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An eigenfunction expansion method to efficiently evaluate spatial derivatives for media with discontinuous properties

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Pseudo-Spectral methods are often used as an alternative to the Finite Difference Time Domain (FDTD) method to model wave propagation in heterogeneous moving media. The FDTD method is robust and accurate but is numerically expensive. Pseudo-Spectral methods make use of the wavelike nature of the solution to obtain more efficient time-domain algorithms. The most straightforward of the Pseudo-Spectral methods is the Fourier method in which a spatial Fourier transform is used to evaluate the spatial derivatives in the wave equation. Whereas this method is accurate for a weakly heterogeneous moving medium, it degenerates for media with discontinuous properties. The eigenfunction expansion method presented here is a way to accurately and efficiently evaluate spatial derivatives in media with interfaces. As in the Fourier method, transforms may be calculated using FFT's and spatial sampling is limited only by the Nyquist condition. The performance of the method is shown in a time-domain implementation for media with discontinuous density and sound speed.

1 Introduction

Wave propagation problems that do not have analytical solutions may be solved by numerical methods. For problems where Green's functions are known, the governing acoustical equation in its integral form can be solved by discretizing interfaces separating sub-domains (e.g. the boundary element method). For problems where Green's functions are numerically too expensive to evaluate, domain discretization methods can be used (e.g. finite element (FE) or finite difference (FD) methods). Generalized FEM and FD methods can be numerically expensive. A way to more efficiently apply domain discretization methods is to make use of the wavelike nature of the solution. One such method is the Pseudo-Spectral (PS) method [1]. For a homogeneous medium, spatial derivatives of the solution at a certain time can accurately be calculated by the simplest PS method, the Fourier PS method. Since spatial Fourier transforms are used, the spatial resolution is bounded by the Nyquist criterion (i.e. 2 points per wavelength). The signal is required to have compact support. This method is more efficient and requires less storage than the finite differences time domain (FDTD) method. The Fourier PS method is still accurate for a weakly non-homogeneous medium [2], but fails due to Gibbs' phenomenon if the medium properties are discontinuous. The Gibbs' phenomenon can be controlled in the Fourier PS method by low-pass filtering (while sacrificing accuracy at the higher frequencies). A post-processing method can be applied, but is computationally inefficient [3]. For a solution which does not have spatial local support, spatial derivatives can be derived using Chebyshev polynomials. This will however require a higher spatial resolution than in the Fourier method (π points per wavelength), a more stringent stability criterion and a multiple subdivision of the spatial domain [1].

A way to solve wave propagation in discontinuous media accurately and efficiently is by using a generalized eigenfunction expansion. This method is an extension of the Fourier method to discontinuous media. The Fourier method appears as the special case of no discontinuity. The generalized (continuum) eigenfunctions are solutions to the wave equation with the discontinuous media. In this paper, the 1D continuum eigenfunction expansion (CEE) for two discontinuous media will be derived for the wave equation. Some numerical key-issues are addressed and results of calculations for dis-

continuous media are shown. Results of calculations for a medium with a slowly varying sound speed are presented. The numerical efficiency of the CEE time domain method is compared with that of the FDTD method.

2 Theory

We consider 1D wave propagation in semi-infinite fluid media, see Fig 1.

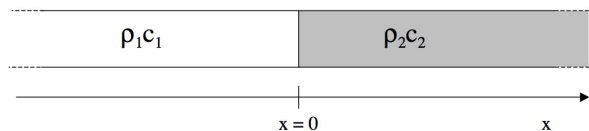


Figure 1: The 1D domain is subdivided in two semi-infinite media, 1 and 2.

Wave propagation is governed by the wave equation:

$$\left[\frac{d}{dx} \left(\frac{1}{\rho(x)} \frac{d}{dx} \right) - \frac{1}{\rho(x)c(x)^2} \frac{d^2}{dt^2} \right] p(x, t) = 0, \quad (1)$$

where $c(x)$ and $\rho(x)$ are the piecewise constant wave speed and density (given by c_j and ρ_j for $j = 1, 2$) and $p(x, t)$ is the pressure. To solve this equation in the time domain, the spatial derivative operator on $p(x, t)$ will be calculated using the continuum eigenfunction expansion method. The continuum eigenfunctions satisfy the eigenvalue equation

$$[L - \epsilon R] \psi(\epsilon, x) = 0, \quad (2)$$

with $L = \frac{d}{dx} \left(\frac{1}{\rho} \frac{d}{dx} \right)$, $\psi(\epsilon, x)$ the eigenfunctions, $R = \frac{1}{\rho c^2}$ and ϵ the eigenvalues. Two orthogonal continuum eigenfunctions that are solutions to Eq (2) are:

$$\psi_+(\epsilon, x) = N_+(\epsilon) \begin{cases} \alpha_1 e^{\frac{\sqrt{\epsilon}}{c_1} x} + \beta_1 e^{-\frac{\sqrt{\epsilon}}{c_1} x} & x < 0 \\ e^{\frac{\sqrt{\epsilon}}{c_2} x} & x > 0 \end{cases} \quad (3)$$

$$\psi_-(\epsilon, x) = N_-(\epsilon) \begin{cases} e^{-\frac{\sqrt{\epsilon}}{c_1} x} & x < 0 \\ \alpha_2 e^{-\frac{\sqrt{\epsilon}}{c_2} x} + \beta_2 e^{\frac{\sqrt{\epsilon}}{c_2} x} & x > 0 \end{cases},$$

where $\epsilon \in (-\infty, 0)$. The coefficients $N_+(\epsilon)$ and $N_-(\epsilon)$ in Eq (3) are normalization constants chosen so that the orthogonality condition

$$\int_{-\infty}^{\infty} \overline{\psi_{\pm}(\epsilon, x)} \psi_{\pm}(\epsilon', x) \frac{dx}{\rho c^2} = \delta(\epsilon - \epsilon') \quad (4)$$

is satisfied. Here the overbar denotes the complex conjugate. The coefficients α_1 , β_1 , α_2 and β_2 can be calculated by the continuity of pressure and normal velocity at $x = 0$.

We can now decompose a function $p(x, t)$, the solution of Eq (1) at a certain time, onto the orthogonal eigenfunctions by:

$$P_{\pm}(\epsilon, t) = \int_{-\infty}^{\infty} p(x, t) \overline{\psi_{\pm}(\epsilon, x)} \frac{dx}{\rho c^2}, \quad (5)$$

where

$$p(x, t) = \sum_{\pm} \int_{-\infty}^0 P_{\pm}(\epsilon, t) \psi_{\pm}(\epsilon, x) d\epsilon. \quad (6)$$

The operator $Lp(x, t)$ then follows from Eq (2) as:

$$Lp(x, t) = \sum_{\pm} \int_{-\infty}^0 \frac{\epsilon}{\rho c^2} P_{\pm}(\epsilon, t) \psi_{\pm}(\epsilon, x) d\epsilon. \quad (7)$$

Thus, the operator including the spatial derivative is calculated by transforming $p(x, t)$ through the orthogonal eigenfunctions, multiplying the transformed function $P_{\pm}(\epsilon, t)$ by $\frac{\epsilon}{\rho c^2}$ and performing the inverse transform to get $Lp(x, t)$. Inserting the eigenfunctions, we can calculate $Lp(x, t)$ by:

$$Lp(x, t) = \begin{cases} -\int_0^{\infty} \frac{k_1^2}{\rho_1 \pi} \left(P_1 + \frac{\beta_1}{\pi \alpha_1} \overline{P_1} + \frac{1}{\pi \alpha_2} P_2 \right) e^{jk_1 x} dk_1 & x < 0 \\ -\int_0^{\infty} \frac{k_2^2}{\rho_2 \pi} \left(P_2 + \frac{\beta_2}{\pi \alpha_2} \overline{P_2} + \frac{1}{\pi \alpha_1} P_1 \right) e^{jk_1 x'} dk_1 & x' > 0, \end{cases} \quad (8)$$

where $\epsilon = -k_j^2 c_j^2$ and we integrate over k_1 , $P_1 = \int_{-\infty}^0 p(x, t) e^{-jk_1 x} dx$, and $P_2 = \int_0^{\infty} p(x' \frac{c_2}{c_1}) e^{-jk_1 x'} dx'$. From Eq (8), it is clear that the spatial derivative operator is evaluated in the wave number domain k_1 .

3 Numerical implementation

To obtain $Lp(x, t)$ numerically from Eq (8), fast Fourier transforms (FFTs) are used because of their computational efficiency. We assume that our $p(x, t)$ has compact support for x between $-X$ and U . When calculating P_1 , we therefore need to integrate from $-X$ to U . This is done by using zero values for $p(x, t)$ for $x > 0$.

$$P_1 = \int_{-\infty}^0 p(x, t) e^{-jk_1 x} dx \quad (9)$$

$$\approx \frac{p(0, t)}{2} + \Delta x_1 \sum_{l=0}^{N_X-1} p(l\Delta x_1 - X, t) e^{-j \frac{2\pi l m}{N}},$$

where N is the total number of discrete spatial points, N_X the number of points for $x < 0$, N_U the number of points for $x > 0$ and $N = N_X + N_U - 1$. At $x = 0$, half the value of p is taken, corresponding to a triangular integration. By the discontinuity of $p(x, t)$ at $x = 0$ in the transform of Eq (9), wave number components are erroneously obtained. The errors will be canceled by wave number components of the other two parts in the integrals of Eq. (8). The values of $\overline{P_1}$ are obtained by taking the complex conjugate of P_1 , multiplied by $e^{jk_1(U-X)}$. For P_2 , integration is done over $p(x' \frac{c_2}{c_1})$, implying that medium 2 has a different spatial sampling than medium 1. It is a consequence of harmonizing the wave number discretization in both media to k_1 , which physically means that the implemented spatial discretization of both media captures the same maximum frequency. For P_2 , we use zero values for $p(x' \frac{c_2}{c_1})$ for $x < 0$ and $p(0, t)/2$ at $x = 0$. Values of $\overline{P_2}$ are obtained similar to $\overline{P_1}$. Two Fourier transforms are thus needed to transform $p(x, t)$ to the wave number domain and after having multiplied by coefficients in the wave number domain, two inverse Fourier transforms are left to obtain $Lp(x, t)$. The spatial discretization should obey Nyquist criterion, i.e. 2 points per wavelength.

4 Calculation results

The 1D CEE method to calculate the second spatial derivative will be validated here for several cases.

For a homogeneous medium, i.e. $\alpha_1 = 1$, $\beta_1 = 0$, $\alpha_2 = 1$ and $\beta_2 = 0$, Eq (8) returns to: $Lp(x, t) = -\int_{-\infty}^{\infty} \frac{k^2}{2\pi\rho} P e^{jkx} dk$ for all x with $P = \int_{-\infty}^{\infty} p(x, t) e^{-jkx} dx$. This is called the Fourier PS method, and only requires one Fourier transform and one inverse Fourier transform to obtain $Lp(x, t)$. The results of the CEE method will be shown along with the results from the Fourier PS method.

4.1 Spatial derivative

We consider a wave with a Gaussian shape propagating from medium 1 to medium 2, which we describe analytically as:

$$p(x, t) = \begin{cases} \alpha_1 e^{-a(x-(x_0+c_1 t))^2} + \beta_1 e^{-a(x+(x_0+c_1 t))^2} & \text{for } x < 0 \\ e^{-a(\frac{c_1}{c_2} x - (x_0+c_1 t))^2} & \text{for } x > 0. \end{cases} \quad (10)$$

with α_1 and β_1 as in Eq (3) and $x_0 = -64\Delta x_1$. The frequency content of the signal is determined by a , and set to $a = \left(\frac{c_1}{1000\Delta x_1}\right)^2$. With the CEE method, we can calculate $Lp(x, t)$ at every instant t . Figure 2a shows $p_n(x, t_1)$ with $t_1 = (68\Delta x_1/c_1)$ s using Eq (10), for $\rho_2 = 2\rho_1$ with constant c and $c_2 = 2c_1$ with constant ρ . The pressure is normalized as $p_n(x, t_1) = p(x, t_1)/|\hat{p}(x, t_1)|$, where $\hat{p}(x, t_1)$ denotes the maximum value.

The operator $Lp_n(x, t_1)$ is now calculated analytically, $Lp_n(x, t_1)_{an}$, using the CEE method, $Lp_n(x, t_1)_{CEE}$,

and using the Fourier PS method, $Lp_n(x, t_1)_{FPS}$. The operators have been normalized as

$Lp_n(x, t_1) = Lp(x, t_1)/|\hat{L}p(x, t_1)_{an}|$. The chosen spatial discretization Δx_1 results in a sample frequency as $f_s = \frac{c_1}{\Delta x_1}$. Figure 2b shows $Lp_n(x, t_1)$ for the two different cases. Figure 2c shows absolute error in $Lp_n(x, t_1)$, expressed by $20\log_{10}|Lp_n(x, t_1)_{an} - Lp_n(x, t_1)_{CEE}|$ for the CEE method, and Fig 2d shows this absolute error as a function of the frequency up to $f_s/2$. The error using the CEE method is, for the two cases considered, very low and rather flat over the frequency band. The error can be shown to be related to the level of $p(x, 0)$ at $f_s/2$. The grid resolution in the Fourier method is equal to the grid resolution in the CEE method apart from the different sound speed case, where an equidistant grid in the Fourier method is used. In the Fourier PS method for the different density case, the operator L has been evaluated in two steps; i.e. a subsequent calculation of two first spatial derivatives. The error using the Fourier method is substantial compared to the CEE method, and is very large around the media interface.

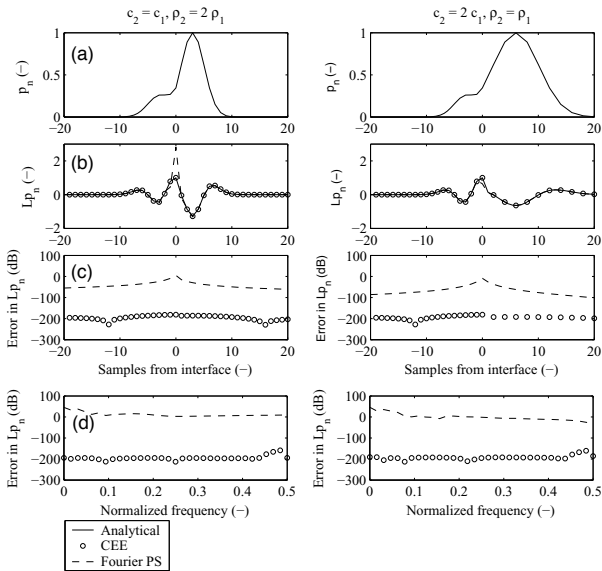


Figure 2: Calculation of $Lp_n(x, t_1)$: (a) analytical normalized pressure p_n ; (b) normalized operator Lp_n from analytical, CEE and Fourier PS methods; (c) $20 \log |Lp_n(x)_{an} - Lp_n(x)_{CEE}|$ and $20 \log |Lp_n(x)_{an} - Lp_n(x)_{FPS}|$; (d) $20 \log |Lp_n(f)_{an} - Lp_n(f)_{CEE}|$ and $20 \log |Lp_n(f)_{an} - Lp_n(f)_{FPS}|$.

4.2 Time-domain implementation

So far, the evaluation of the first operator of Eq (1) has been discussed. For an efficient evaluation of the second operator of Eq (1), use has been made of the k -space method. This method uses the analytical solution of the wave equation in the wave number-time ($k-t$) domain and has been used in the Fourier PS method before (e.g. [2]). We apply it here to the CEE method. After multiplying Eq (1) by $\psi_{\pm}(\epsilon, x)$ and integrating over x we get:

$$\left[\frac{k^2}{\rho} + \frac{1}{c^2 \rho} \frac{d^2}{dt^2} \right] P_{\pm}(\epsilon, t) = 0. \quad (11)$$

The solution to this equation can be written as:

$$P_{\pm}(\epsilon, t) = A_{\pm}(\epsilon) e^{j c_1 k_1 t}. \quad (12)$$

After some algebra, we can write:

$$\frac{1}{c^2 \rho} \frac{p(x, t + \Delta t) - 2p(x, t) + p(x, t - \Delta t)}{\Delta t^2} = \sum_{\pm} \int_{-\infty}^0 \left(-\frac{k^2}{\rho} \text{sinc}^2(c_1 k_1 \Delta t / 2) P_{\pm}(\epsilon, t) \right) \psi_{\pm}(\epsilon, x) d\epsilon. \quad (13)$$

The left hand side of Eq (13) can be seen as a finite difference representation of the time derivative operator. The difference between Eq (13) and a traditional second order finite difference representation in time (known as the leapfrog iteration) is the $\text{sinc}^2(c_1 k_1 \Delta t / 2)$ term at the right hand side of Eq (13). In contrast to leapfrog iteration, no error in the time stepping is introduced by the k -space method, since Eq (12) is exact. Given that c is constant in both media, the k -space method is unconditionally stable [2]. The numerical time step Δt is bounded by the Nyquist criterion as well, and has here been chosen to be $\Delta t = \Delta x_1 / (2c_1)$. The time domain calculation is started with Eq (10) and t runs from $0\Delta t$ to $2500\Delta t$. Figure 3a shows the analytical solution at $t = 1000\Delta t$ for the two cases considered above, i.e. $\rho_2 = 2\rho_1$ with constant c and $c_2 = 2c_1$ with constant ρ , showing a reflected and transmitted wave. The accuracy of the CEE k -space method, Eq (13), is studied by comparing the analytical transmission coefficient with the calculated transmission coefficient.

$$T_{an} = \frac{2\rho_2 c_2}{\rho_2 c_2 + \rho_1 c_1} \\ T_{CEE} = \frac{\mathcal{F}_t(p(II, t))}{\mathcal{F}_t(p(I, t))}, \quad (14)$$

where \mathcal{F}_t is the Fourier transform with respect to time, $p(I, t)$ is the pressure of the incident wave recorded at a position I with $x < 0$, and $p(II, t)$ the pressure of the transmitted wave recorded at a position II with $x > 0$. Figure 3b shows T_{an} , T_{CEE} and T_{FPS} (calculated similarly as T_{CEE}) for the two cases studied. The accuracy for the CEE k -space method is fine, as expected. The accuracy breaks down close $f_s/2$, where f_s is the sample frequency related to the spatial discretization. The Fourier PS k -space method shows to be a low frequency approximation of the correct solution (as also shown in [3]).

The leapfrog iteration method is known to be dispersive. To display the accuracy of the CEE k -space method regarding dispersion, the relative phase error ϵ_{ϕ} using both methods is calculated by:

$$\begin{aligned}\epsilon_\phi(f) &= 100 \left(\frac{\Delta\phi - \Delta\phi_{an}}{\Delta\phi_{an}} \right) \\ &= 100 \left| \frac{\phi[\mathcal{F}_t(p(II, t))] - \phi[\mathcal{F}_t(p(I, t))] - \omega\mathcal{T}}{\omega\mathcal{T}} \right|\end{aligned}\quad (15)$$

where $\phi[y]$ the phase of y and \mathcal{T} the travel time between points II and I . Along with the relative phase error for the k -space method, the relative phase error using the leapfrog iteration method (by omitting the $\text{sinc}^2(c_1 k_1 \Delta t/2)$ term in Eq (13)) is shown in Fig 3c, using $\Delta t = \Delta x_1/(10c_1)$. The results show that whereas the phase error using the leapfrog method is around -0.4 % at $f_s/2$, the error using the k -space method is negligible. The Fourier PS ϵ_ϕ results for the $c_2 = 2c_1$ case can be attributed to the fact that the medium interface in this method is situated between two spatial grid points.

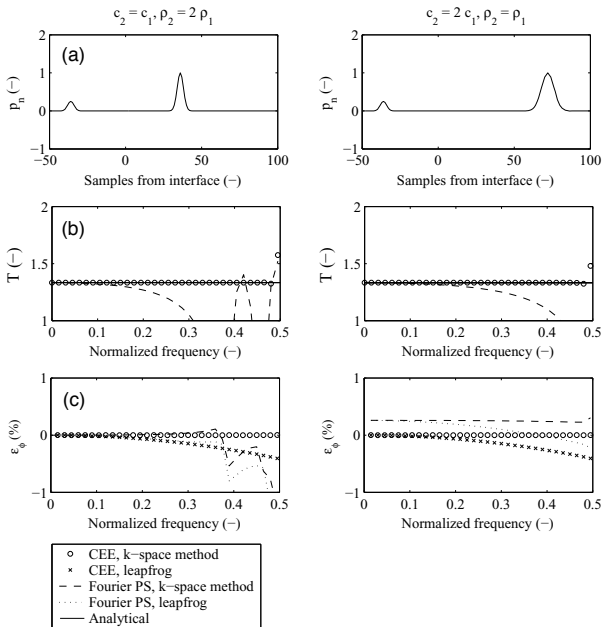


Figure 3: Results of time domain calculations: (a) analytical normalized pressure $p_n(x, 1000\Delta t)$; (b) transmission coefficient T from analytical, CEE and Fourier PS methods; (c) relative phase error ϵ_ϕ , from CEE $_{k\text{-space}}$, CEE $_{\text{leapfrog}}$, Fourier PS $_{k\text{-space}}$, Fourier PS $_{\text{leapfrog}}$ methods.

4.3 Slowly varying medium sound speed

The advantage of the CEE method over boundary discretization methods arises when the medium properties smoothly vary spatially. For smoothly varying medium properties, the Fourier PS method will return a good approximation of the second spatial derivative operator, see e.g. [4]. Since the CEE method is based on Fourier transforms, discontinuous media problems with smoothly varying media properties are expected to be well resolved using the CEE method for media with piecewise constant properties. In this section, it will

be studied whether this is the case by varying the medium sound speed $c(x)$ smoothly in domain 2. Results of calculations with the CEE and Fourier PS methods will be compared to a second order finite difference time domain (FDTD) method, which reads:

$$\begin{aligned}p(x, t + \Delta t) - 2p(x, t) + p(x, t - \Delta t) \\ = \frac{\Delta t^2 c(x)^2}{\Delta x^2} (p(x + \Delta x, t) - 2p(x, t) + p(x - \Delta x, t))\end{aligned}\quad (16)$$

The FDTD has been implemented with $f_{sFDTD} = 16f_{sCEE}$ Hz and $\Delta t_{FDTD} = \Delta x_{FDTD}/(10c_1)$, with f_s related to the spatial discretization. The FDTD results up to $f_{sFDTD}/32$ have a small amplitude and phase error and will therefore serve as a reference. The sound speed profile has first been chosen to be a shifted and low pass filtered version of $c_2 = 2c_1$ (a first order Butterworth filter with a cut-off frequency of $f_s/20$ has been used). Figure 4a displays the normalized sound speed profile for this case, with $c_n(x) = c(x)/c_1$. The time domain calculations were executed with initial values $p(x, 0)$ as from Eq (10) with $a = 2(f_s/1000)^2$. Figure 4b shows the transmission coefficients from the FDTD, CEE and Fourier PS calculations. For the latter two, which are equal for this case, both the k -space method and the leapfrog iteration in time have been calculated for. Since $c(x)$ increases in medium 2, the k -space method has a more stringent stability criterion (see [2]), and $\Delta t = \Delta x_1/(10c_1)$ has been chosen for the k -space and the leapfrog iteration method. The results show that the error in the CEE and Fourier PS methods are small, apart from frequencies close to the sample frequency, as we have seen in the former section. In Fig 4c, the relative phase error is calculated, where the phase change $\Delta\phi_{FDTD}$ has been used as a reference. The relative phase error in the k -space method is smaller than in the leapfrog method, but not as small as in section 4.2. The reason is that the Green's function in $k-t$ space, as used in the k -space method, is not exact any longer.

As a second sound speed profile, we take the former sound speed profile and add c_1 to the values in medium 2, see second subplot of Fig 4a. From the T and relative phase error results, we notice that the Fourier PS results show similar deviations as for the single discontinuity as in section 4.2. The error in T and relative phase error in the CEE method are comparable with the errors in the former sound speed profile case. Numerical tests indicate that a more abrupt transition in the sound speed will increase the required number of points per wavelength.

4.4 Numerical efficiency

The CEE method is developed to obtain an efficient wave propagation computation through discontinuous inhomogeneous fluid media. To indicate the efficiency of the calculations in section 4.3, the computation time from CEE and second order accurate FDTD methods are compared. For a similar accuracy, the number of points per wavelength in the FDTD was found to be 12 times larger than in the CEE method, while keeping the same ratio $\Delta t/\Delta x$ in both methods. For this

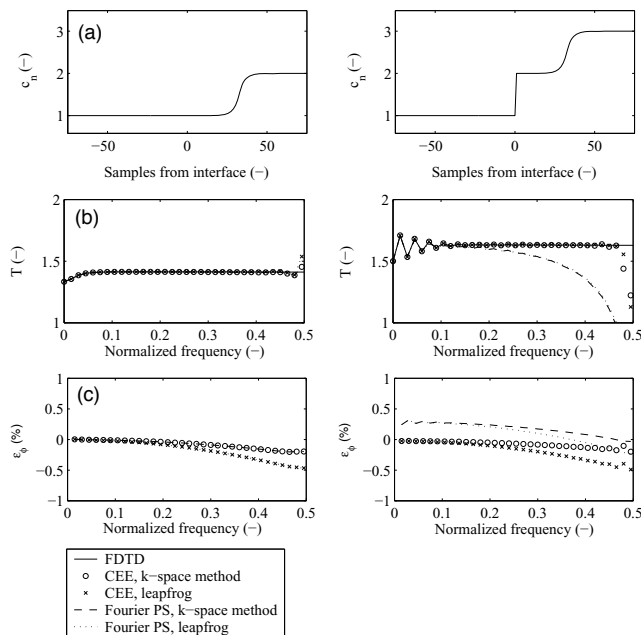


Figure 4: Results of time domain calculations: (a) normalized sound speed profiles $c_n(x)$; (b) transmission coefficient T from analytical, CEE and Fourier PS methods; (c) relative phase error ϵ_ϕ , from CEE and Fourier PS methods.

1D problem, the ratio 12 also holds for the required storage capacity of both methods. The number of operations in the CEE method N_{CEE} can be estimated by $N_t C_{CEE} N_x \log_2(N_x)$, with N_t the number of time steps, N_x the number of spatial points, $N_x \log_2(N_x)$ the approximate number of multiplications for a FFT and C_{CEE} a constant.

For the number of operations in the FDTD method, N_{FDTD} , we can then write $12N_t C_{FDTD} 12N_x$. The ratio N_{FDTD}/N_{CEE} was found to be 16 from the MATLAB implementation, with $N_x = 512$. This ratio depends on both N_x and the chosen numbers of points per wavelength in both methods. As shown by Liu, Pseudo-Spectral methods are even more rewarding for higher dimensions [5].

5 Conclusions

To model wave propagation through discontinuous inhomogeneous fluid media in the time domain, the use of a continuum eigenfunctions expansion (CEE) can be useful to calculate the spatial derivative operator of the wave equation of the solution at every time step. The solution is decomposed through the orthogonal set of continuum eigenfunctions, and the spatial derivative operator is taken in the transformed (wave number) domain. As for the Fourier Pseudo-Spectral (PS) method, integral transforms can be evaluated by making use of fast Fourier transforms, but in contrast to the Fourier PS method, the used eigenfunctions account for the discontinuity of the media properties. Calculations for one dimensional problems show that the continuum eigenfunction expansion method yields accurate results for

wave propagation in a two fluid problem, where density and wave speed are discontinuous across the media interface. Also, for an additional smoothly varying medium property (here c), the CEE method was shown to be accurate. The CEE, where slightly more than 2 points per wavelength are required, is computationally faster and requires less storage than the FDTD method. The CEE method applied to higher dimensions is currently under development.

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