

On the relation between sources and initial conditions for the wave and diffusion equations



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ABSTRACT

In seismic forward modeling and fluid–flow simulations, sources and initial conditions are two approaches to initiate the perturbation of the medium in order to compute synthetic seismograms and pore–pressure maps of a reservoir, respectively. Assuming delta functions in time and space, source and initial particle velocity are equivalent in the first case (wave equation), while in the second case (diffusion equation) source and diffusion field are equivalent. The differential equation based on fractional derivatives unifies both cases but those equivalences break down when the order of the derivative is not a natural number. A simulation example, based on the fractional wave equation, illustrates the implementation of the source with a band-limited time history on a numerical mesh. In this case, the implementation of the initial condition requires a numerical calculation since the medium is heterogeneous. Body forces and stress sources (e.g., earthquakes) can easily be related in uniform media. A 1D example shows such a relation.

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1. Introduction

The correct source modeling in direct grid methods is essential in hydrocarbon prospecting and earthquake seismology to compute synthetic seismograms, as well as in reservoir simulations, where the governing equations are based on the diffusion equation [1,2]. The initiation of the wavefield by sources or initial conditions is partially outlined in the literature but not fully detailed and verified. In most cases, there is not even the complete information (e.g., wave shape, frequency) to reproduce the results, yet being this aspect of numerical modeling essential.

We show in this work the equivalences and the differences between the two approaches by using the 1D differential equation, which allows us to provide simple but insightful mathematical demonstrations. First, we consider the wave equation with a source term (the inhomogeneous equation) and initial conditions. We obtain the solution by performing a double Fourier transform to the wavenumber–Laplace domain, and by means of the residue theorem we get the explicit closed-form solution in the space–time domain. The same procedure is applied to the diffusion equation. We generalize the approach by considering the fractional differential equations, which include both the wave and diffusion equation.

Details of the source implementation in a 2D full-wave modeling algorithm based on the fractional differential equation are shown, where the spatial derivatives are computed with the Fourier pseudospectral method and the fractional time

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derivative is approximated with the Grünwald–Letnikov series [3]. The Fourier method used here is accurate (negligible numerical dispersion) up to the maximum wavenumber of the mesh that corresponds to a spatial wavelength of two grid points [2]. A final 1D example shows the relation between body forces and stress sources.

2. The wave equation

Let us consider the 1D wave equation

$$u_{,tt} - c^2 u_{,xx} = S(x, t), \quad -\infty < x < +\infty, \quad t \geq 0, \tag{1}$$

where $u = u(x, t)$ is the response variable (e.g., the displacement field), $c > 0$ is a characteristic velocity,

$$S(x, t) = S_0 \delta(x) \delta(t), \tag{2}$$

is the source term and δ denotes the Dirac generalized function [2].

We consider the initial conditions (suitable for a PDE of the second order in time)

$$\begin{aligned} u(x, 0) &= U_0 \delta(x), \\ u_{,t}(x, 0) &= V_0 \delta(x). \end{aligned} \tag{3}$$

To be clear, let us perform a dimensional analysis of the above equations. We have

$$\begin{aligned} c &= [LT^{-1}], & S &= [T^{-2}], & \delta(x) &= [L^{-1}], & \delta(t) &= [T^{-1}], \\ S_0 &= [LT^{-1}], & U_0 &= [L], & V_0 &= [LT^{-1}]. \end{aligned}$$

We denote the solutions separately due to S_0 , U_0 and V_0 by $\mathcal{G}_*^w(x, t)$, $\mathcal{G}_{1C}^w(x, t)$ and $\mathcal{G}_{2C}^w(x, t)$, respectively. They are referred to as the *Green functions* for the corresponding Boundary Value Problems of the wave equation. The upper index w refers generically to the wave equation, the lower index “*” refers to the non-homogeneous wave equation with the source term and both vanishing initial conditions, while 1C and 2C refer to the homogeneous wave equation with the first and the second non vanishing initial condition, respectively (the so-called first and second Cauchy problems).

Let us introduce the Fourier transform with respect to x and the Laplace transform with respect to t of the response variable using the following notation

$$\widehat{u}(\kappa, t) := \int_{-\infty}^{+\infty} e^{-i\kappa x} u(x, t) dx, \quad \widetilde{u}(x, t) := \int_0^{\infty} e^{-st} u(x, t) dt,$$

where κ is the wavenumber, s is the Laplace variable and $i = \sqrt{-1}$.

Applying the Fourier transform to (1) gives

$$\widehat{u}_{,tt} + c^2 \kappa^2 \widehat{u} = S_0 \delta(t), \tag{4}$$

Applying the Laplace transform to this equation yields

$$s^2 \widetilde{u} - U_0 s - V_0 + c^2 \kappa^2 \widetilde{u} = S_0. \tag{5}$$

Eq. (5) gives the combined Laplace–Fourier transform of the solution of (1) with conditions (2) and (3):

$$\widetilde{u}(\kappa, s) = \frac{U_0 s + V_0 + S_0}{s^2 + c^2 \kappa^2}. \tag{6}$$

From this result, we already see that the initial condition $V_0 \neq 0$ provides a Green function similar to that provided by the source $S_0 \neq 0$, that is $\mathcal{G}_*^w(x, t) \propto \mathcal{G}_{2C}^w(x, t)$.

To be clear, a check of the correctness of the dimensional analysis of Eq. (6) can be done taking into account

$$\kappa = \left[\frac{1}{L} \right], \quad s = \left[\frac{1}{T} \right], \quad \widetilde{u} = [LT].$$

It can be seen that (6) satisfies the dimensional analysis.

Let us now consider $U_0 = V_0 = 0$ in order to derive the Green function $\mathcal{G}_*^w(x, t)$ corresponding to the source. For this aim let us first perform the inverse Fourier transform of (6). We have

$$\widetilde{u}(x, s) = \frac{S_0}{2\pi c^2} \int_{-\infty}^{\infty} \frac{\exp(i\kappa x)}{\kappa^2 + s^2/c^2} d\kappa. \tag{7}$$

We use the residue theorem to solve this equation. The denominator has two poles, $\kappa = is/c$ and $\kappa = -is/c$, which correspond to the residues

$$\frac{\exp(-sx/c)}{2is/c} \quad \text{and} \quad -\frac{\exp(-sx/c)}{2is/c},$$

respectively. Since the previous integral is $2\pi i \sum$ residues,

$$\begin{aligned} \tilde{u}(x, s) &= \frac{S_0}{2sc} \exp(-sx/c), \quad x \geq 0, \\ \tilde{u}(x, s) &= \frac{S_0}{2sc} \exp(+sx/c), \quad x < 0. \end{aligned} \tag{8}$$

Inverting the Laplace transform, we get

$$g_*^w(x, t) = \frac{S_0}{2c} [H(t + x/c) + H(t - x/c)], \tag{9}$$

where H denotes the (unit-step) Heaviside function. Thus Eq. (9) provides the Green function for the wave equation (1) with the source term and vanishing initial conditions. The same result can be obtained by performing at first the inverse Laplace transform of (6), giving

$$\hat{u}(\kappa, t) = \frac{S_0}{c\kappa} \sin(c\kappa t), \quad t \geq 0, \tag{10}$$

and then performing the inverse Fourier transform.

Replacing S_0 by V_0 gives the Green function for the *homogeneous wave equation* with the initial conditions $U_0 = 0, V_0 \neq 0$, namely

$$g_{2c}^w(x, t) = \frac{V_0}{2c} [H(t + x/c) + H(t - x/c)]. \tag{11}$$

On the other hand, if $S_0 = V_0 = 0$, we derive the Green function of the *homogeneous wave equation* with the initial conditions $U_0 \neq 0, V_0 = 0$, namely $g_{1c}^w(x, t)$. We have from (6)

$$\tilde{\hat{u}}(\kappa, s) = \frac{U_0 s}{s^2 + c^2 \kappa^2}. \tag{12}$$

Now

$$\begin{aligned} \tilde{u}(x, s) &= \frac{U_0}{2c} \exp(-sx/c), \quad x \geq 0, \\ \tilde{u}(x, s) &= \frac{U_0}{2c} \exp(+sx/c), \quad x < 0, \end{aligned} \tag{13}$$

so that

$$g_{1c}^w(x, t) = \frac{U_0}{2c} [\delta(t + x/c) + \delta(t - x/c)]. \tag{14}$$

It is clear the relation between $g_*^w(x, t), G_{2c}^w(x, t)$ given by (9), (11), respectively and $g_{1c}^2(x, t)$ given by (14) since, formally

$$\frac{d}{dt} H(t) = \delta(t).$$

Note that the three Green functions can be alternatively re-written as

$$\begin{aligned} g_*^w(x, t) &= \frac{S_0}{2c} [H(x - ct) - H(x + ct)], \\ g_{1c}^w(x, t) &= \frac{U_0}{2} [\delta(x - ct) + \delta(x + ct)], \\ g_{2c}^w(x, t) &= \frac{V_0}{2c} [H(x - ct) - H(x + ct)], \end{aligned} \tag{15}$$

where we have used the properties $\delta(ax) = |a|^{-1}\delta(x)$ and $\delta(x) = \delta(-x)$.

If represented as functions of x for fixed t (snapshot), the Green functions $g_*^w(x, t)$ and $g_{2c}^w(x, t)$ yield a box function of width $2ct$ centered at $x = 0$, while $g_{1c}^w(x, t)$ represents two spikes (deltas) located at ct and $-ct$.

We can recover from the above analysis the classical d'Alembert result on the solution for the Cauchy problem of the homogeneous wave equation,

$$u_{,tt} - c^2 u_{,xx} = 0, \quad -\infty < x < +\infty, \quad t \geq 0, \tag{16}$$

coupled with the initial conditions

$$\begin{aligned} u(x, 0) &= \Phi(x), \\ u_{,t}(x, 0) &= \Psi(x), \end{aligned} \tag{17}$$

that is

$$u(x, t) = \frac{1}{2} [\Phi(x - ct) + \Phi(x + ct)] + \frac{1}{2c} \int_{x-ct}^{x+ct} \Psi(\xi) d\xi. \tag{18}$$

In fact, we easily recognize that the above solution is given by

$$u(x, t) = G_{1C}^w(x, t) * \Phi(x) + G_{2C}^w(x, t) * \Psi(x), \tag{19}$$

with $U_0 = V_0 = 1$ in the Green functions. Here we have used the usual notation for the space convolution of two (absolutely integrable) functions

$$f(x) * g(x) := \int_{-\infty}^{+\infty} f(\xi) g(x - \xi) d\xi = \int_{-\infty}^{+\infty} f(x - \xi) g(\xi) d\xi, \tag{20}$$

where here “*” denotes time convolution.

3. The diffusion equation

Let us consider the 1D diffusion equation

$$u_{,t} - d u_{,xx} = S(x, t), \quad -\infty < x < +\infty, \quad t \geq 0, \tag{21}$$

where $u = u(x, t)$ is the response variable (e.g., the pressure field), $d > 0$ is a diffusion coefficient,

$$S(x, t) = S_0 \delta(x) \delta(t), \tag{22}$$

is the source term and δ denotes the Dirac generalized function.

We consider the initial condition (suitable for a PDE of the first order in time)

$$u(x, 0) = U_0 \delta(x). \tag{23}$$

To be clear, let us perform a dimensional analysis of the above equations. We have

$$\begin{aligned} d &= [L^2 T^{-1}], & S &= [T^{-1}], & \delta(x) &= [L^{-1}], & \delta(t) &= [T^{-1}], \\ S_0 &= [L], & U_0 &= [L]. \end{aligned}$$

We denote the solutions separately due to S_0 and U_0 by $\mathcal{G}_*^d(x, t)$ and $\mathcal{G}_C^d(x, t)$, respectively. They are referred to as the *Green functions* for the corresponding Boundary Value Problems of the diffusion equation. The upper index d refers generically to the diffusion equation, the lower index “*” refers to the non-homogeneous diffusion equation with the source term and vanishing initial condition while C refers to the homogeneous diffusion equation with the second non vanishing initial condition (the so-called first and second Cauchy problems). Applying the Fourier transform to (21) gives

$$\widehat{u}_{,t} + d\kappa^2 \widehat{u} = S_0 \delta(t), \tag{24}$$

Applying the Laplace transform to this equation yields

$$\widetilde{s\widehat{u}} - U_0 + d\kappa^2 \widetilde{\widehat{u}} = S_0. \tag{25}$$

Eq. (25) gives the combined Laplace–Fourier transform of the solution of (21) with conditions (22) and (23):

$$\widetilde{\widehat{u}}(\kappa, s) = \frac{U_0 + S_0}{s + d\kappa^2}. \tag{26}$$

From this result, we already see that the initial condition $U_0 \neq 0$ provides a Green function similar to that provided by the source $S_0 \neq 0$, that is $\mathcal{G}_*^d(x, t) \propto \mathcal{G}_C^d(x, t)$.

To be clear, a check of the correctness of the dimensional analysis of Eq. (26) can be done taking into account

$$\kappa = \left[\frac{1}{L} \right], \quad s = \left[\frac{1}{T} \right], \quad \widetilde{\widehat{u}} = [LT].$$

It can be seen that (26) satisfies the dimensional analysis.

Let us now consider $U_0 = 0$ in order to derive the Green function $\mathcal{G}_*^d(x, t)$ corresponding to the source. For this aim let us first perform the inverse Fourier transform of (26). We have

$$\widetilde{u}(x, s) = \frac{S_0}{2\pi d} \int_{-\infty}^{\infty} \frac{\exp(i\kappa x)}{\kappa^2 + s/d} d\kappa. \tag{27}$$

We use the residue theorem to solve this equation. The denominator has two poles, $\kappa = is^{1/2}/\sqrt{d}$ and $\kappa = -is^{1/2}/\sqrt{d}$, which correspond to the residues

$$\frac{\exp\left(-s^{1/2}x/\sqrt{d}\right)}{2is^{1/2}/\sqrt{d}} \quad \text{and} \quad -\frac{\exp\left(-s^{1/2}x/\sqrt{d}\right)}{2is^{1/2}/\sqrt{d}},$$

respectively. Since the previous integral is $2\pi i \sum$ residues,

$$\begin{aligned} \tilde{u}(x, s) &= \frac{S_0}{2s^{1/2}\sqrt{d}} \exp\left(-s^{1/2}x/\sqrt{d}\right), \quad x \geq 0, \\ \tilde{u}(x, s) &= \frac{S_0}{2s^{1/2}\sqrt{d}} \exp\left(+s^{1/2}x/\sqrt{d}\right), \quad x < 0. \end{aligned} \tag{28}$$

Inverting the Laplace transform, we get

$$g_*^d(x, t) = S_0 \frac{1}{2\sqrt{\pi dt}} \exp\left(-\frac{x^2}{4dt}\right). \tag{29}$$

Similarly

$$g_c^d(x, t) = U_0 \frac{1}{2\sqrt{\pi dt}} \exp\left(-\frac{x^2}{4dt}\right). \tag{29'}$$

Thus Eqs. (29) and (29') provide, apart the factors S_0 and U_0 , the well-known Gaussian probability density with variance $\sigma^2 = 2dt$, a classical result! The same result can be obtained by performing at first the inverse Laplace transform of (26), giving

$$\hat{u}(\kappa, t) = S_0 \exp(-dt\kappa^2) \quad t \geq 0, \tag{30}$$

and then performing the inverse Fourier transform.

4. Time fractional diffusion-wave equation

The above analysis may be generalized by replacing the time derivatives of order 1 and 2 with Caputo derivatives of order β with $0 < \beta \leq 1$ and $1 < \beta \leq 2$, respectively. We write

$$D_t^\beta u - d u_{,xx} = S(x, t), \quad -\infty < x < +\infty, \quad t \geq 0, \tag{31}$$

where $u = u(x, t)$ is the response variable (e.g., the dilatation field in Carcione et al. [4], Eq. (24)), $d > 0$ is a positive constant (of dimension $[L^2T^{-\beta}]$), and D_t^β denotes the time-fractional derivative of order β in the Caputo sense. Here

$$S(x, t) = S_0\delta(x)\delta(t), \tag{32}$$

is the source term and δ denotes the Dirac generalized function.

For the initial conditions we must distinguish the case $0 < \beta \leq 1$ that requires only one initial condition $u(x, 0) = U_0\delta(x)$ and the case $1 < \beta \leq 2$ that requires two initial conditions. $\{u(x, 0) = U_0\delta(x), \quad u_t(x, 0) = V_0\delta(x)\}$.

Consequently, the combined Fourier–Laplace transform of the solution reads

$$\tilde{u}(\kappa, s) = \frac{U_0s^{\beta-1} + V_0s^{\beta-2} + S_0}{s^\beta + d\kappa^2}, \tag{33}$$

where we must put $V_0 \equiv 0$ in the case $0 < \beta \leq 1$ in order to take into account that the second initial condition is dropped. Thus, from the dimensional analysis of Eq. (33) we recognize that whereas in the case $\beta = 1$ we had only one independent Green function, in the case $0 < \beta < 1$ we have two independent Green functions. Similarly, whereas in the case $\beta = 2$ we had two independent Green function, in the case $1 < \beta < 2$ we have three independent Green functions. All these Green functions turn out to be Wright functions of the second kind related to the auxiliary functions introduced by Mainardi in the 90s [5].

From Eq. (33), we can see that for $\beta = 1$, the source is equivalent to the initial condition U_0 , while for $\beta = 2$, the source is equivalent to the initial condition V_0 .

5. Examples

The numerical method described here is a simple implementation of a finite difference method for the equation of motion. It is used just for illustration aims because the main focus of the paper is not on numerical methods. For more advanced

methods the reader can consult the book by Li and Zheng [3]. In the discrete space–time case, the implementations of source and initial condition are not equivalent since a delta function cannot be used due to aliasing problems. The fact that the field is sampled at discrete points imposes a maximum frequency and/or wavenumber that can propagate without aliasing. If the maximum grid size is dx and the minimum velocity is c_0 , the maximum frequency imposed by the Nyquist theorem is

$$f_{\max} = \frac{c_0}{2dx}. \tag{34}$$

This means that a band-limited time history $h(t)$ is required and

$$S(x, z, t) = S_0\delta(x)\delta(z)h(t), \tag{35}$$

where the spectrum of $h(t)$ cannot have significant amplitudes for frequencies greater than f_{\max} , while the maximum wavenumber that the grid can “support” is π/dx [2].

Let us consider the fractional 2D dilatation formulation of elasticity in the (x, z) -plane to illustrate the point. The governing equation is [4]

$$D_t^\beta \epsilon - \Delta_\rho(\rho M \epsilon) = S, \quad M = \frac{M_0}{\rho} \omega_0^{\beta-2}, \tag{36}$$

where ϵ is the dilatation field, $\Delta_\rho = \partial_x \rho^{-1} \partial_x + \partial_z \rho^{-1} \partial_z$, ρ is the mass density, M_0 is the bulk modulus and ω_0 is a reference frequency. If $\beta = 2$ we have the wave equation for a lossless medium. The source time history is the so-called Ricker wavelet,

$$h(t) = \left(a - \frac{1}{2}\right) \exp(-a), \quad a = \left[\frac{\pi(t - t_s)}{T}\right]^2, \tag{37}$$

where $T = 1/f_0$ is the period of the wave and we take $t_s = 1.5T$. Then, the duration of the time history of the source is $3T$.

In this case, Eq. (33) reads in a homogeneous medium,

$$\tilde{u}(\kappa, s) = \frac{U_0 s^{\beta-1} + V_0 s^{\beta-2} + S_0 \tilde{h}}{s^\beta + (M_0/\rho) \omega_0^{\beta-2} \kappa^2}. \tag{38}$$

We discretize Eq. (36) at $t = n dt$, $x = i dx$ and $z = j dz$, where dt is the time step, (dx, dz) is the size of a spatial cell and n, i and j are natural numbers. The computation of the fractional derivative is based on the Grünwald–Letnikov approximation [4,2]. The spatial derivatives are calculated with the Fourier method by using the fast Fourier transform (FFT) [2]. The Fourier pseudospectral method has spectral accuracy for band-limited signals. Then, the results are not affected by spatial numerical dispersion.

We consider an interface separating two half spaces, with the same density and sound velocity ($\rho = 2500 \text{ kg/m}^3$ and $c_0 = 3200 \text{ m/s}$, respectively) but different quality factors, $Q = 100$ (upper medium, $\beta = 1.99363$) and $Q = 10$ (lower medium, $\beta = 1.93655$). It is $Q = 1/\tan \xi$ and $M_0 = \rho c_0^2 \cos^2(\xi/2)$, where $\xi = \pi(1 - \beta/2)$ [4]. Moreover, $\omega_0 = 2\pi f_0$, where f_0 is the peak frequency of the source. A dilatational source with $S_0 = 1$ and $f_0 = 60 \text{ Hz}$ is applied at the interface. We consider a numerical mesh with uniform vertical and horizontal grid spacings $dx = dz = 9 \text{ m}$, 117×117 grid points, and the time stepping algorithm uses $dt = 0.2 \text{ ms}$. Fig. 1 shows snapshots of the dilatation field at 50 ms (the source duration) and 160 ms, where it can clearly be seen that the wavefield is more damped in the lower half space due to the lower quality factor. In order to properly implement the perturbation as an initial condition, the correct approach is to consider the field shown in Fig. 1(a) as the initial condition. In this case there is no analytical or semi-analytical solution because of the fact that the medium is heterogeneous. In a homogeneous medium an analytical Green function $g(t)$ can be computed and the perturbation can be initiated with a temporal delta. In this case, for instance $\beta = 2$, source and initial condition (particle velocity) are equivalent and the final solution can be obtained by a time convolution between $g(t)$ and the time history $h(t)$, i.e., $g * h$, since the differential equation is linear, i.e., the Fourier superposition principle holds.

Assume now the equations of elasticity in 1D space,

$$u_{,tt} = \frac{1}{\rho} \sigma_{,x} + S, \quad \sigma = M_0 u_{,x} + m, \tag{39}$$

where u is the displacement, σ is the stress, M_0 is a bulk modulus and m is a moment–tensor like source to model earthquakes [2]. The source S is a body force (per unit volume in 3D space). Combining the preceding equations and assuming a uniform medium, we obtain

$$u_{,tt} = c^2 u_{,xx} + S + \frac{1}{\rho} m_{,x}, \tag{40}$$

where $c^2 = M_0/\rho$. Performing a double transform, we obtain

$$\tilde{u}(\kappa, s) = \frac{U_0 s + V_0 + S_0 + i\kappa m_0/\rho}{s^2 + c^2 \kappa^2}, \tag{41}$$

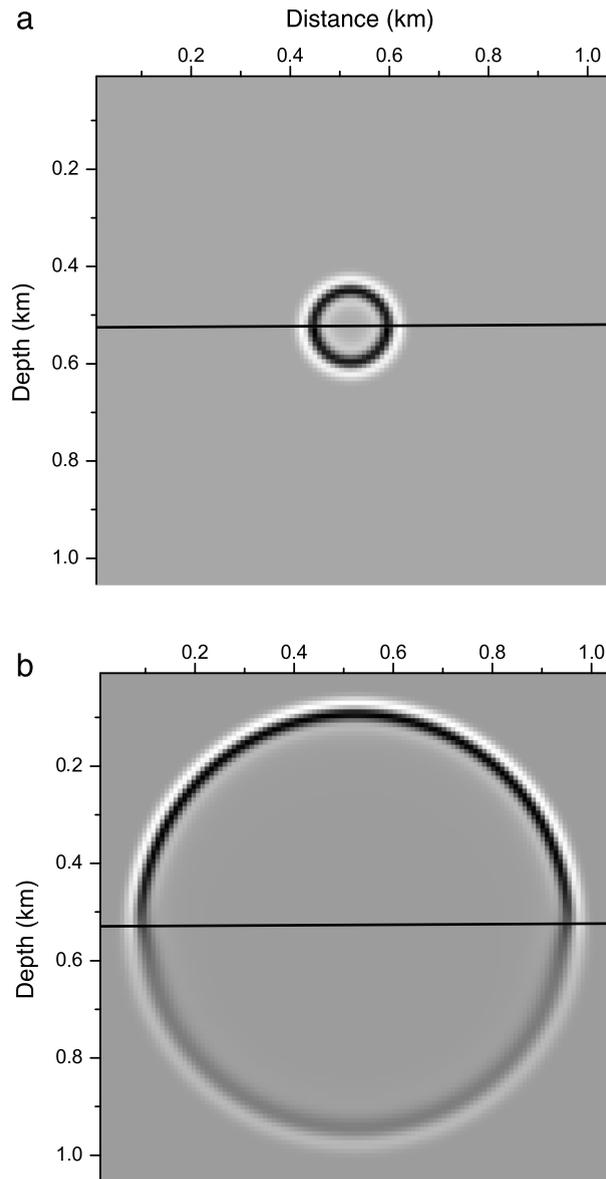


Fig. 1. Snapshot of the wavefield at 50 ms (a) and 160 ms (b).

where we have assumed $S = S_0\delta(x)\delta(t)$ and $m = m_0\delta(x)\delta(t)$. Eq. (41) equals Eq. (6) for $m_0 = 0$. If we have the solution for S , i.e., the Green function \mathcal{G}_*^w (see Eq. (9)), we obtain the solution for the source m as $\mathcal{G}_{*,x}^w/\rho$, i.e., we get

$$\frac{m_0}{2\rho c^2} [\delta(t + x/c) - \delta(t - x/c)]. \tag{42}$$

6. Conclusions

A wavefield, either wave-like or diffusion, can be initiated by sources and initial conditions. We have shown the equivalence in the continuum, where a source term is equivalent to the time derivative of the field (wave equation) and to field itself (diffusion equation) for delta functions in time and space. In the discrete case, the source time history is band-limited and the equivalence can be established only in uniform media. In heterogeneous media, an initial condition has to be computed numerically and this approach is general, i.e., it can be applied to the fractional differential equation. One example illustrates such an implementation. We also show that body forces and stress sources (e.g., earthquakes) can be related in uniform media. The methods have been shown for a point source, but it can easily be extended to the case of a spatially distributed source.

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