1971); Li and Key (2007). A few inversions have been performed using the standard finite-element approach (Askan *et al.* 2007). However, with the regaining of importance of land exploration and the need for better reservoir characterisation, these techniques might become crucial to better model the propagation and diffusion phenomena around interfaces and in anisotropic media. In global seismology, the spectral finite-element method with a spectral convergence in the standard space has reached a mature level (Komatitsch and Vilotte 1998; Komatitsch and Tromp 2002; Chaljub *et al.* 2007). This method has been applied in an inversion scheme at lithospheric scales (Fichtner *et al.* 2008; Tape *et al.* 2009). DGFEM implementations that provide additional properties and flexibilities have been proposed (Käser *et al.* 2007; De la Puente *et al.* 2008). The first preliminary attempts of this method for seismic imaging have been performed (de la Puente *et al.* 2010). The relative advantages of the different finite-element methods for inversion remain an active research topic.

7 SOME MODELLING AND IMAGING CONSIDERATIONS

When modelling approaches form the kernel of an inversion/ imaging problem, some extra considerations can influence our choice, depending on the size of the model space. In elastodynamics and electromagnetism imaging methods, the earth model contains from less than 100 unknowns in very small real-sized cases, to hundreds of millions in large real-sized cases. When the forward modelling is fast enough and with a reduced number of unknowns, the objective function of the inverse problem can be minimised with a global optimisation technique, such as a grid search or Monte Carlo sampling (Press 1968; Silva and Hohmann 1983; Hong and Sen 2009), or a semi-global method, such as simulated annealing or genetic algorithms (Sen and Stoffa 1995), where the sampling strategy of the model space depends on the values of the objective function. These (semi-)global optimisations are interesting because they only rely on the value of the misfit function. To converge, these methods require a number of simulations that is often larger than the number of unknowns. Unfortunately, they can be implemented only with small cases under certain simplifications. Classically, a 1D assumption is made, and the spectral methods are good candidates. The FDM and the finite-volume and finite-element methods are often still too expensive to allow (semi-)global searches.

In more complex settings, we revert to local optimisation due to computational constraints. Local techniques without the estimation of the gradient, such as the simplex method, are limited to a few parameters. This leaves us with gradient optimisation. This adds some burdens on the implementation, as the gradient of the misfit function with respect to model parameters needs to be evaluated and numerical differentiation is not a real option due to its cost. Computing the Jacobian matrix of the misfit function, namely the Fréchet derivatives with respect to the model parameters, is often not possible because it would require a large number of simulations, although there are cases where it is manageable (Chen *et al.* 2007). With a limited number of pa-

rameters, closed-form estimation of the Fréchet derivatives can be done with the spectral methods, as mentioned previously. An alternative consists of directly evaluating the gradient with the adjoint-state technique (Chavent 2009). The discretisation of the equations 7, 8, 9, or 10 leads to the formal system $\mathbf{L}\mathbf{p} = \mathbf{f}$. The adjoint system is given by $\mathbf{L}^T\mathbf{q} = \mathbf{g}$, where \mathbf{q} is the adjoint (back-propagated) fields, \mathbf{g} the source of the adjoint system, which depends on the residuals between the observed and computed data from the fields \mathbf{p} , and T the transposition. The gradient with respect to a model parameter m is then given by $\mathbf{q}^T\partial_m\mathbf{L}\mathbf{p}$. Several comments that may guide our modelling choice can now be made:

- The forward (direct) and backward (adjoint) systems are similar. They are conjugated, and consequently they have the same dispersion curve. The methods described for the forward system can be used directly to solve the backward system. However, the source term of the backward system is generally less localised than the source term of the forward system. This may become a challenge with spectral methods. Moreover, it is recommended to derive the adjoint system from the discretised system (Chavent 2009). This can be numerically difficult or expensive with certain approaches, such as spectral methods or sophisticated spatial and temporal schemes; e.g., with some FDM schemes on irregular grids, and some high-order time-integration schemes.

- In the time domain, the adjoint system is solved backwards. This means that computing the gradient requires the incident fields at all of the time steps. This is a burden compared to the frequency domain, where all of the frequencies can be treated separately. When an efficient frequency solver exists, such as in diffusive electromagnetism, the frequency domain is then the domain of choice. Note that the situation becomes more complicated when a time window is applied to the data, e.g., to remove the air wave. When the I/O becomes a bottle-neck with the time-domain approach, check-pointing methods can be applied, as recalled by Symes (2007); however, this increases the computational effort and the complexity of the implementation.

- In the frequency domain, the matrix \mathbf{L} is independent of the source locations. With a direct solver, the LU matrix decomposition is then carried out only once, making this implementation attractive. In 3D geometries, however, the parallelisation of the direct solver is quite challenging, and this requires a very large amount of memory. This approach is a priori not a real option in diffusive electromagnetism, where fast iterative solvers exist. In acoustics, with fixed-spread acquisition, the direct-solver approach can be an option when very few frequencies are used, as in certain FWIs (see examples in Brossier *et al.* (2010)). This, however, relies heavily on the hardware architecture, and especially the speed of communication.

- Often, the data contain a large number of sources. The forward and backward systems can be very efficiently parallelised over the sources. Moreover, the computational domain can be adapted to the shot acquisition, which leads to an efficient implementation, especially when the computational and inversion grids can be decoupled. Time-domain and frequency-domain implementations with an iterative solver take advantage of this feature when dealing with large real datasets. For the frequency, the algorithm can also be

parallelised over the frequencies. This favours frequency-domain implementation when an efficient solver exists. This explains why frequency-domain approaches are favoured in diffusive electromagnetism; moreover, just a sparse set of frequencies are often used. In elastodynamics, no sufficiently efficient 3D frequency-domain iterative solver exists yet to compete with time-domain implementation when a large band-frequency window needs to be modelled, such as for RTM. When only a very few frequencies are used, such as with certain (acoustic) FWI, iterative solvers can be an option. Nevertheless, time-domain implementations are currently the most common choices.

- The gradient will be efficiently evaluated when the matrix $\partial_m \mathbf{L}$ is very sparse. High-order time or spatial schemes reduce the sparsity of these matrices. The adjoint state technique can, for instance, be relatively inefficient with spectral methods, such as the reflectivity method. The FDM and finite-element high-order spatial schemes are generally not an issue. However, parallel implementations by domain decomposition can significantly increase inter-node communication. The local nature of the DGFEM appears to be an advantage. In the time domain, the complexity added by the high-order time scheme, such as a high-order ADER scheme, needs to be evaluated. Currently, as far as we know, only low-order time schemes are used in inversion.

With large inverse problems, these considerations around the gradient computation appear to be in favour of the FDM, or the finite-volume or finite-element methods for spatial discretisation. The choice between frequency-domain and time-domain formulations is problem dependent. Physical or (pre)-processing considerations should influence the choice, as these can influence the behaviour of the numerical implementation.

8 CONCLUSIONS

In this review, three main modelling approaches have been presented. First, spectral methods can give very efficient and accurate solutions; however, their lack of flexibility limits their applications to very specific earth geometries, e.g., a layered earth. Secondly, the discretisation of the strong formulation of the PDEs was discussed. This corresponds to the pseudo-spectral, finite-difference method and finite-volume method. On a structured meshing, and notably a regular or stretched grid, these approaches are easy to implement and are relatively flexible. They are currently the methods of choice for large-scale modelling and inversion in exploration geophysics, and especially in the marine environment. They may however demand very fine discretisation when the earth model contains large contrasts, and accurately modelling the responses around a sharp interface is quite challenging. Thirdly, we discussed the weak formulation, namely the finite-element methods with continuous and discontinuous approaches. The use of test functions gives us more freedom, and the integral form provides us flexibility in the meshing. However, they lead to numerical challenges: they are more difficult to implement than methods related to the strong formulation, they are often more expensive in computational time and memory, and they are more complicated to use because the accuracy of the response depends on the quality of the meshing.

This classification helps in our understanding of the advantages and limitations of each particular method for the modelling of specific physical phenomena. The choice of the modelling approach depends in particular on the needed accuracy, the efficiency in the evaluation of the solution and the gradient of the misfit function in an inversion algorithm, and the simplicity of use. Although this was not really discussed, the efficiency can depend considerably on the hardware architecture. Some of the new types of hardware architecture require new modelling implementations to be used efficiently, as, for example, graphical processor units, which can require specific developments. Similarly, the practical implementation will probably be adapted to the data acquisition. Densely sampled acquisition in exploration geophysics, with or without blending, or in lithospheric investigations with the recent deployment of sensors, as for the US array experiment, challenge our modelling choice. This appears to indicate that developments in modelling and the associated inversion approaches remain crucial for the improvement of our sub-surface knowledge, and particularly for the extraction of more information from the ever larger datasets we record.

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