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The Complex-Step-Finite-Difference method

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SUMMARY

We introduce the Complex-Step-Finite-Difference method (CSFDM) as a generalization of the well-known Finite-Difference method (FDM) for solving the acoustic and elastic wave equations. We have found a direct relationship between modelling the second-order wave equation by the FDM and the first-order wave equation by the CSFDM in 1-D, 2-D and 3-D acoustic media. We present the numerical methodology in order to apply the introduced CSFDM and show an example for wave propagation in simple homogeneous and heterogeneous models. The CSFDM may be implemented as an extension into pre-existing numerical techniques in order to obtain fourth- or sixth-order accurate results with compact three time-level stencils. We compare advantages of imposing various types of initial motion conditions of the CSFDM and demonstrate its higher-order accuracy under the same computational cost and dispersion–dissipation properties. The introduced method can be naturally extended to solve different partial differential equations arising in other fields of science and engineering.

Key words: Numerical solutions; Wave propagation.

1 INTRODUCTION

The study of integro-differential equations to model real or ideal problems is nowadays the most powerful tool to predict the behaviour of any known system. The exact solution of the mathematical problem is called the analytical solution. Usually this analytical solution is extremely difficult to find for realistic problems, often impossible; for this reason the numerical solution takes so much importance. The numerical solution gives an approximation to the analytical solution usually transforming the continuous domain into a discrete domain that can be later solved on a computer, for example, Finite-Difference method (FDM), Finite-Element method (FEM), Spectral-Element method (SEM), Finite-Volume method (FVM) and Discontinuous-Galerkin method (DGM) among many others.

The FDM is one of the simplest, most intuitive and easiest to implement numerical method. Its origins date back to the times of Isaac Newton (1642–1727) and Gottfried Leibniz (1646–1716) who are recognized as the fathers of the differential calculus, and the concept of the derivative. The FDM is based on the concept of the finite difference (FD) operator, hence its name: finite, because it transforms an infinite dimensional problem (continuous problem) into a finite dimensional problem (discrete problem) and difference, because it computes derivatives using subtractions. The FDM approximates derivatives of an ordinary differential equation (ODE) and/or partial differential equation (PDE) by divided differences defined at the so-called grid points (refereed as spatial discretization).

Despite the FDM being one of the oldest numerical techniques, it remains as one of the most powerful (in terms of computational cost) methods for solving differential equations. Also, despite its limitations, the FDM remains one of the most popular methods because of it being relatively straightforward and intuitively understanding from a physical point of view.

Simulations to the wave equation can be carried out using various FD discretizations and compared to the analytical solutions in order to determine whether or not reliable results are obtained. Not all of the FD discretizations that can be made by combining various approximations to the wave equation are useful. To determine whether a certain FD discretization can be applied to the problem, we have to use the concepts of convergence, consistency, stability, dispersion, dissipation and attenuation properties of the numerical solution.

In this study we extend the concept of the FDM for solving differential equations using the recent generalization of the Complex-Step method (CSM) by Abreu *et al.* (2013). Originally formulated for imaginary perturbations by Squire & Trapp (1998), the generalization of the CSM was made considering a complex step in a strict sense, which permits to find various approximations for the first- and second-order derivatives of any complex-valued analytic function using its real and imaginary parts. Many of these approximations help to avoid term cancellation errors inherent to classic FD approximations, as well as permit the computation of second-order derivatives using a single step and reaching sixth-order accuracy in a compact three levels stencil.

In this study we introduce the Complex-Step-Finite-Difference method (CSFDM) and illustrate its accuracy for solving the acoustic wave propagation problem in one, two and three dimensions within a homogeneous medium and also propose its correct use for the generalization of well-known numerical techniques like the FEM, SEM and DGM in order to solve the elastic wave propagation problem in 3-D heterogeneous media. In Section 2 we first describe basic concepts of FD and CS approximations for first- and second-order derivatives in order to develop basic intuition in the nature of the CSM. In Section 3 we derive discretizations of the 1-D wave equation (first-order and second-order) using FD and CS approximations. In this section we establish the methodology for implementing the CSFDM; we also illustrate some simulation examples using the FDM and the CSFDM. In Section 4 we illustrate numerical simulations of the 2-D and 3-D acoustic wave equation using the standard FDM and the CSFDM, discussing similarities and differences among their propagation properties. In Section 5 we generalize well-known computational techniques for solving the elastic wave propagation problem in a 3-D heterogeneous medium. Finally, in Sections 6 and 7 we draw a general overview and conclusions from this study, respectively.

2 FINITE-DIFFERENCE AND COMPLEX-STEP DERIVATIVE APPROXIMATIONS

Derivative approximations are one of the basic pillars for computational physics nowadays. The accurate and stable calculation of derivative approximations is crucial to obtain reliable results when modelling a physical system. FD approximations are the most basic and intuitive way to represent approximate values of derivatives of any order.

The simplest FD approximation for first-order derivatives, obtained from Taylor's series, is called the *forward* FD approximation and is given by the following expression:

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} + \mathcal{O}(\Delta x), \tag{1}$$

where Δx refers to the *differential step* and the symbol $\mathcal{O}$ refers to the *approximation error*.

The forward approximation is a first-order approximation ($\mathcal{O}(\Delta x)$) which uses information at two levels of the function, that is, at x and $x + \Delta x$. In other words, to obtain approximate values of the first derivative of f at the point x, we need information of the function at x and at a different point $x + \Delta x$. Clearly, the error made in the approximation depends on how big we choose Δx to be.

Eq. (1) can be easily obtained from the Taylor series expansion of $f(x + \Delta x)$ and neglecting all the terms related to higher-order derivatives and expressing all of them as $\mathcal{O}(\Delta x)$.

In the same way, using the Taylor's series of $f(x - \Delta x)$ and reordering, we can find the *backward* FD approximation given by the following expression:

$$f'(x) = \frac{f(x) - f(x-\Delta x)}{\Delta x} + \mathcal{O}(\Delta x). \tag{2}$$

Combining Taylor series of $f(x + \Delta x)$ and $f(x - \Delta x)$ we can obtain the *centred* FD approximation:

$$f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2). \tag{3}$$

Note that eq. (3) is a second-order approximation ($\mathcal{O}(\Delta x^2)$) by the price of using more information of the function than the forward approximation; that is, we need information at two different points ($x + \Delta x$ and $x - \Delta x$) from the evaluation point (x).

In the same way, combining Taylor series of $f(x + \Delta x)$ and $f(x - \Delta x)$ we can obtain the most simple FD approximation for second-order derivatives, given by the following expression:

$$\begin{aligned} f''(x) &= \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \\ &= \frac{f(x+\Delta x) - f(x) - (f(x) - f(x-\Delta x))}{\Delta x^2} + \mathcal{O}(\Delta x^2). \end{aligned} \tag{4}$$

Note that the numerator of eq. (4) is simply the difference between forward and backward first-order derivative approximations. Many different FD approximations can be made by simply combining Taylor's series expansions of function's values (e.g. $f(x + \Delta x)$, $f(x - \Delta x)$, $f(x + 2\Delta x)$, $f(x \pm \frac{2}{3}\Delta x)$, ...), different from the evaluation point x.

Usually, the order of the error in FD approximations is related to the number of differential steps taken away from the evaluation point (x). It is easy to check that FD approximations for first- and second-order derivatives can be computed within three evaluation levels of the function ($f(x - \Delta x), f(x), f(x + \Delta x)$) with at most an accuracy of second-order ($\mathcal{O}(\Delta x^2)$).

FD approximations can be used to compute derivative values of any order and with any desired accuracy, with the price of requiring information of the function away from the evaluation point.

Most naturally, derivatives of analytic functions are approximated by FD techniques using real numbers, but the less intuitive idea of using an imaginary number in analytic functions differentiation has been shown capable of overcoming the term cancellation problems inherent to all FD approximations, as well as reducing the associated approximation error (e.g. Abreu *et al.* 2013). Squire & Trapp (1998) presented a method for computing first-order derivatives of any real analytic function using the Taylor's series expansion of the imaginary perturbation of the function. The method was formally named the CSM.

The CSM uses a purely imaginary number $\mathbf{i}$ ($\mathbf{i}^2 = -1$) for computing the first- and second-order derivatives of real functions. The CSM can be easily derived from the Taylor's series expansion of $f(x + \mathbf{i}\Delta x)$, taking the imaginary part and reordering to obtain the following expression for first-order derivatives approximations:

$$f'(x) = \frac{\mathfrak{Im}(f(x + \mathbf{i}\Delta x))}{\Delta x} + \mathcal{O}(\Delta x^2), \tag{5}$$

where $\mathfrak{Im}$ refers to the imaginary part of the function. Note that x is set to be a real number.

Eq. (5) was obtained for the first time by Squire & Trapp (1998). Using the same Taylor's expansion of $f(x + \mathbf{i}\Delta x)$ but taking the real part, we can obtain an expression for second-order derivatives approximations given by the following expression:

$$f''(x) = \frac{2(f(x) - \mathfrak{Re}(f(x + \mathbf{i}\Delta x)))}{\Delta x^2} + \mathcal{O}(\Delta x^2), \tag{6}$$

where $\mathfrak{Re}$ refers to the real part of the function.

Eqs (5) and (6) are the most basic equations that can be found using the Taylor's expansion of $f(x + \mathbf{i}\Delta x)$. The numerical advantages of the CSM are clear: eq. (5) shows a single term in the numerator rather than a difference showed in eq. (1) (and inherent to all FD approximations), and hereby circumvents the instability related to term cancellation errors, besides being more accurate (see Abreu *et al.* 2013, for further details).

The generalization of the CSM made by Abreu *et al.* (2013) consisted in taking a complex step in a strict sense, that is, replacing the imaginary differential step $\mathbf{i}\Delta x$ by a proper complex step $h + \mathbf{i}v$ where $h, v \in \mathbb{R}$ and $h, v \to 0$.

Following, we rewrite the approximations listed in Abreu *et al.* (2013) and used in this study by omitting all the equivalent expressions considering $\mathfrak{Im}(f(x \pm h + \mathbf{i}v)) = -\mathfrak{Im}(f(x \pm h - \mathbf{i}v))$.

$$f'(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v))}{v} + \mathcal{O}(h, v^2), \tag{7}$$

$$f'(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) + \mathfrak{Im}(f(x - h + \mathbf{i}v))}{2v} - \left(\frac{3h^2 - v^2}{6}\right) f'''(x) + \mathcal{O}(5h^4 - 10h^2v^2 + v^4), \tag{8}$$

$$f''(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) - \mathfrak{Im}(f(x - h + \mathbf{i}v))}{2hv} - \frac{(h^2 - v^2)}{3!} f^{iv}(x) + \mathcal{O}\left(3h^4 - 10h^2v^2 + 3v^4\right). \tag{9}$$

Note that if we set $v = \sqrt{3}h$ and $v = h$ in eqs (8) and (9) respectively, the approximation error becomes $\mathcal{O}(h^4)$.

Using eqs (8) and (9) and the most convenient relationship between h and v, we are able to compute fourth-order accurate values of a first-order and second-order derivatives respectively, only requiring two levels of information of the function ($x + h + \mathbf{i}v$ and $x - h + \mathbf{i}v$) different from the evaluation point of the derivative (x).

Approximations found by Abreu *et al.* (2013) are not all the approximations that can be found for computing first- and second-order derivatives. Eqs (7)–(9) can be rewritten including the initial and/or centre point to include more information of the function into the discretization:

$$f'(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) + \mathfrak{Im}(f(x + \mathbf{i}v))}{2v} + \mathcal{O}(h, v^2). \tag{10}$$

$$f''(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) - \mathfrak{Im}(f(x + \mathbf{i}v))}{hv} + \mathcal{O}(h, v^2). \tag{11}$$

$$f'(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) + \mathfrak{Im}(f(x + \mathbf{i}v)) + \mathfrak{Im}(f(x - h + \mathbf{i}v))}{3v} - \left(\frac{2h^2 - v^2}{6}\right) f'''(x) + \mathcal{O}(10h^4 - 20h^2v^2 + 3v^4). \tag{12}$$

$$f'''(x) = \frac{\mathfrak{Im}(f(x + h + \mathbf{i}v)) - 2\,\mathfrak{Im}(f(x + \mathbf{i}v)) + \mathfrak{Im}(f(x - h + \mathbf{i}v))}{h^2 v} + \mathcal{O}(h^2 - 2v^2). \tag{13}$$

Note that the expression for the third-order derivative (eq. (13)) is just a simple three levels scheme.

We can write a more general and accurate approximation for the first-order derivative given by the following expression:

$$\begin{aligned} f'(x) = {} & \left(\frac{3h^2 - v^2}{3h^2 v}\right) \mathfrak{Im}(f(x + \mathbf{i}v)) + \frac{v}{6h^2}[\mathfrak{Im}(f(x + h + \mathbf{i}v)) + \mathfrak{Im}(f(x - h + \mathbf{i}v))] \\ & - \left(\frac{v^2(5h^2 - 7v^2)}{5!3}\right) f^{v}(x) + \left(\frac{7h^4v^2 - 35h^2v^4 + 18v^6}{7!3}\right) f^{vii}(x) + \mathcal{O}(h^8, v^8). \end{aligned} \tag{14}$$

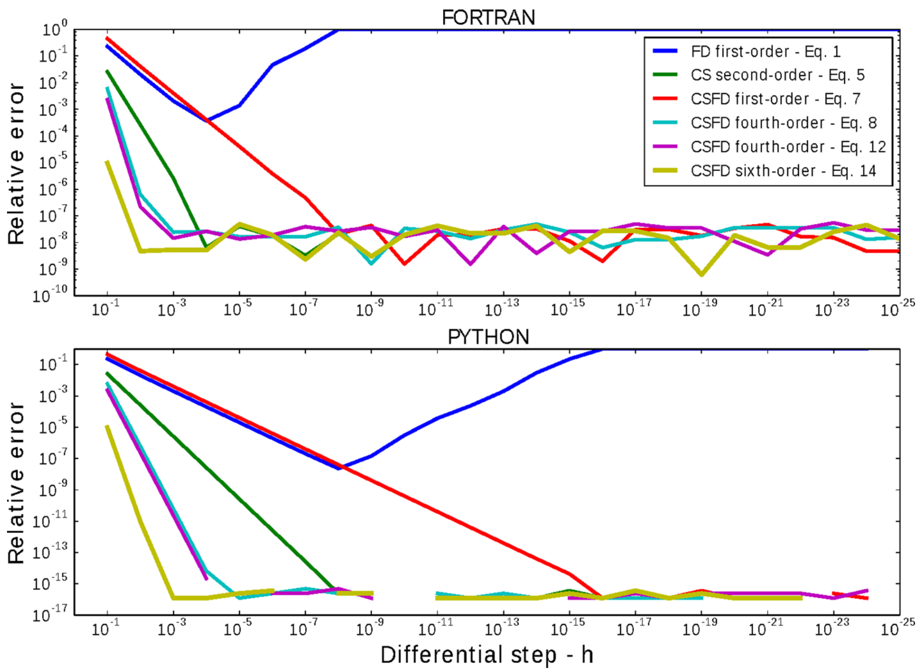

Figure 1. Derivative approximation validation and comparison using gnu gfortran compiler and Python.

Note that in eq. (14) we can choose the weights of each term $\Im\mathfrak{m}(f(x+h+\mathbf{i}v))$, $\Im\mathfrak{m}(f(x-h+\mathbf{i}v))$ and $\Im\mathfrak{m}(f(x+\mathbf{i}v))$ and the approximation will remain fourth-order accurate. If we choose $5h^2-7v^2=0$ the error in the approximation is clearly $\mathcal{O}(h^6)$, in a compact three level stencil. Eq. (14) is apparently the most accurate approximation for first-order derivatives that can be found with complex-steps in a compact three level stencil.

Because expressions 10, 12 and 14 for computing first-order derivatives are not listed in Abreu *et al.* (2013), we perform a numerical test: we use an analytic test function used by Lyness & Sande (1971), and subsequently by many authors, that has become an established de-facto standard in numerical differentiation:

$$f(x)=\frac{e^x}{\sin^3(x)+\cos^3(x)}.$$

Consistent with previous work on complex variable differentiation, we evaluate the function at the test point $x=1.5$, which has the following values for the first and second derivatives: $f'(x)=3.622$ and $f''(x)=14.5683$.

Simulations have been carried out in Fortran90 language and using the GNU Fortran compiler gfortran with standard double precision format for all variables. Also, in order to make comparisons with the Fortran compiler gfortran, we use Python language with its default floating point precision for making calculations.

Results are displayed in Fig. 1, where the differential step h starts from $1e^{-1}$ and decreases geometrically to $1e^{-25}$. The v value is taken as $v=h$, unless a better and specific choice of v versus h must be adopted in order to increase the order of the accuracy, as indicated in the description of eqs (10), (12) and (14). All plotted errors are relative errors.

We can appreciate similar results with both programming languages. The forward FD approximation totally collapses when reaching the variable precision used. We can also appreciate, as expected, that the most accurate approximation is expression 14, and none of the CS approximations collapses by truncation error.

Before we proceed, in order to develop intuition in the geometrical interpretation of the CS derivative approximation, note that the imaginary part of the imaginary perturbation can be represented as an approximate increment in the vertical axis simply made by equating eq. (1) and eq. (5) (see Fig. 2).

3 FINITE-DIFFERENCE AND COMPLEX-STEP-FINITE-DIFFERENCE METHODS APPLIED TO THE 1-D WAVE EQUATION

Numerical analysis of the one dimensional (1D) first-order and second-order wave equations is one of the basis for most of the numerical methods that are implemented in realistic 3-D media (acoustic or elastic) in the field of geophysics.

The 1-D second-order scalar wave equation, also called the 1-D two-way wave equation, is given by the following mathematical expression:

$$\frac{\partial^2 u}{\partial t^2}=c^2\frac{\partial^2 u}{\partial x^2}, \tag{15}$$

where $u=u(x,t)$ is the displacement field, x is the space variable, t is the time variable and c is the propagation velocity.

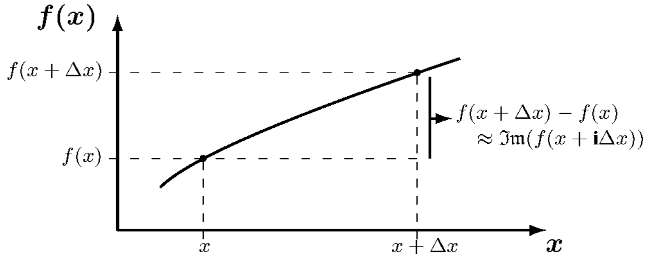

Figure 2. Geometric representation of the Complex Step.

To solve the PDE (15) we need an initial condition of displacement and velocity or a time-dependent function which generates the motion at certain time levels and at certain locations. In this study we refer both as *motion conditions*.

Eq. (15) subject to initial conditions of displacement and speed,

$$u(x,0) = f(x) \quad \text{and} \quad \dot{u}(x,0) = g(x), \tag{16}$$

is called *the initial value problem*.

The time-dependent source of motion ($u(x_s, t)$) can be applied over a single point (x_s), usually referred as a point source, or over a set of points of the whole spatial domain.

The mathematical expression for the 1-D elastic wave equation is the same for the 1-D acoustic wave equation with the only difference in the velocity propagation term. In an elastic medium we can find different types of 1-D waves, for example *P*, *SV* and *SH* waves. All of these waves belong to the same mathematical expression (eq. 15), with different particle motion and wave speed:

$$c = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad \text{for a } P \text{ wave}, \tag{17}$$

$$c = \sqrt{\frac{\mu}{\rho}} \quad \text{for a } SV \text{ and } SH \text{ waves}, \tag{18}$$

where λ and μ are Lame elastic parameters and ρ is the density.

Generalization of eq. (15) to non-constant coefficients, that is, taking into account variations of speed (heterogeneous media), is given by the following expression:

$$\frac{\partial^2 u}{\partial t^2} = \nabla \cdot (c(x)^2 \, \nabla u), \tag{19}$$

where the operator ∇ is the gradient and $\nabla \cdot$ is the divergence. Note that the velocity is not longer constant and this change is taken into account by the divergence operator.

Eq. (15) and/or eq. (19) are called two-way wave equations: this means that they involve a *differential operator* that propagates a wave in two directions (positive and negative directions).

If we rearrange and factorize eq. (15) we can write the following

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = \left(\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} \right) u = \left[\left(\frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) \right] u = 0. \tag{20}$$

The two differential operators in which the two-way wave equation (eq. 15) can be decomposed are called one-way wave differential operators. We can write these one-way differential operators by the following expression:

$$\frac{\partial u}{\partial t} = \pm c \frac{\partial u}{\partial x}. \tag{21}$$

Expression 21 is called the one-way wave equation, also called the first-order wave equation, which propagates the wave in a single direction only (positive or negative).

The first-order and second-order wave equations are the basis of any numerical experiment design in computational wave propagation. Despite both wave equations (one-way and two-way) are hyperbolic PDE, they possess different propagation properties: whereas the first-order wave equation propagates the wave-field in a single direction only (positive or negative) and do not suffer reflections on fixed boundaries, the second-order wave equation propagates the wave-field in two directions (positive and negative) and suffers reflections on fixed boundaries.

Before we proceed, note that the second-order wave equation could be written as follows:

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = \frac{1}{2} \left[\left(\frac{\partial}{\partial t} + \mathbf{i} \frac{\partial}{\partial t} \right) \left(\frac{\partial}{\partial t} - \mathbf{i} \frac{\partial}{\partial t} \right) - c^2 \left(\frac{\partial}{\partial x} + \mathbf{i} \frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial x} - \mathbf{i} \frac{\partial}{\partial x} \right) \right] u = 0, \tag{22}$$

where time and space variables are considered to be complex numbers each.

3.1 Finite-difference discretizations to the 1-D wave equations

The most basic FD discretizations to the one-way and two-way wave equations are made by combining forward, backward and centred FD approximations for time and/or space derivatives. All of these combinations are tested in order to determine whether they produce a reliable solution to the initial value problem. Table 1 illustrates the very well known discretizations and its respective name for the first-order wave equation. Forward and backward Euler discretizations are unconditional unstable but they can be modified in order to efficiently solve the problem, which leads to the Lax-Friedrichs method (see Thomas 1995, for further details).

In order to illustrate a FD discretization and its direct connection with CSFD discretizations, we write the most basic FD approximation to the one-way wave equation, made by using the forward approximation (eq. 1) for time and space derivatives of the equation. After rearranging we can obtain the following mathematical expression:

$$u_x^{t+\Delta t} = \mathrm{S}\, u_{x+\Delta x}^t + (1-\mathrm{S})u_x^t + \mathcal{O}(\Delta t, \Delta x), \tag{23}$$

where $\mathrm{S} = \frac{c\Delta t}{\Delta x}$ is called the *Courant number* and/or *stability factor*. The parameter Δx is referred as the *grid spacing* and Δt as the *time step*.

Eq. (23) is a stable and convergent FD discretization to the one-way wave equation and is known as the *upwind* discretization, which is first-order accurate in time and space.

Using the centred approximation (eq. 3) at both sides of the one-way wave equation, the following expression is obtained:

$$u_x^{t+\Delta t} = \mathrm{S}\, \left(u_{x+\Delta x}^t - u_{x-\Delta x}^t\right) + u_x^{t-\Delta t} + \mathcal{O}(\Delta t^2, \Delta x^2). \tag{24}$$

Eq. (24) is the well known *leapfrog* discretization to the one-way wave equation and it is of second-order accurate in time and space (see Strang 2007, for further details).

Expressions 23 and 24 can be respectively written in a general operator form as follows:

$$\Delta_t^+ u_x^t = \mathrm{S}\, \Delta_x^+ u_x^t + \mathcal{O}(\Delta t, \Delta x), \tag{25}$$

$$\Box_t\, u_x^t = \mathrm{S}\, \Box_x\, u_x^t + \mathcal{O}(\Delta t^2, \Delta x^2), \tag{26}$$

where

$$\Delta_x^+ f(x) = f(x+\Delta x) - f(x), \tag{27}$$

$$\Box_x^n\, f(x) = f(x + n\Delta x) - f(x - n\Delta x). \tag{28}$$

We can also discretize the second-order wave equation (eq. 15), using the centred FD approximation for the second-order derivative (eq. 4) in time and space,

$$u_x^{t+\Delta t} = \mathrm{S}^2 \left(u_{x+\Delta x}^t + u_{x-\Delta x}^t\right) + 2(1-\mathrm{S}^2)\, u_x^t - u_x^{t-\Delta t} + \mathcal{O}(\Delta t^2, \Delta x^2). \tag{29}$$

Eq. (29) is a convergent and stable FD discretization and is known as the *leapfrog* approximation for the second-order wave equation (see Strang 2007).

In order to numerically solve the second-order wave equation (eq. 15) using the FD discretization (29) we need two initial conditions; these initial conditions are given by the initial displacement of the particle ($u(x, 0)$) and velocity ($\dot{u}(x, 0)$) and/or in case of a point source, only displacement values over certain time levels and space location are required ($u(x_s, t)$).

We can write discretization (29) in a general operator form as follows:

$$\Delta_t^+ \circ \Delta_t^-\, u_x^t = \mathrm{S}^2\, \Delta_x^+ \circ \Delta_x^-\, u_x^t + \mathcal{O}(\Delta t^2, \Delta x^2), \tag{30}$$

or

$$\Box_x^{1/2} \circ \Box_x^{1/2}\, u_x^t = \mathrm{S}^2\, \Box_x^{1/2} \circ \Box_x^{1/2}\, u_x^t + \mathcal{O}(\Delta t^2, \Delta x^2), \tag{31}$$

where $\circ$ is the convolution operation.

It is well known that the upwind and leapfrog (for the one-way and two-way wave equations) approximations are stable, non-dispersive and non-dissipative for the maximum Courant number ($\mathrm{S} = 1$), which is given for the case of the homogeneous media (see Thomas 1995, for details).

Table 1. Velocity and density parameters of the simulation.

	Layer	Halfspace
P-wave velocity	1125 m s^{-1}	5468 m s^{-1}
S-wave velocity	625 m s^{-1}	3126 m s^{-1}
Density	1600 kg m^{-3}	1800 kg m^{-3}

We can write, for the case of homogeneous media, the upwind discretization (eq. 23) and the leapfrog discretization for the second-order wave equation (eq. 29) using operators as follows, respectively

$$\rhd_t u_x^t = \rhd_x u_x^t + \mathcal{O}(\Delta t, \Delta x), \tag{32}$$

$$\lhd\rhd_t u_x^t = \lhd\rhd_x u_x^t + \mathcal{O}(\Delta t^2, \Delta x^2), \tag{33}$$

where

$$\rhd_x f(x) = f(x + \Delta x), \tag{34}$$

$$\lhd\rhd_x^n f(x) = f(x + n\Delta x) + f(x - n\Delta x). \tag{35}$$

3.2 Complex-Step-Finite-Difference discretizations to the 1-D wave equations

In this section, we follow a similar strategy given in Section 3.1 for FD discretizations: We combine various CS approximations for the first- and second-order derivatives to the first-order and second-order wave equations. We only considered explicit schemes in this study.

We name our introduced approximations the Complex-Step-Finite-Difference (CSFD) discretizations to the one-way and two-way wave equations.

Following, we present a list of the CSFD discretizations for the first-order wave equation using operators:

$$\rhd_t \,\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) = \mathrm{S} \rhd_x \,\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) + \mathcal{O}(\Delta t, \Delta x), \tag{36}$$

$$\lhd\rhd_t \,\mathfrak{Im}\left(u_{x+\mathbf{i}\sqrt{3}\Delta x}^{t+\mathbf{i}\sqrt{3}\Delta t}\right) = \mathrm{S} \lhd\rhd_x \,\mathfrak{Im}\left(u_{x+\mathbf{i}\sqrt{3}\Delta x}^{t+\mathbf{i}\sqrt{3}\Delta t}\right) + \mathcal{O}(\Delta t^4, \Delta x^4), \tag{37}$$

$$\lhd\rhd_t \,\mathfrak{Im}\left(u_{x+\mathbf{i}\sqrt{2}\Delta x}^{t+\mathbf{i}\sqrt{2}\Delta t}\right) = \mathrm{S} \lhd\rhd_x \,\mathfrak{Im}\left(u_{x+\mathbf{i}\sqrt{2}\Delta x}^{t+\mathbf{i}\sqrt{2}\Delta t}\right) + (\mathrm{S}-1)\mathfrak{Im}\left(u_{x+\mathbf{i}\sqrt{2}\Delta x}^{t+\mathbf{i}\sqrt{2}\Delta t}\right) + \mathcal{O}(\Delta t^4, \Delta x^4). \tag{38}$$

Using approximations 11 and 9 in time and space, respectively, for the second-order wave equation, we can write the following discretizations in an operator form

$$\Delta_t^+ \mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) = \mathrm{S}^2\, \Delta_x^+ \mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) + \mathcal{O}(\Delta t, \Delta x), \tag{39}$$

$$\Box_t \,\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) = \mathrm{S}^2 \Box_x \,\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) + \mathcal{O}(\Delta t^4, \Delta x^4). \tag{40}$$

3.3 Comparison between the Finite-Difference and the Complex-Step-Finite-Difference methods for the 1-D wave equation

We compare all the previous discretization for the Courant number of one (S = 1), which is translated to modelling the wave propagation problem in homogeneous media. The main reason for this is to establish the most general similitude between FD and CSFD discretizations: It can be easily appreciated that all of the discretizations constructed can be reduced to the upwind and the leapfrog discretizations (for the first- and second-order wave equations) in homogeneous media.

Recall the general FD expression for the second-order wave equation (eq. 29)

$$\mathrm{val}(x, t + \Delta t) = \mathrm{S}^2[\mathrm{val}(x + \Delta x, t) + \mathrm{val}(x - \Delta x, t)] + 2(1 - \mathrm{S}^2)\,\mathrm{val}(x, t) - \mathrm{val}(x, t - \Delta t),$$

where val(x, t) represents the numerical value of the displacement to be propagated.

Also, recall the CSFD expression for the first-order wave equation (eq. 37) written in a general operator form as follows:

$$\mathrm{val}(x, t + \Delta t) = \mathrm{S}[\mathrm{val}(x + \Delta x, t) + \mathrm{val}(x - \Delta x, t)] - \mathrm{val}(x, t - \Delta t). \tag{41}$$

Both expressions are equivalent for S = 1, that is, there is an equivalence for the maximum Courant number in both expressions, reproducing same results by solving the second-order wave equation with the FDM and by solving the first-order wave equation with the Complex-Step-Finite-Difference method (CSFDM).

Note also that modelling the first-order wave equation using the upwind discretization (eq. 25) is exactly the same as modelling the second-order wave equation using discretization 39 (for S = 1), with the only difference being the numerical value to be propagated (displacements values with the FDM and values of the imaginary part of the imaginary perturbation of the displacement with the CSFDM), that is, both methods solve a different PDE following an equivalent solution structure. It means that we can model the two-way wave equation in a single direction using the CSFDM just like FD does with the one-way wave equation.

The same kind of analogy can be made for the discretization 33 of the second-order wave equation in homogeneous media and the CSFD discretizations 37 and 38. Those expressions are equivalent for $S = 1$, that is, they produce the same operation over different values, which means we can model the one-way wave equations in two directions using the CSFDM just like FDM does it for the two-way wave equation.

CSFD numerical simulations to the second-order wave equation using discretization 40 will involve the parasitic wave intrinsic to the leapfrog scheme to the one-way wave equation (see Thomas 1995, for more information about the parasitic wave). The effects of the parasitic mode can be solved introducing numerical dissipation. To this end and following the same approach of the Lax–Friedrich method (see Thomas 1995), we construct the following approximation:

$$\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t-\Delta t+\mathbf{i}\Delta t}\right) \approx \frac{1}{2}\left(\mathfrak{Im}\left(u_{x+\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) + \mathfrak{Im}\left(u_{x-\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right)\right), \tag{42}$$

which is the spatial mean of $\mathfrak{Im}(u_{x+\mathbf{i}\Delta x}^{t-\Delta t+\mathbf{i}\Delta t})$ at the previous time level. Thus, discretization 40 can be written as follows

$$\mathfrak{Im}\left(u_{x+\mathbf{i}\Delta x}^{t+\Delta t+\mathbf{i}\Delta t}\right) - \frac{1}{2}\mathfrak{Im}\left(u_{x+\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t} + u_{x-\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) = S^2\left(\mathfrak{Im}\left(u_{x+\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right) - \mathfrak{Im}\left(u_{x-\Delta x+\mathbf{i}\Delta x}^{t+\mathbf{i}\Delta t}\right)\right) + \mathcal{O}(\Delta t, \Delta x). \tag{43}$$

Discretization 43 is an analogous CSFD discretization to the popular Lax-Friedrich method for the one-way wave equation. A clear advantage is that discretization 43 propagates the wave in a single direction only, that is, using this discretization we are able to propagate the second-order wave equation without reflection, that is, there is no need of absorbing boundary conditions. Both directions are obtained by just interchanging signs in the velocity term (c). Although the first-order CSFD approximation 43 represents a new way of propagating the second-order wave equation in a single direction, it is low accurate in space and time, which makes it unsuitable for most realistic problems.

3.4 Numerical examples: 1-D wave equations simulations

Numerical examples are performed using an initial displacement function $f(x, 0)$ and a point source $f(x_s, t)$ as initial motion conditions in homogeneous media. The main advantage of the CSFDM over FDM is the order of accuracy reached with the difference operator used: we can obtain second-order accurate values at single step, that is, using two levels of information in time and space, and sixth-order of accuracy at two steps, that is, using only three levels of information in time and space. Another advantage is related to the methodology applied to impose initial motion conditions as illustrated in the next section.

3.4.1 Numerical methodology

The numerical methodology presented in this study for using CSFD approximations is rather different from all previous known FD analyses. As mentioned before, it is well known that there are several FD discretizations to the wave equation which solve the problem in an efficient way, for instance: the staggered grid, upwind, leapfrog, Lax-Wendroff, Lax-Friedrichs, MacCormack and Beam-Warming among many others methods.

In the most basic fashion, all of these methods use a *displacement* condition as an input to numerically propagate the wave. This displacement condition is given as an initial displacement ($f(x, 0)$) for the first-order wave equation, an initial displacement and velocity ($\dot{f}(x, 0)$) for the second-order wave equation or a time-dependent source ($f(x_s, t)$) for both cases (x_s is the application point of the source). All of these different FD discretizations are just simply *difference operators* (e.g. eqs 26 and 30) which solve the wave propagation problem in a convergent, consistent and stable way.

In order to propagate the imaginary part of the imaginary perturbation (in time and/or space) of the displacement required by the CSFDM, we have to construct the initial condition equivalent to those given by the FDM: In case of initial displacement ($u(x, 0)$), we just have to build its respective imaginary part of the imaginary perturbation in space ($\mathfrak{Im}(u(x + \mathbf{i}\Delta x, 0))$) at each corresponding grid point (see Fig. 3). In case of a point source, we have a time-dependent function evaluated at certain spatial grid point ($u(x_s, t)$) over different time

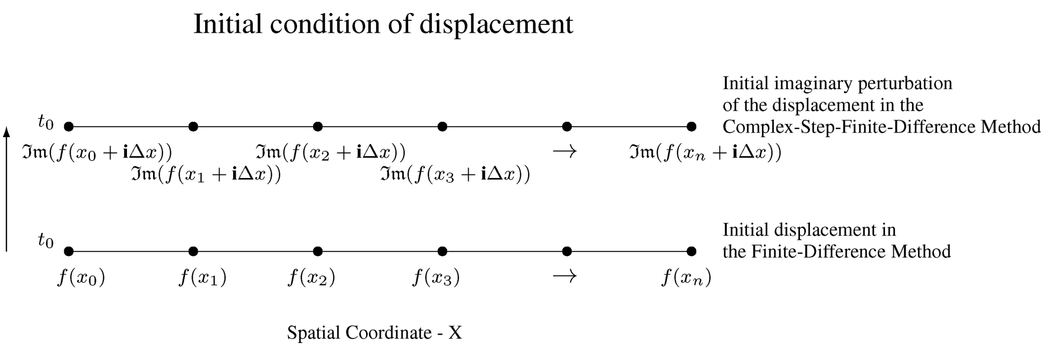

Figure 3. Initial conditions of displacement given in the FD and the CSFDMs: A replacement of the initial displacement $f(x, t_0)$ given in the FDM by its respective imaginary part of the imaginary perturbation in space ($\mathfrak{Im}(f(x + \mathbf{i}\Delta x, t_0))$) is made in the CSFDM as an initial step of the process.

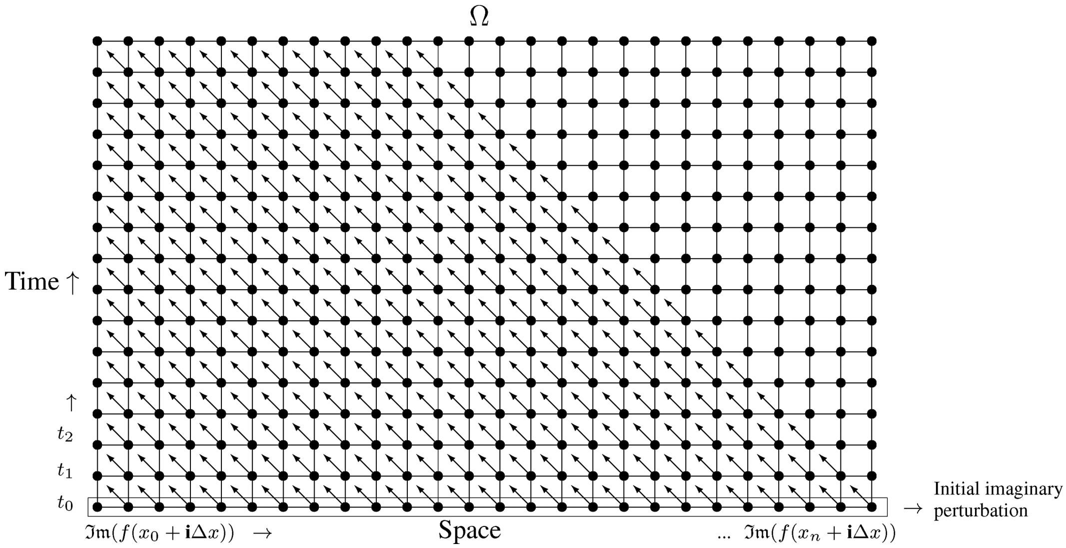

Figure 4. One-way wave simulation process in the CSFDM: propagation of the imaginary part of the imaginary perturbation in space in case of a given initial displacement.

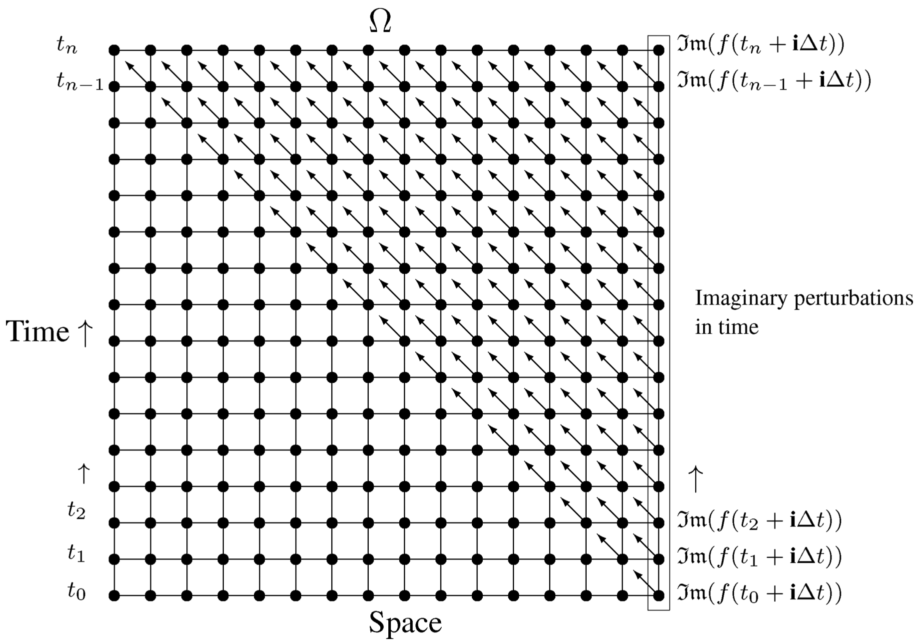

Figure 5. One-way wave simulation process in the CSFDM: propagation of the imaginary part of the imaginary perturbation in time in case of a given point source.

levels. In this case, we have to build its respective imaginary part of the imaginary perturbation in time ($\mathfrak{Im}(u(x_s, t + \mathbf{i}\Delta t))$) at each time level.

It is important to recall that we are not doing any change of domain from the real space ($\mathbb{R}$) to the complex space ($\mathbb{C}$). Spatial grid points remain the same, the only change that we apply is the numerical value to be propagated by the application of the selected *difference operator*.

The numerical methodology for using *higher-order accurate* CSFD discretizations is slightly different from *second-order* accuracy. In order to get higher-order accurate solutions we have to build the imaginary part of the imaginary perturbation, that is, $\mathfrak{Im}(u(x + \mathbf{i}v_x, 0))$ and/or $\mathfrak{Im}(u(x_s, t + \mathbf{i}v_t))$, where v_x and/or v_t are the most convenient values that produce the higher-order accuracy into the discretization.

A basic application of the FDM applied to the wave equation is to compute/propagate displacements at each time level and to compute velocities and/or accelerations using those displacement values. Unlike the FDM, the main application of the CSFDM presented in this study is to compute/propagate the imaginary part of the imaginary perturbation of the displacement (in time or space) and to be able to compute displacement, gradient, velocity, acceleration and/or acceleration values at each time level using those imaginary perturbation values.

Figs 4 and 5 illustrate the one-way wave propagation process of the imaginary part of the imaginary perturbation in space and time, respectively, given in the CSFDM.

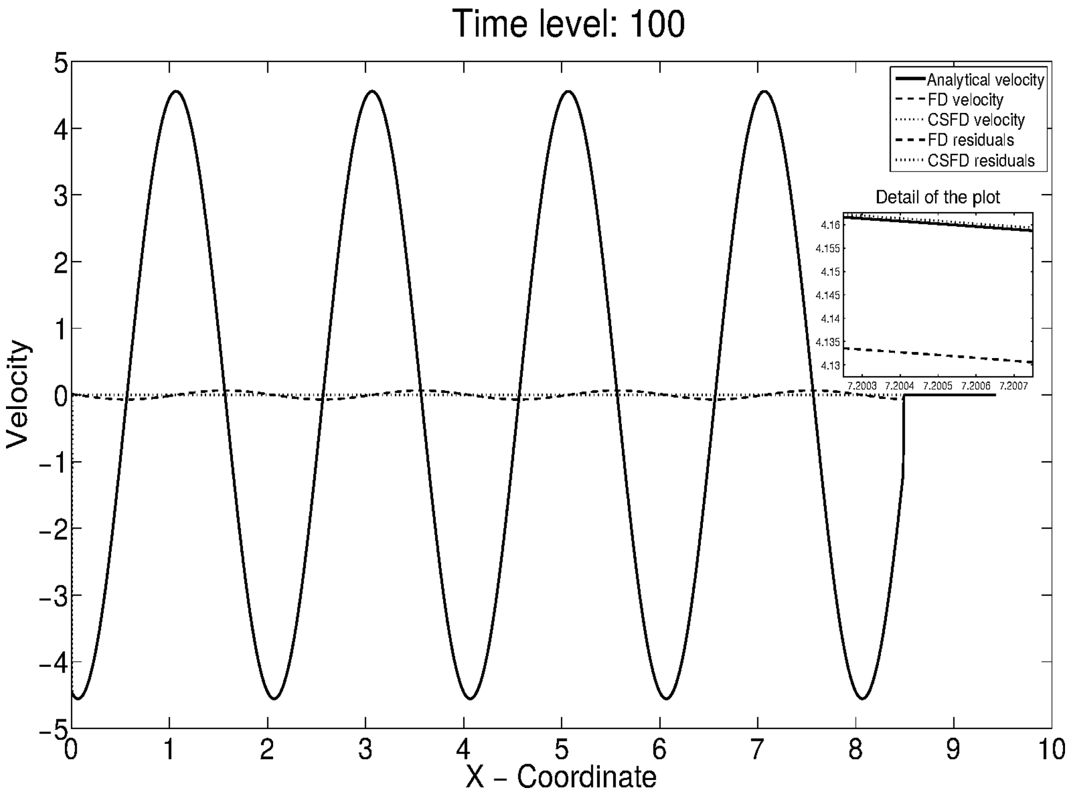

Figure 6. Velocity calculation comparisons using forward FD operator in the one-way wave simulation process with an initial condition: $f(x, 0) = \sin \pi x$. It can be appreciated how the CSFDM reproduces second-order accurate numerical values and the conventional FDM only first-order accurate values.

3.4.2 Initial condition: plane wave

For the first example, we solve the one-way wave equation considering the following initial displacement:

$$u(x, 0) = \sin \pi x, \quad \text{for} \quad 0 \le x \le 3\pi. \tag{44}$$

The analytical displacement solution to the initial value problem is obtained applying the d'Alembert general formula.

$$u(x, t) = \cos(\pi x + \pi c t), \quad \text{for} \quad 0 \le x \le 3\pi \quad \text{and} \quad t > 0, \tag{45}$$

with analytical velocity given by

$$\dot{u}(x, t) = -\pi c \sin(\pi x + \pi c t), \quad \text{for} \quad 0 \le x \le 3\pi \quad \text{and} \quad t > 0. \tag{46}$$

For numerical computations we use a regular grid: Total grid length 3π km. Number of space discretizations 1000 ($\Delta x = 0.0094$ km), number of time discretizations 500 ($\Delta t = 0.0065$ s) and wave speed equal to 1.450 km s^{-1} (Courant number equal to one, S = 1).

As mentioned in previous sections, the methodology presented here to compare results between FD and CSFD is simple: with the FDM we use eq. (44) as an initial motion condition, whereas with the CSFDM we have to construct initial conditions similar to those given.

The idea is to compute for each initial displacement given ($u(x + n\Delta x, 0)$ with $n = 0, \ldots, N$) its corresponding imaginary part of the imaginary perturbation (in space), that is

$$\Im\mathfrak{m}(u(x + n\Delta x + \mathbf{i}\Delta x, 0)) \quad \text{with} \quad n = 0, \ldots, N, \tag{47}$$

as an initial step of the process. In this first specific example, the condition is given by

$$\Im\mathfrak{m}(\sin(\pi(x + n\Delta x) + \mathbf{i}\Delta x, 0)) \quad \text{with} \quad n = 0, \ldots, 1000. \tag{48}$$

After this, any efficient difference operator can be used to propagate the wave in time.

Note that CSFDM mainly differs of FDM in setting initial conditions: because we make an imaginary perturbation in space in eq. (47), dividing by Δx we get displacement gradients at each time level. Boundary conditions will be related to *displacement gradient* values. In order to get velocity values we have to use the first-order wave equation.

We compare velocity values instead of displacement values (see Fig. 6). The reason of this is to highlight the advantages for computing derivative values using complex steps. Displacement values can be computed by the following expression:

$$u_x^{t+\Delta t} = u_x^t + \Im\mathfrak{m}\left(u_x^{t+\mathbf{i}\Delta t}\right) + \mathcal{O}(\Delta t^2), \tag{49}$$

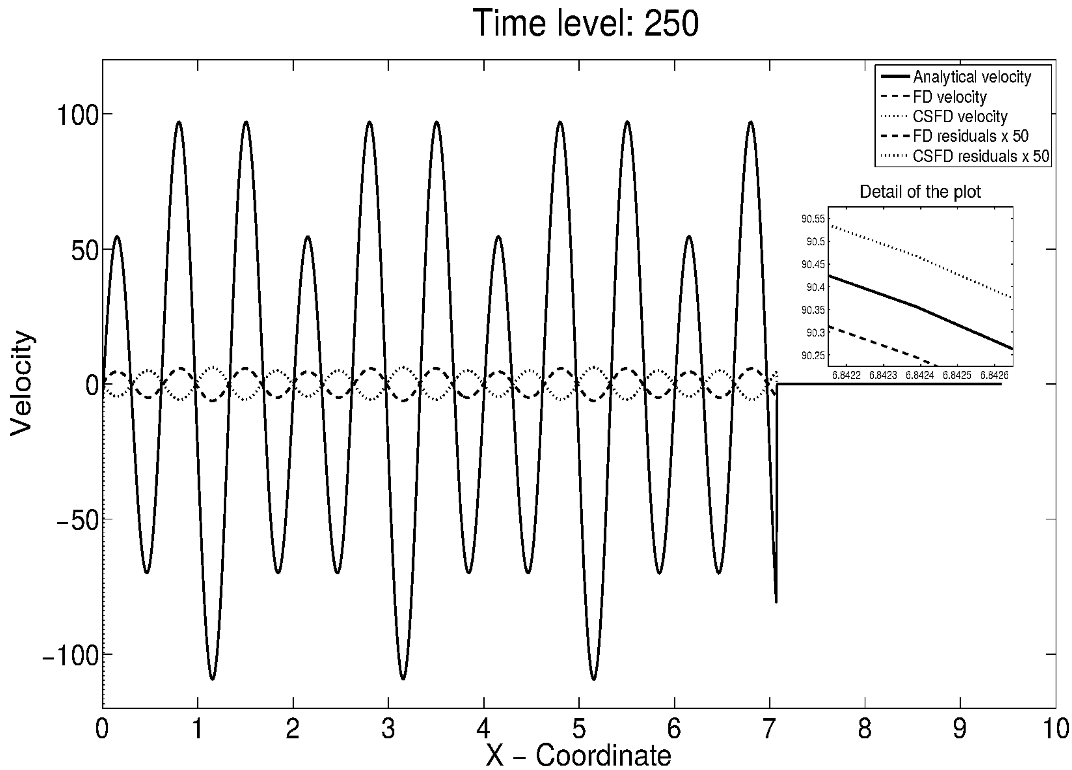

Figure 7. Velocity calculation comparisons using the forward FD operator in the one-way wave simulation process with an initial condition: $f(x, 0) = 3\sin 2\pi x + 6\cos 3\pi x$. It can be appreciated how the CSFDM reproduces second-order accurate numerical values using a single time level approximation (eq. 5) such as the conventional FD using three time levels (eq. 3).

using the initial displacement ($u(x, 0)$) and using the computed imaginary part of the imaginary perturbation (in time) of the displacement at each time level, we can obtain $u_x^{t+n\Delta t}$. We can also compute displacement values using the following expression

$$u_x^{t+\Delta t} = u_x^{t-\Delta t} + 2\,\Im\mathfrak{m}\left(u_x^{t+\mathrm{i}\Delta t}\right) + \mathcal{O}(\Delta t^3). \tag{50}$$

Note that eqs (49) and (50) correspond to numerical integration expressions.

Continuing, as a second example we just use a slightly more complicated initial condition:

$$u(x, 0) = 3\sin 2\pi x + 6\cos 3\pi x, \quad \text{for} \quad 0 \le x \le 3\pi. \tag{51}$$

The analytical solution to the initial value problem is

$$u(x, t) = 3\sin(2\pi x + 2\pi ct) + 6\cos(3\pi x + 3\pi ct), \quad \text{for} \quad 0 \le x \le 3\pi \quad \text{and} \quad t > 0, \tag{52}$$

with analytical velocity

$$\dot{u}(x, t) = 6\pi c\cos(2\pi x + 2\pi ct) - 18\pi c\sin(3\pi x + 3\pi ct), \quad \text{for} \quad 0 \le x \le 3\pi \quad \text{and} \quad t > 0. \tag{53}$$

The CSFDM reproduces the same results as the FDM using a single time level only instead of two time levels different from the evaluation point of the derivative (see Fig. 7). Here is one of the advantages of the CSFDM over the FDM; we can obtain same order of accuracy with different information. Note also that the residuals are orthogonal, the same relationship between pure real and pure imaginary numbers.

3.4.3 *Initial condition: source (time-dependent function)*

In this section, we show that we can use the CSFDM to place an input source (time-dependent function) at a single point to efficiently solve the point source wave propagation problem.

The methodology for a single point source is similar to the previous case: The idea is to compute for a certain time-dependent function $f(x_s, t)$ its corresponding imaginary part of the imaginary perturbation in time ($\Im\mathfrak{m}(f(x_s, t + \mathbf{i}\Delta t))$), as an initial step of the process. Later, we can use any efficient difference operator to propagate the wave, just like in the initial displacement case.

In order to illustrate this case, we use a Ricker source:

$$f(x_s, t) = \delta(x - x_s)\left(1 - 2f_0^2(t - t_0)^2\right)\exp\left(-f_0^2(t - t_0)^2\right), \tag{54}$$

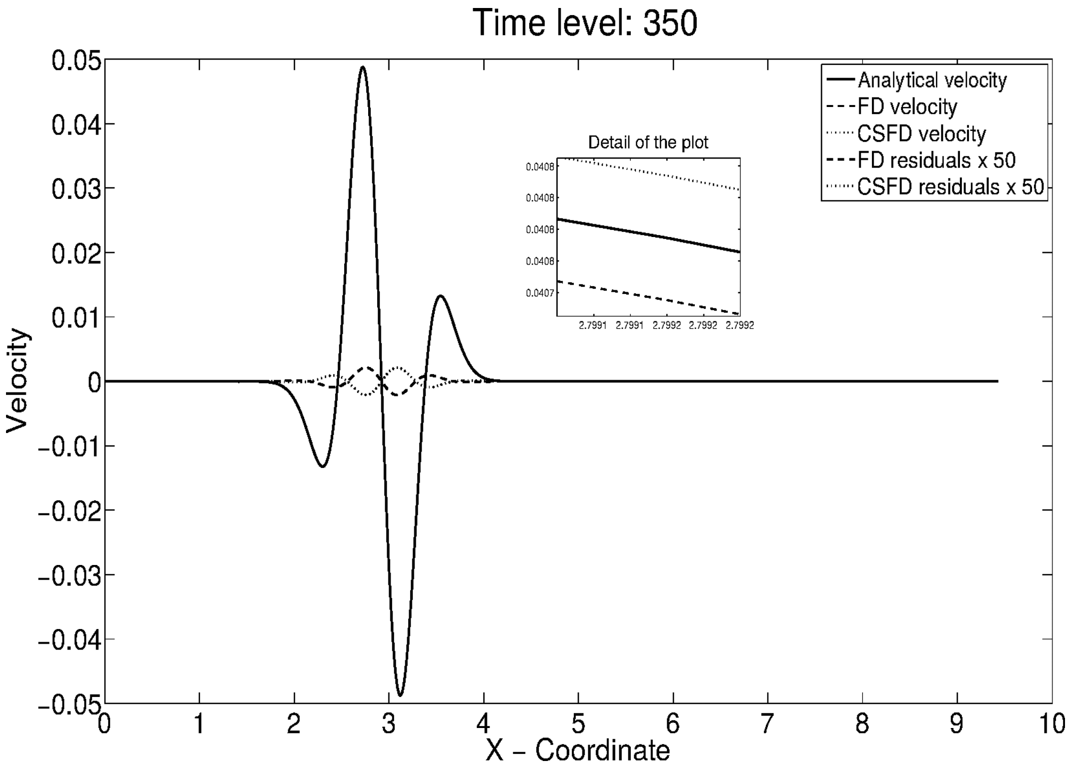

Figure 8. Velocity calculation comparisons using the forward FD operator in time and space in the one-way wave simulation process of a Ricker source. It can be appreciated how the CSFDM reproduces second-order numerical values using a single level approximation (eq. 5) such as the conventional FD using three time levels velocity approximation (eq. 3).

where δ is the Dirac delta function, f_0 is the dominant frequency and set in our example to $f_0 = 1/(40\Delta t)$, t_0 is the time delay (convenient to express it as multiple of $1/f_0$) and set to be $t_0 = 4/f_0$. We use the same spatial domain used in the initial displacement example.

Fig. 8 illustrates numerical results using a one-way propagation scheme. We can appreciate how the CSFDM reproduces the same velocity values as the FDM, that is, FD velocity values are computed using the centred approximation (eq. 3) and CSFD velocity values using one time level approximation (eq. 5). An important fact to highlight in Figs 7 and 8 is that FD and CSFD residuals are orthogonal.

Figs 9 and 10 illustrate results using the FD leapfrog discretization (eq. 24) for the second-order wave equation. We can appreciate how the CSFDM reproduces the solution in both directions and sixth-order accurate velocity values are obtained by using only three levels of information and compared with second-order FD velocity values using the same amount of time levels (see Fig. 9). Fourth-order acceleration values are computed using three time levels CS approximations and compared with second-order FD results (see Fig. 10).

We have seen that the CSFD discretizations 37 and 38 (equivalent for S = 1) propagate values by following the approximate structure solution to the second-order wave equation given by the ordinary FDM (eq. 30), so the absence of parasitic modes in the CSFD solution is not surprising. In fact, CSFDM permits to numerically describe two-way wave propagation with a first-order wave equation.

3.5 Boundary conditions

In all previous examples a rigid boundary was used but CSFD discretizations are not limited to rigid boundary conditions. It is well known that some FD discretizations for the one-way wave equation produces no reflection in a 1-D medium and no reflection in certain angles in 2-D and 3-D media (e.g. Clayton & Engquist 1980). The same principle is used in the CSFDM: In order to avoid reflections we may use a simple discretization for the one-way wave equation on the boundaries (e.g. eq. 39) or a simple paraxial approximation given by Clayton & Engquist (1980) and Reynolds (1978) among many others. Always taking into account the numerical value being propagated (imaginary part of the imaginary perturbation in time or space).

4 FINITE-DIFFERENCE AND COMPLEX-STEP-FINITE-DIFFERENCE METHODS APPLIED TO THE 2-D AND 3-D ACOUSTIC WAVE EQUATION

In order to introduce the CSFDM in a higher dimensional medium, in this section, we adopt a more general expression for the acoustic wave equation than the 1-D case presented before. The acoustic wave equation in a 1-D, 2-D or 3-D medium describes a longitudinal motion, that is, the directions of the particle motion and propagation are the same. Physical examples of acoustic motion are states of the matter like gases

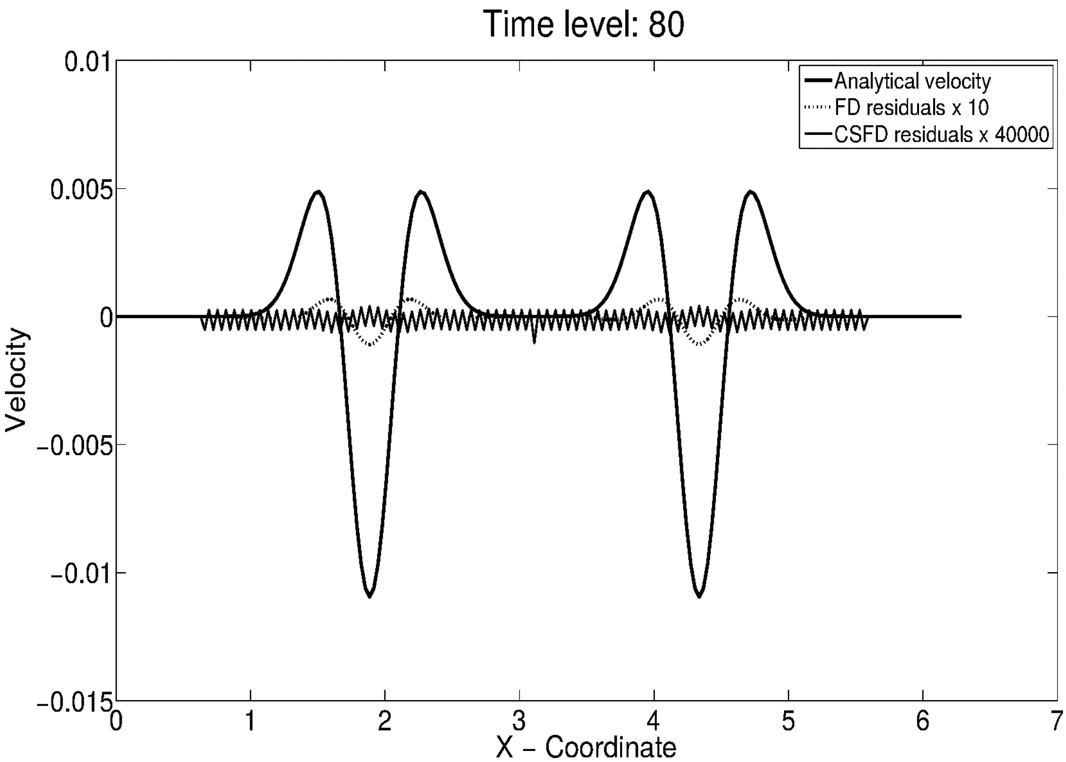

Figure 9. Velocity calculation comparisons using the leapfrog FD discretization for the second-order wave equation in homogeneous media. Second-order accurate velocity values are computed using the centred FD approximation (eq. 3) and the sixth-order CS approximation (eq. 14).

and liquids that, except for viscous stresses, do not respond to shear strain. The restoring force responsible for wave propagation phenomena is a result of a pressure change (normal stress) in the body.

The multidimensional second-order (two-way) acoustic wave equation is given by the following mathematical expression (Cohen 2002),

$$\frac{1}{\kappa(\boldsymbol{x})}\frac{\partial^2 \mathrm{P}}{\partial t^2}(\boldsymbol{x}, t) - \nabla\cdot\left(\frac{1}{\rho(\boldsymbol{x})}\nabla \mathrm{P}(\boldsymbol{x}, t)\right) = f(\boldsymbol{x}, t), \tag{55}$$

where P is the pressure, the operator $\nabla = (\partial/\partial x_1, \ldots, \partial/\partial x_d)^T$ is the gradient, the operator $\nabla\,\cdot$ is the divergence, ρ is the density and κ is the bulk modulus, both strictly positive functions of position the vector $\boldsymbol{x}$.

The velocity (c) of sound wave propagation is given by

$$c(\boldsymbol{x}) = \sqrt{\frac{\kappa(\boldsymbol{x})}{\rho(\boldsymbol{x})}}. \tag{56}$$

In the absence of sources ($f(\boldsymbol{x}, t)$), the motion conditions are given by

$$\mathrm{P}(\boldsymbol{x}, 0) = \mathrm{P}_0(\boldsymbol{x}), \quad \frac{\partial \mathrm{P}}{\partial t}(\boldsymbol{x}, 0) = \mathrm{P}_1(\boldsymbol{x}).$$

The first-order multidimensional wave equation or one-way acoustic wave equation is given by the following mathematical expression:

$$\frac{1}{\sqrt{\kappa(\boldsymbol{x})}}\frac{\partial \mathrm{P}}{\partial t}(\boldsymbol{x}, t) - \nabla\cdot\left(\frac{1}{\sqrt{\rho(\boldsymbol{x})}}\mathrm{P}(\boldsymbol{x}, t)\right) = f(\boldsymbol{x}, t), \tag{57}$$

In the absence of sources, the initial condition required is given by

$$\mathrm{P}(\boldsymbol{x}, 0) = \mathrm{P}_0(\boldsymbol{x}).$$

Eq. (57) has not been widely used in numerical simulations of wave propagation problems in a 2-D and/or 3-D medium by the FDM due to the intrinsic nature of the method to propagate the wave in a single direction. However, this property of unidirectional propagation has been widely used in the design of non-reflecting (absorbing) boundary conditions (e.g. Clayton & Engquist 1980).

On the other hand, paraxial approximations to the 2-D and 3-D second-order wave equation have been widely used in geophysical imaging/migration (e.g. Claerbout 1986; Tappert 1977). Also, exact one-way wave equations in a 2-D media have been used in the context of the Fourier domain, where the factorization of the wave equation is easily made (e.g. Angus *et al.* 2004).

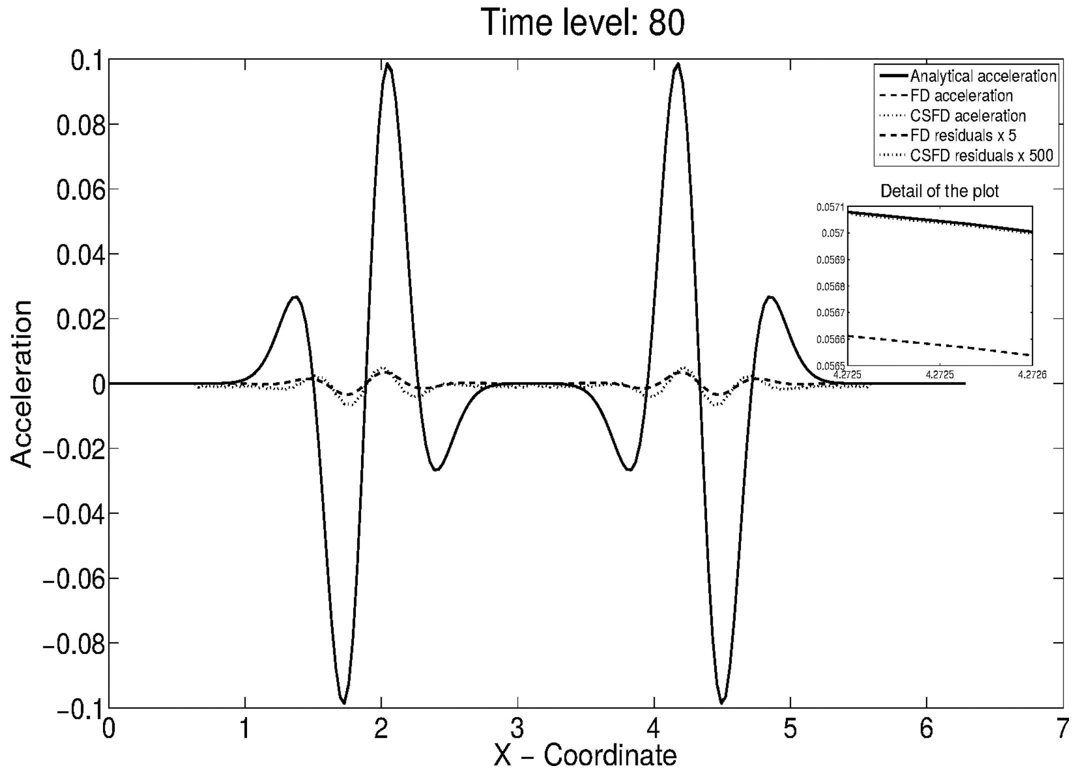

Figure 10. Acceleration calculation comparisons using the leapfrog FD discretization for the second-order wave equation in homogeneous media. Second-order accurate velocity values are computed using the centred FD approximation (eq. 3) and fourth-order accurate values using the CS approximation (eq. 8).

Commonly, first-order hyperbolic systems of coupled PDE are used to solve the wave propagation problem (e.g. Virieux 1986; Moczo *et al.* 2004). This is not the case of eq. (57), which is a higher dimensional non-coupled PDE.

4.1 Finite-Difference and Complex-Step-Finite-Difference discretizations to the 2-D acoustic wave equation

The most basic FD discretizations to the 2-D one-way homogeneous wave equation are made applying the forward (eq. 1) and the centred (eq. 3) approximations to the first-order derivative in time and space, which leads to the following expressions, respectively

$$\left(\Delta_t^+ - \mathrm{S}\left(\Delta_x^+ + \Delta_z^+\right)\right)\mathrm{P}_{x,z}^t + \mathcal{O}(\Delta t, \Delta x, \Delta z) = 0, \tag{58}$$

$$(\Box_t - \mathrm{S}(\Box_x + \Box_z))\mathrm{P}_{x,z}^t + \mathcal{O}(\Delta t^2, \Delta x^2, \Delta z^2) = 0. \tag{59}$$

Using the centred FD approximation for the second-order derivative (eq. 4) in time and space we can find the following FD discretization for the 2-D two-way homogeneous wave equation

$$\left(\Box_t^{1/2} \circ \Box_t^{1/2} - \mathrm{S}^2\left(\Box_x^{1/2} \circ \Box_x^{1/2} + \Box_z^{1/2} \circ \Box_z^{1/2}\right)\right)\mathrm{P}_{x,z}^t + \mathcal{O}(\Delta t^2, \Delta x^2, \Delta z^2) = 0. \tag{60}$$

In homogeneous media we can write eqs (58) and (60) as follows

$$(\rhd_t - \mathrm{S}(\rhd_x + \rhd_z))\mathrm{P}_{x,z}^t + \mathcal{O}(\Delta t, \Delta x, \Delta z) = 0, \tag{61}$$

$$(\lhd\rhd_t - \mathrm{S}^2(\lhd\rhd_x + \lhd\rhd_z))\mathrm{P}_{x,z}^t + \mathcal{O}(\Delta t^2, \Delta x^2, \Delta z^2) = 0. \tag{62}$$

The CSFD discretizations to the 2-D first-order wave equation using approximations 7 and 8 in time and space are given by the following expressions, respectively,

$$(\rhd_t - \mathrm{S}(\rhd_x + \rhd_z))\Im\mathrm{m}\left(\mathrm{P}_{x+\mathbf{i}\Delta x, z+\mathbf{i}\Delta z}^{t+\mathbf{i}\Delta t}\right) + \mathcal{O}(\Delta t, \Delta x, \Delta z) = 0, \tag{63}$$

$$(\lhd\rhd_t - \mathrm{S}(\lhd\rhd_x + \lhd\rhd_z))\Im\mathrm{m}\left(\mathrm{P}_{x+\mathbf{i}\sqrt{3}\Delta x, z+\mathbf{i}\sqrt{3}\Delta z}^{t+\mathbf{i}\sqrt{3}\Delta t}\right) + \mathcal{O}(\Delta t^4, \Delta x^4, \Delta z^4) = 0. \tag{64}$$

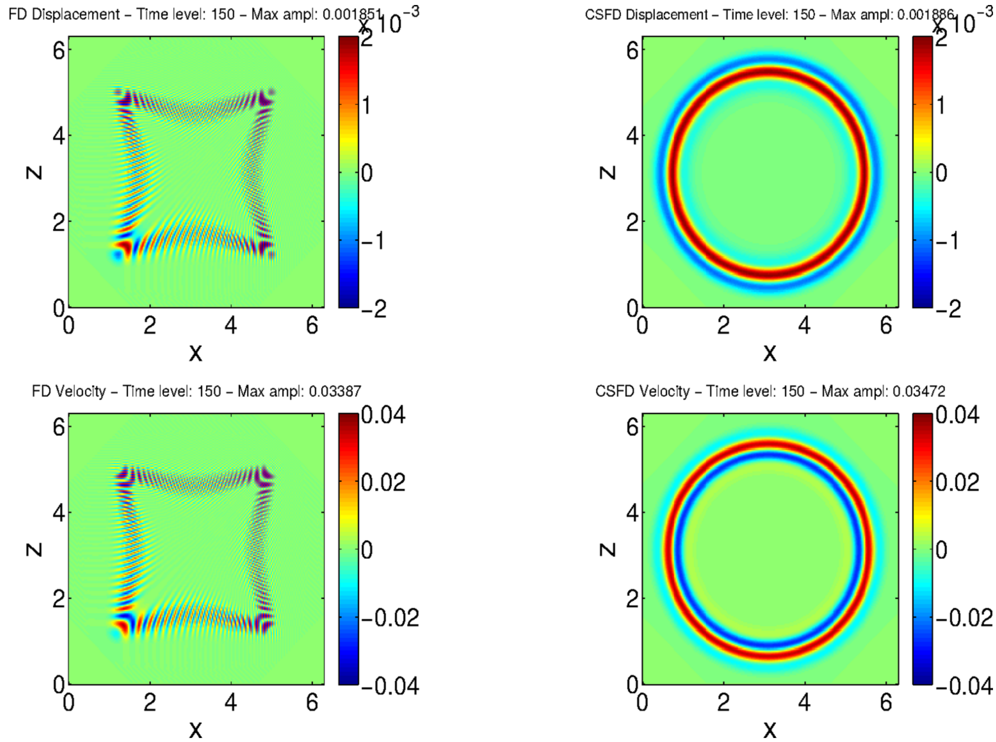

Figure 11. One-way 2-D acoustic wave equation snapshot simulation using the FDM and CSFDM: we can appreciate how the FDM propagates the wave in an angle of 45°, 135°, 225° and 315° only, unlike the CSFDM that correctly propagates the wave in all directions.

For the 2-D second-order wave equation we can find the following discretizations using approximations 9 and 11 (over time and space), respectively,

$$\left(\Delta_t^+ - \mathrm{S}^2\left(\Delta_x^+ + \Delta_z^+\right)\right)\mathfrak{Im}\left(\mathrm{P}^{t+\mathbf{i}\Delta t}_{x+\mathbf{i}\Delta x,z+\mathbf{i}\Delta z}\right) + \mathcal{O}(\Delta t, \Delta x, \Delta z) = 0, \tag{65}$$

$$(\Box_t - \mathrm{S}^2(\Box_x + \Box_z))\mathfrak{Im}\left(\mathrm{P}^{t+\mathbf{i}\Delta t}_{x+\mathbf{i}\Delta x,z+\mathbf{i}\Delta z}\right) + \mathcal{O}(\Delta t^2, \Delta x^2, \Delta z^2) = 0. \tag{66}$$

We have seen in previous sections the equivalence of modelling the 1-D second-order wave equation using the FDM and the 1-D first-order wave equation using the CSFDM. This can also be appreciated in the 2-D case: by simple inspection we see that eqs (62) and (64) produce the same operation but over different numerical values and with different accuracy. Another important difference is the power of the Courant number: It can be easily checked that the maximum value is $\mathrm{S} \leq 1/\sqrt{2}$ for the two-way wave equation (solved with the FDM), for which we get the characteristic solution (see Thomas 1995; Inan & Marshall 2011, for details) and $\mathrm{S} \leq 1/2$ for the one-way wave equation (solved with the CSFDM). It means we get the same results for the maximum Courant number of both schemes but over different time scales, as long as the motion conditions in both schemes are the same. The same analogy can be made for discretizations to the one-way wave equation using the FDM and the two-way wave equation using the CSFDM: we get exactly the same operation over different numerical values and different powers of the Courant number. In other words, the CSFDM solves the second-order wave equation by a discretization that has equivalent dispersion properties of the FD discretization to the one-way wave equation and the other way around, interchanging PDEs and methods.

4.1.1 Numerical example

In order to illustrate the FD and CSFD leapfrog discretizations to the one-way wave equation in a 2-D space (eqs 59 and 64, respectively), we present numerical simulations for a Ricker point source in a homogeneous medium: length in the x direction: $L_x = 2\pi$ km, length in the z direction: $L_z = L_x$, number of space discretizations: $nx = 200$ and $nz = nx$ ($\Delta x = \Delta z = 0.0314$ km), number of time levels: $nt = 200$, wave speed $c = 1.45\,\mathrm{km\,s^{-1}}$, Courant number: $\mathrm{S} = 0.5$, and time step $\Delta t = \mathrm{S}\Delta x/c$. The Ricker point source (eq. 54) has the following parameters: dominant frequency $f0 = 1/(10\Delta t)$ and time delay $t0 = 4/f0$.

It is well known that the leapfrog FD scheme in a 2-D space propagates the wave in 45°, 135°, 225° and 315° only and the rest of the space is filled by parasitic modes, unlike the CSFDM that properly propagates the wave in all directions (Fig. 11). Like mentioned in the 1-D case, the superiority of the leapfrog scheme for the second-order wave equation (eq. 60) over the leapfrog for the first-order wave equation (eq. 59) is regarding the presence of high-order oscillations that does not affect the convergence of the second-order leapfrog and it does for the first-order leapfrog [see Strikwerda (2004) page 195 for further details].

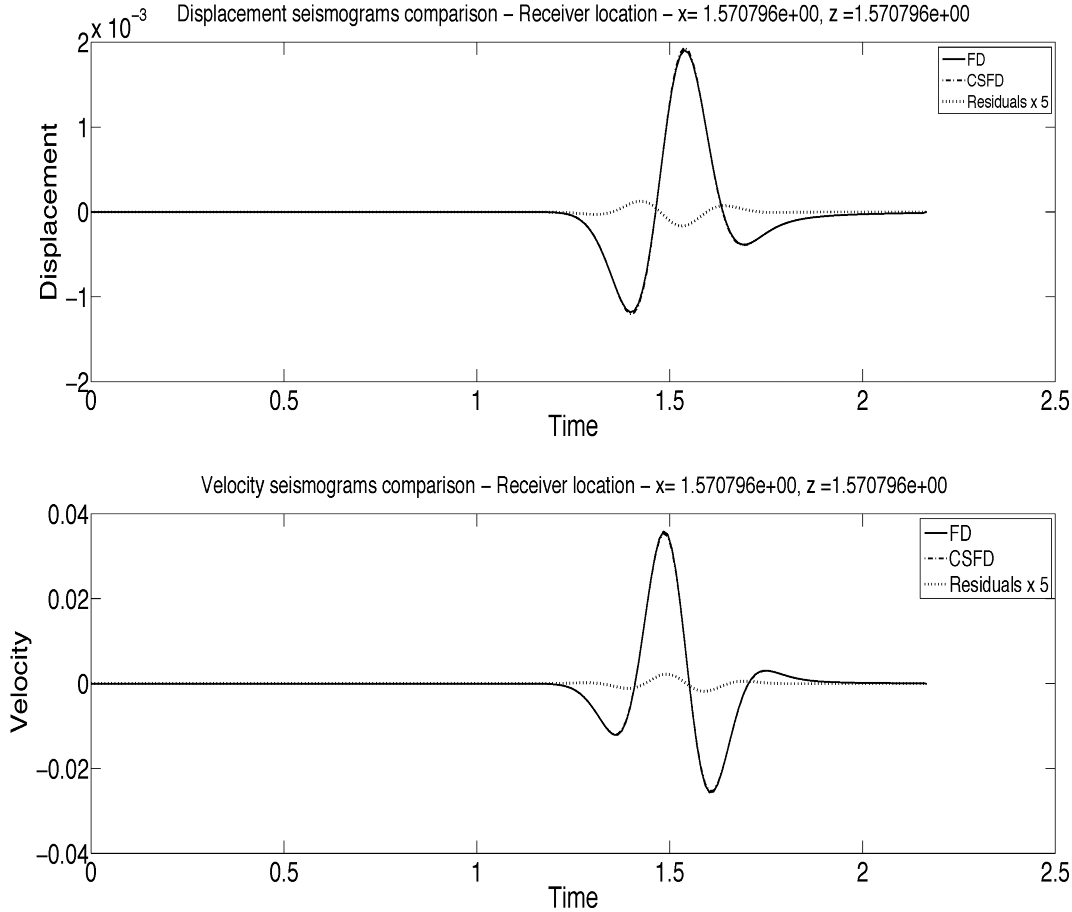

Figure 12. One-way 2-D acoustic wave equation simulation seismogram comparisons using the FDM and the CSFDM (receiver located at 45°).

Since the FDM properly propagates the first-order wave equation at certain angles (45, 135, 225 and 315), if a receiver is located at an angle of 45°, the solution found by the FDM and the CSFDM fit (Fig. 12). Fig. 13 illustrates seismogram comparisons found with the CSFDM and the analytical solution; as expected, propagating the wave using the maximum Courant number of 0.5, the method reproduces the analytical solution.

4.2 Finite-Difference and Complex-Step-Finite-Difference discretizations to the 3-D acoustic wave equation

FD and CSFD discretizations to the 3-D first- and second-order wave equations can be compared to the 2-D case analysed in the previous section: the main differences are related to inverse propagation properties modelling both wave equations using the two methods, that is, we are able to model the one-way wave equation in two directions and to model the two-way wave equation in a single direction using the CSFDM, which are exactly inverse properties compared to the FDM. On the other hand, another difference among the methods is related to the power of the Courant number and their accuracy.

3-D discretizations in both methods can be easily constructed by simply adding the third spatial coordinate into the different FD and CSFD discretizations presented in the previous section.

In all previous examples, we only considered homogeneous media and the maximum possible Courant number, which in all the discretizations produces the characteristic solution (see Thomas 1995; Strikwerda 2004; Strang 2007; Inan & Marshall 2011, for the dispersion analysis of the different FD discretizations). Like in the 2-D case, the main difference among the methods for the 2-D and 3-D case is related to the power of the Courant number: we can mention, in the 3-D case, the maximum Courant number of the FD discretization to the two-way wave equation is given by $S = 1/\sqrt{3}$. In the analogous CSFD discretization there is no square power of the Courant number, which implies the maximum Courant number to be $S = 1/3$, which is simply translated into a different time scale for the same grid used in both methods.

4.2.1 Numerical example

In order to illustrate the CSFD discretization to the one-way wave equation in a 3-D space, we present numerical simulations for a Ricker point source in a homogeneous medium: Length in the x direction $L_x = 2\pi$ km, length in the y and z direction $L_z = L_y = L_x$, number of space discretizations $nx = 50$ and $nz = ny = nx$ ($\Delta x = \Delta y = \Delta z = 0.0314$ km), number of time levels $nt = 100$, wave speed $c = 1.45\,\mathrm{km\,s^{-1}}$,

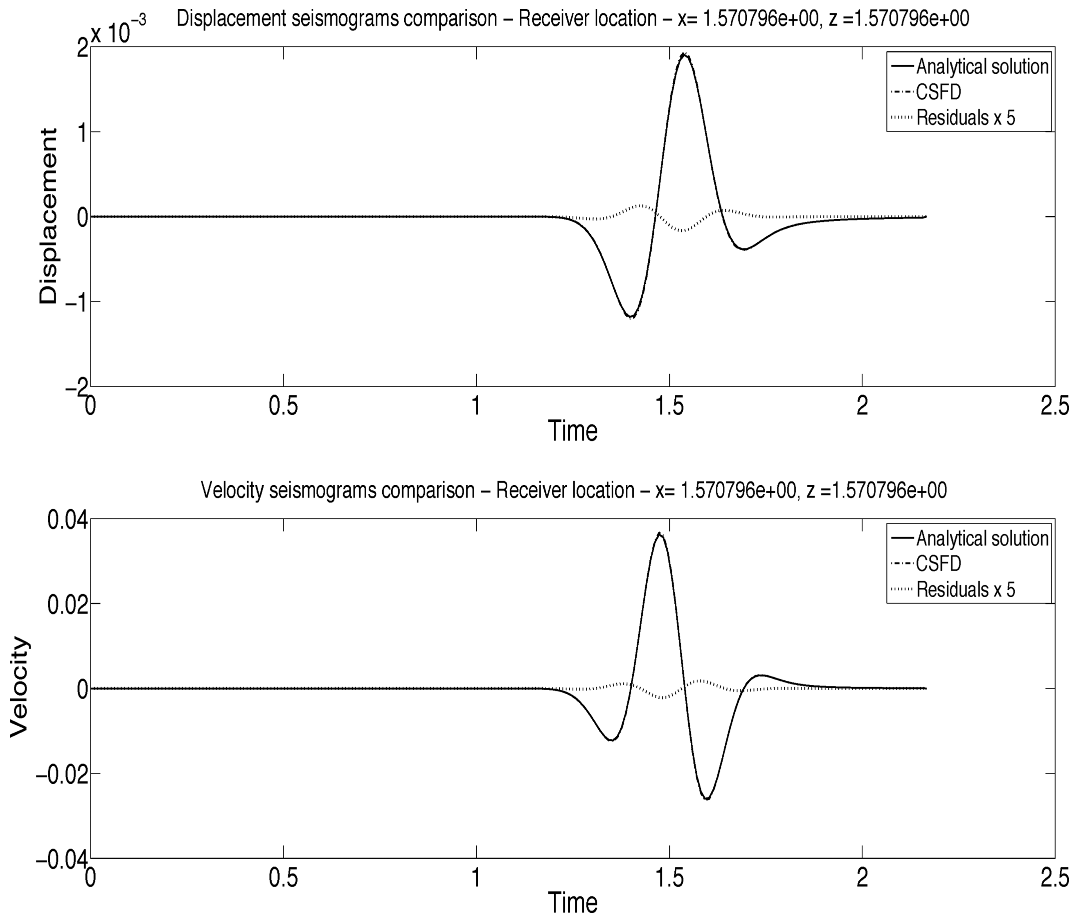

Figure 13. One-way 2-D acoustic wave equation simulation seismogram comparisons using the CFSDM against analytical solutions.

Courant number $S = 1/3$, time step $\Delta t = S\Delta x/c$. As motion condition we consider a Ricker source (eq. 54) with the following parameters: dominant frequency $f0 = 1/(10\Delta t)$ and time delay $t0 = 4/f0$.

Fig. 14 illustrates seismogram comparisons of CSFD results: as expected, using the maximum Courant number of $1/3$, the CSFDM reproduces the analytical solutions.

5 GENERALIZATION OF THE 3-D FINITE-DIFFERENCE, FINITE-ELEMENT, DISCONTINUOUS-GALERKIN AND SPECTRAL-ELEMENT METHODS USING COMPLEX-STEPS

The natural targets for numerical modelling of wave propagation are heterogeneous media. In general heterogeneous media, an analytical solution for the wavefield is not available, and we have to recur to numerical methods. There is not a single numerical method that is suitable for all types of configurations that the physical problem can adopt, that is, there is not a best numerical method that solves all kind of problems. Research scientists must be very aware of the application area that each numerical method possesses to determine which one to use in order to solve the physical problem of interest.

Nowadays exist a huge variety of numerical methods used in computational seismology. The most popular are probably the FD, Finite-Element, Spectral-Element and Discontinuous-Garlerkin methods. Each of them has their own advantages and disadvantages.

Despite the improvement in accuracy in velocity and acceleration solutions by the introduction of complex steps, as showed in previous CSFD discretizations for the one-way and two-way wave equations, the use of CSFD discretizations (based on the introduction of complex steps in the Taylor's series) to the wave equation (one and two-way) is found to show inaccurate results in the presence of heterogeneous media. Abreu (2014) presented a detailed study of stability and dispersion–dissipation properties of possible CSFD discretizations to be used in heterogeneous media. All of them showed disappointing results. However, the performance of the CSFD methodology introduced in this study can be assessed directly from our previous considerations combined with the most popular numerical techniques used nowadays.

Numerical techniques can be easily adapted to the use of complex steps and this modification will principally lead to more accurate fields, while the structure of the numerical solution of each method remains the same, that is, the discretization keeps all the properties of propagation, dispersion–dissipation that the numerical solution possesses. In other words, taking the best of the CSFDM (regarding its higher accuracy) and the best of the working numerical schemes for heterogeneous media (regarding dispersion–dissipation properties).

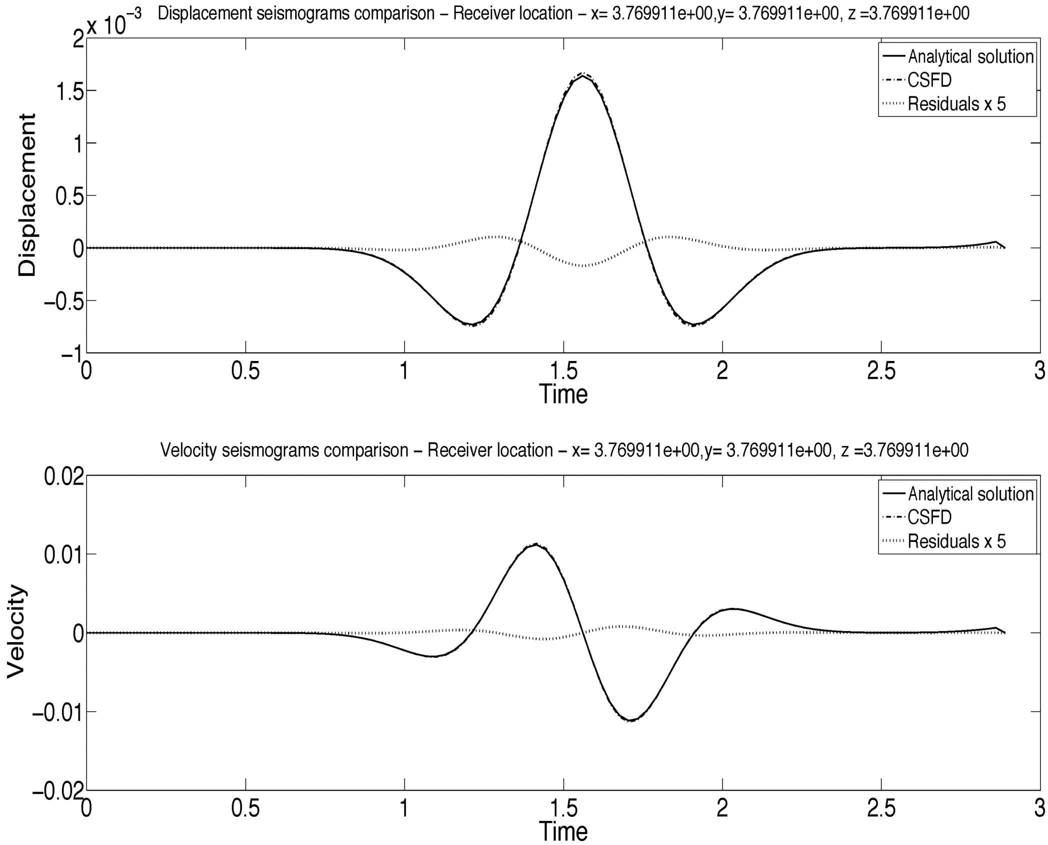

Figure 14. One-way 3-D acoustic wave equation simulation seismogram comparisons using the CFSDM against the analytical solution.

The CSFDM applied in heterogeneous media, presented in this study, does not involve a new differential operator to solve the elastic wave equation in heterogeneous medium. As stated before, the CSFDM can be combined with any known working numerical technique with the only difference in the value to be propagated using the selected scheme, from which we can compute more accurate fields than those obtained by common FD techniques.

In order to illustrate the previous statements, in the next section we describe how to apply the CSFDM to the elastic wave equation in a 3-D heterogeneous medium (for a concise and clear derivation of the equation of motion in elastic medium refer to Slawinski 2010).

5.1 The 3-D elastic wave equation

We consider the displacement formulation of the equation of motion without the body force term, given by the following mathematical expressions (see Moczo *et al.* 2014)

$$\begin{aligned}
\frac{\partial^2 u_x}{\partial t^2} &= \alpha^2\left(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_y}{\partial y\partial x}+\frac{\partial^2 u_z}{\partial z\partial x}\right)+\beta^2\left(\frac{\partial^2 u_x}{\partial y^2}-\frac{\partial^2 u_y}{\partial y\partial x}+\frac{\partial^2 u_x}{\partial z^2}-\frac{\partial^2 u_z}{\partial z\partial x}\right)\\
\frac{\partial^2 u_y}{\partial t^2} &= \alpha^2\left(\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_z}{\partial z\partial y}+\frac{\partial^2 u_x}{\partial x\partial y}\right)+\beta^2\left(\frac{\partial^2 u_y}{\partial z^2}-\frac{\partial^2 u_z}{\partial z\partial y}+\frac{\partial^2 u_y}{\partial x^2}-\frac{\partial^2 u_x}{\partial x\partial y}\right)\\
\frac{\partial^2 u_z}{\partial t^2} &= \alpha^2\left(\frac{\partial^2 u_z}{\partial z^2}+\frac{\partial^2 u_x}{\partial x\partial z}+\frac{\partial^2 u_y}{\partial y\partial z}\right)+\beta^2\left(\frac{\partial^2 u_z}{\partial x^2}-\frac{\partial^2 u_x}{\partial x\partial z}+\frac{\partial^2 u_z}{\partial y^2}-\frac{\partial^2 u_y}{\partial y\partial z}\right),
\end{aligned}\tag{67}$$

where $\alpha=\sqrt{\frac{\lambda+2\mu}{\rho}}$ the *P*-wave velocity and $\beta=\sqrt{\frac{\mu}{\rho}}$ the *S*-wave velocity.

Following Moczo *et al.* (2011), discretizations in space of eq. (67) using the FDM, FEM, SEM and DGM can be represented in a unified form given by the following expressions:

$$\begin{aligned}
\frac{\partial^2 u_x}{\partial t^2} &= \beta^2\Big[r^2\left(D_{xx}\,u_x^t+D_{yx}\,u_y^t+D_{zx}\,u_z^t\right)+D_{yy}\,u_x^t-D_{yx}\,u_y^t+D_{zz}\,u_x^t-D_{zx}\,u_z^t\Big]+\mathcal{O}(\Delta\boldsymbol{x}^m),\\
\frac{\partial^2 u_y}{\partial t^2} &= \beta^2\Big[r^2\left(D_{yy}\,u_y^t+D_{zy}\,u_z^t+D_{xy}\,u_x^t\right)+D_{zz}\,u_y^t-D_{zy}\,u_z^t+D_{xx}\,u_y^t-D_{xy}\,u_x^t\Big]+\mathcal{O}(\Delta\boldsymbol{x}^m),\\
\frac{\partial^2 u_z}{\partial t^2} &= \beta^2\Big[r^2\left(D_{zz}\,u_z^t+D_{xz}\,u_x^t+D_{yz}\,u_y^t\right)+D_{xx}\,u_z^t-D_{xz}\,u_x^t+D_{yy}\,u_z^t-D_{yz}\,u_y^t\Big]+\mathcal{O}(\Delta\boldsymbol{x}^m),
\end{aligned}\tag{68}$$

where the order of the error m depends on the numerical technique chosen and $r^2=\frac{\alpha}{\beta}$.

Each numerical technique differs in the form of the operators $D_{\xi\eta}$ with $\xi, \eta \in \{x, y, z\}$ for approximating derivatives.

Moczo *et al.* (2011) present a very concise and understandable study on the differences of FDM, FEM, SEM and DGM, regarding their accuracy with respect to *P*-wave to *S*-wave speed ratio. In this study, we focus on their similarities. The FDM, FEM, SEM and DGM have in common FD discretizations in time. The most familiar and simplest FD discretization for the second-order time derivative of displacement is the leapfrog approximation (eq. 4).

Unlike differential steps in space or grid spacing (Δx, Δy, Δz), the differential step in time or time step (Δt) is a constant parameter during the entire numerical simulation (at least in the most common numerical applications, however there exist the concept of local time step, for which the methodology presented in this work would not apply). The value of Δt depends on the maximum value of the Courant number that the numerical technique can handle and the spatial steps (grid spacing) chosen by the user of the numerical technique.

Following Moczo *et al.* (2011), we can write the equations of motion (eqs 68) discretizing time using the leapfrog approximation (eq. 4) as follows

$$u_x^{t+\Delta t} - 2u_x^t + u_x^{t-\Delta t} = \Delta t^2\beta^2\Big[r^2\left(D_{xx}\,u_x^t + D_{yx}\,u_y^t + D_{zx}\,u_z^t\right) + D_{yy}\,u_x^t - D_{yx}\,u_y^t + D_{zz}\,u_x^t - D_{zx}\,u_z^t\Big] + \mathcal{O}(\Delta\boldsymbol{x}^m, \Delta t^2),$$

$$u_y^{t+\Delta t} - 2u_y^t + u_y^{t-\Delta t} = \Delta t^2\beta^2\Big[r^2\left(D_{yy}\,u_y^t + D_{zy}\,u_z^t + D_{xy}\,u_x^t\right) + D_{zz}\,u_y^t - D_{zy}\,u_z^t + D_{xx}\,u_y^t - D_{xy}\,u_x^t\Big] + \mathcal{O}(\Delta\boldsymbol{x}^m, \Delta t^2),$$

$$u_z^{t+\Delta t} - 2u_z^t + u_z^{t-\Delta t} = \Delta t^2\beta^2\Big[r^2\left(D_{zz}\,u_z^t + D_{xz}\,u_x^t + D_{yz}\,u_y^t\right) + D_{xx}\,u_z^t - D_{xz}\,u_x^t + D_{yy}\,u_z^t - D_{yz}\,u_y^t\Big] + \mathcal{O}(\Delta\boldsymbol{x}^m, \Delta t^2). \quad (69)$$

The fact that eqs (69) represent a second-order approximation in time is simple: based on displacement values at three time levels ($t - \Delta t$, t, $t + \Delta t$), we are able to compute velocity and acceleration values using leapfrog approximations for the first- and second-order derivatives up to second-order accuracy only.

A different approach, suggested in this study, is to apply the concept of the CSFDM and to propagate the imaginary part of the imaginary perturbation in time and/or space of the displacement, and to be able to compute velocity, acceleration and/or strain values at each time level. As already showed in the homogeneous case, using these imaginary part based values, we are able to compute motion fields with higher accuracy than by using displacements.

Note that like in the acoustic case, the FDM, FEM, SEM and DGM are simply difference (or summation) operators that propagate displacement values at different time levels by following an approximate efficient and convergent solution to the elastic wave equation in an isotropic medium.

Following Moczo *et al.* (2011), we can use a unified symbolic expression for all numerical methods as follows

$$u_\xi^{t+\Delta t} = \text{numerical scheme}\ \left\{u_\eta^{t-\Delta t}, u_\zeta^t\right\}, \quad (70)$$

or, equivalently

$$u(I, J, K, t + \Delta t) = \text{numerical scheme}\ \{u(I, J, K, t - \Delta t), u(I, J, K, t)\}, \quad (71)$$

with $\xi, \eta, \zeta \in \{x, y, z\}$ and $u^{t+\Delta t}$, u^t, $u^{t-\Delta t}$ represent displacement components at relevant grid positions around (I, J, K) at times $t + \Delta t$, t and $t - \Delta t$, respectively.

Using each different technique's numerical operator, we can propagate the imaginary part of the imaginary perturbation in time or space. Before we proceed, like in the acoustic case, note that propagating the imaginary perturbation *does not* affect the dispersion properties of each method, that is, the only difference is in the accuracy of the solutions that we are able to obtain.

We can write the most general symbolic expression for the CSFM applied to the elastic wave equation as follows:

$$\mathfrak{Im}\left(u_\xi^{t+\Delta t+\mathrm{i}\Delta t}\right) = \text{numerical scheme}\left\{\mathfrak{Im}\left(u_\eta^{t+\mathrm{i}\Delta t}\right), \mathfrak{Im}\left(u_\zeta^{t-\Delta t+\mathrm{i}\Delta t}\right)\right\}, \quad (72)$$

for a perturbation in time (time-dependent point source), and

$$\mathfrak{Im}\left(u_{\xi+\mathrm{i}\xi}^{t+\Delta t}\right) = \text{numerical scheme}\left\{\mathfrak{Im}\left(u_{\eta+\mathrm{i}\eta}^{t}\right), \mathfrak{Im}\left(u_{\zeta+\mathrm{i}\zeta}^{t-\Delta t}\right)\right\}, \quad (73)$$

for a perturbation in space (initial plane wave source).

The terms $\mathfrak{Im}(u_{\xi+\mathrm{i}\xi}^{t+\Delta t})$, $\mathfrak{Im}(u_{\eta+\mathrm{i}\eta}^{t})$ and $\mathfrak{Im}(u_{\zeta+\mathrm{i}\zeta}^{t-\Delta t})$ refer to the imaginary part of the imaginary perturbation in space for relevant grid points $\xi, \eta, \zeta \in \{x, y, z\}$ that each different numerical scheme requires.

5.1.1 Case of a point source:

In case of a point source we compute the perturbation of the displacement in time, that is, $\mathfrak{Im}(u_\xi^{t+\mathrm{i}\Delta t})$.

Because we cannot compute fourth-order or sixth-order accurate values for first- and second-order derivatives using the same relation between the differential steps of the CS approximation (h, v), we have to decide, at the beginning of the simulation process, which value are we interested in: displacement, velocities or accelerations. Having decided the field that we want to compute with fourth (or sixth) order accuracy, we can proceed to perform the numerical simulation.

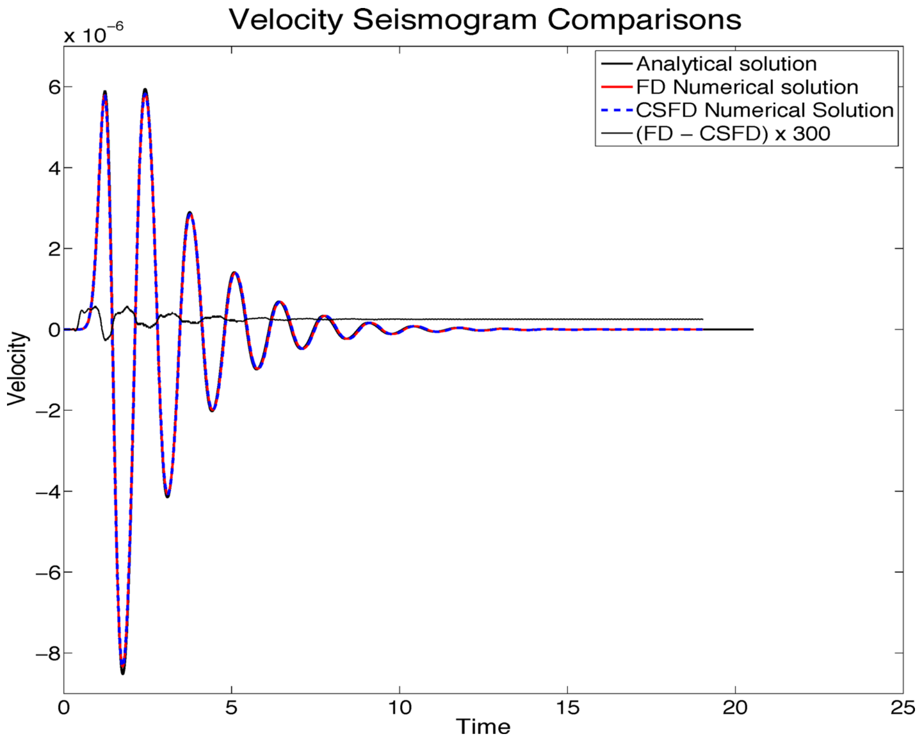

Figure 15. Single layer over a halfspace simulation using the Spectral-Element method. Velocity solutions are computed using a second-order FD and sixth-order CSFD approximations.

5.1.2 Case of an initial plane wave:

In case of a plane wave, we compute the perturbation of the displacement in space, that is, $\mathfrak{Im}(u^{t+\Delta t}_{\xi+\mathbf{i}\xi})$, with $\xi \in \{x, y, z\}$. Like in the point source case, we have to decide the order of the derivative that we want to approximate with a four (or sixth) order accuracy. Having decided, we can perform the numerical simulation with the only difference, from a regular simulation, in the numerical value to be propagated.

5.1.3 Numerical simulations

Usually, existing numerical schemes have been carefully benchmarked against analytical solutions for particular model geometries (flat layers) or pseudo-analytical solutions for the common approximation of Earth's heterogeneity through a layered halfspace. In this section, we apply the CSFDM to a conceptually simple example of a heterogeneous medium: a layer over an elastic halfspace.

We emphasize that we do not develop any new differential operator to solve the elastic wave equation in heterogeneous medium. The structure of the numerical solution of each method remains the same, that is, the discretization keeps all the properties of propagation, dispersion–dissipation that the numerical solution possess. The only difference is given by the value to be propagated using the selected numerical scheme, from which we can compute more accurate fields than those given by common FD techniques. In other words, with the combination of the CSFDM over a pre-existing numerical technique, we only improve the accuracy of the method for computing certain fields.

The physical model of our example consists of a homogeneous elastic layer over halfspace: layer thickness 200 m. Density and elastic velocity vales are presented in Table 1.

The source is a time-dependent function defined by a Garbor signal as follows

$$s(t) = e^{-\left(\frac{2\pi f_p(t-t_s)}{\gamma}\right)^2} \cos 2\pi f_p(t - t_s) + \Psi, \tag{74}$$

with parameters: $\gamma = 1, f_p = 0.45$ Hz, $\Psi = \frac{\pi}{2}$ and $t_s = 1$ s. The source time function is exited at the depth of 600 m.

The size of the computational model is 31000 m. At the top of the computational model applies the free surface condition. At the bottom of the computational model non-reflecting boundary conditions are applied (one-way approximation of the wave equation).

One receiver is located at the free surface. The model is discretized with a regular grid spacing of 35 m. 6 GLL points per element, a Courant number of 0.5 and time discretization of 0.0056 s are used. The source and interface are located at the closest GLL points. Total simulation time of 19 s.

Fig. 15 shows results from a simulation using the SEM. Velocity values are computed using the second-order leapfrog approximation (eq. 3) and the sixth-order CSFD approximation (eq. 14).

Due to that the analytical solution is computed using a pseudo-analytical method (obtained from Moczo *et al.* 2004); We cannot control how accurate the solution is. However, we found a good agreement with results obtained using FD and CSFD approximations for velocity values. Theoretically, CSFD results are more accurate than those found by FD, as shown in the homogeneous case, when an exact solution to the wave propagation problem was available. The differences between the solutions found using FD and CSFD approximations for velocity values are in the order of 2×10^{-9}.

6 GENERAL DISCUSSION

In this study, we have presented a new methodology in order to improve the accuracy of pre-existing numerical techniques widely used to solve the elastic wave propagation phenomena in heterogeneous media. All the mentioned numerical techniques that can be generalized by the use of complex steps have been well benchmarked. The use of complex steps will only represent slightly different seismograms (more accurate fields), which led us to state that for any numerical technique implemented in realistic media, the key feature to study and enhance are dispersion–dissipation properties, over time and space domains (as studied by Abreu 2014; Moczo *et al.* 2014), instead of looking to reproduce more accurate values. We also emphasize that the introduction of higher accurate schemes alone, for instance in time, may not bring substantial improvement in the numerical method, unless the dispersion–dissipation properties are favourable to improve the numerical technique.

The most appropriate numerical scheme used to solve the wave propagation phenomena should minimize differences between numerical and analytical dispersion–dissipation properties, besides being more accurate and faster from the computational point of view. In this sense, the finding of better numerical methods should be considered as a minimization problem.

7 CONCLUSIONS

Based on the work by Abreu *et al.* (2013), we have introduced the CSFDM to solve with higher-order accuracy the acoustic wave equation in 1-D, 2-D and 3-D homogeneous medium and the elastic wave equation in general heterogeneous media using compact stencils. Making the use of complex numbers in numerical modelling of wave propagation and using difference operators, this work extends the well known FDM, FEM, SEM and DGM to the use of complex-steps approximations and permits to compute more accurate results under the same computational requirements and dispersion–dissipation properties. Advantages of the introduced CSFDM are the separation between gradients and velocities as initial motion conditions of the wave propagation problem. The introduced numerical method is based on a generalization of the standard FDM and therefore its implementation is rather simple and straightforward. The benchmarking of the CSFDM against the standard SEM for a simple scenario shows an excellent agreement. We have introduced, from a methodological and theoretical point of view, the correct use of complex-step derivatives in numerical simulations of seismic wave propagation using the FEM, SEM and DGM. This study shows how to obtain up to sixth-order accurate velocity values, in a compact three levels stencil, making slight modifications of any of the previous mentioned techniques. Although we have focused our attention in the acoustic and elastic wave equations, it is expected that complex steps can be naturally extended to find more accurate solutions for various PDEs found in the geophysical field, such as Navier–Stokes equations and shallow water equations among many others. A wide possible range of applications of the CSFDM is yet to be explored. Further studies are required to fully understand the complete potential of the use of complex numbers in numerical modelling.

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