ON INCLUSION OF SOURCE IN THE SYSTEM OF FIRST-ORDER LINEAR WAVE EQUATIONS

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Abstract

Simulating propagation of acoustic waves via solving a system of three-coupled first-order linear differential equations using a k-space pseudo-spectral method is popular for biomedical applications, firstly because of availability of an open-source toolbox for implementation of this numerical approach, and secondly because of its efficiency. The k-space pseudo-spectral method is efficient, because it allows coarser computational grids and larger time steps than finite difference and finite element methods for the same accuracy. The goal of this study is to compare this numerical wave solver with an analytical solution to the wave equation using the Green’s function for computing propagation of acoustic waves in homogeneous media. This comparison is done in the frequency domain. Using the k-Wave solver, a match to the Green’s function is obtained after modifying the approach taken for including mass source in the linearised equation of continuity (conservation of mass) in the associated system of wave equations.

1. Introduction

A numerical approach based on a k-space pseudo-spectral method was proposed for solving the coupled first-order linear differential equations for wave propagation [1, 2]. The proposed approach is exact for homogeneous media, unconditionally stable for the sound speeds below the nominal sound speed used in the k-space scheme, and accurate for weakly heterogeneous media like soft tissues [1, 2]. Using pseudo-spectral approaches, the spatial gradient of a field is approximated using the information from the entire field [1]. This is in contrast with finite difference or finite element methods, in which the spatial gradient at each point is computed based on only the information on nearby points [3, 4]. Furthermore, a k-space correction to the spatial gradients allows using larger time steps than pseudo-spectral methods for the same accuracy [1, 2, 5].

An open-source toolbox for a numerical implementation of this approach is popular in the fields related to biomedical acoustics [5, 6]. The goal of this study is to numerically investigate accuracy of the k-space pseudo-spectral approach for solving the three-coupled first-order linear wave equations in homogeneous media. For measuring accuracy of this numerical approach, the acoustic waves approximated using this approach will be compared to an analytical solution to the wave equation using the Green’s function [7, 8]. These comparisons will be done for approximating propagation of acoustic waves induced by an excitation of a point source using a time-varying ultrasonic pulse. The k-Wave toolbox will be used for performing the simulation experiments in 2D and 3D cases.
and for different excitation pulses and Courant-Friedrichs-Lewy (CFL) numbers [5, 6]. The results show that the numerical approach proposed in [1, 2] is accurate for homogeneous media, i.e., the acoustic waves approximated using this numerical approach match the analytic solution to the wave equation using the Green’s function for homogeneous media. More importantly, for obtaining this match, the approach taken for including source in the equation of continuity (conservation of mass) in the system of three-coupled first-order linear wave equations in the k-Wave toolbox was revisited and modified. (cf. Eq. 2.19 in the k-Wave user manual [10].)

One important application of simulating time-varying ultrasound pulses is quantitative reconstruction of acoustic properties of tissues using full-Wave inversion [12, 13, 14, 15, 16, 17, 18, 19, 20, 11].

Section 2 first describes the system of three-coupled first order linear wave equations for propagation of acoustic waves, and then a numerical implementation of this system using a k-space pseudo-spectral method is described, and an inclusion of time-varying sources to this system of equations is modified and explained. An analytic solution to the wave equation using the Green’s function, which will be used as the benchmark, is also explained in this section. The numerical results will be given in section 3. A discussion of the results follows in section 4.

2. Wave equation for homogeneous media

2.1. Wave equation in the continuous domain. This section explains formula describing the acoustic wave propagation in homogeneous media. Let \( x = (x^1, ..., x^d) \) denote a spatial position in \( \mathbb{R}^d \) with \( d \) the number of dimensions. (\( d \in \{2, 3\} \).) An emission element is excited by an ultrasonic pulse \( s(x, t) \) in times \( t \in (0, T_s) \). Here, the emission element is assumed isotropic and a point at position \( x_e \) for simplicity, but an extension to an emission element with finite volume is straightforward. The propagation of the induced pressure can be defined using the second-order wave equation in the form

\[
\frac{1}{c^2} \frac{\partial^2}{\partial t^2} p(x, t) - \nabla^2 p(x, t) = s(x, t),
\]

where \( p \) denotes the acoustic pressure, and \( c \) is the sound speed which is assumed homogeneous. By ignoring the dependence on \( x \) and \( t \), \( p \) is the scalar acoustic pressure with units of kg m\(^{-2-d}\) s\(^{-2}\), and the excitation pulse \( s \) is a scalar with units of kg m\(^{-d}\) s\(^{-2}\). The three-coupled first-order linear acoustic propagation equations can be defined in the form

\[
\begin{align*}
\frac{\partial}{\partial t} u(x, t) &= -\frac{1}{\rho_0} \nabla p(x, t) \\
\frac{\partial}{\partial t} \rho(x, t) &= -\rho_0 \nabla u(x, t) + s_M(x, t) \\
p(x, t) &= c(x)^2 \rho(x, t),
\end{align*}
\]

(2)

Here, \( \rho_0 \) is the ambient density with units of kg m\(^{-d}\), and is assumed homogeneous. By ignoring the dependence on \( x \) and \( t \), \( \rho \) and \( u \) denote the acoustic density and particle velocity vectors with components in units of kg m\(^{-d}\) and ms\(^{-1}\), respectively. Also, \( s_M(x, t) \) denotes the time-varying mass source which represents the time rate of the input of mass per unit volume, and is in units of kg m\(^{-d}\) s\(^{-1}\). The relation between the mass source and the excitation pulse satisfies

\[
s(x, t) = \frac{\partial s_M(x, t)}{\partial t}.
\]

(3)
Here, for a point source at position $x_e$, the excitation is defined as

$$s(x, t) = \delta(x - x_e) \ s(t),$$

where $s(t)$ has a time duration $T_s$. Also, the pressure field $p(x, t)$ is recorded for time $T$ with $T \gg T_s$.

2.2. Wave equation in the discretised domain. This section explains a discretisation of the wave equation [2]. Let $X = (X^1, \ldots, X^d)$ denote the position of the grid points for a $d$-dimensional grid with $X^\zeta$ the position $X$ along the Cartesian coordinate $\zeta \in \{1, \ldots, d\}$. We also use $n \in \{1, \ldots, N_s, \ldots N_T\}$ for the sampled times within the times $t \in \{0, \ldots, T_s, \ldots T\}$ (The same notations will be used for quantities in the continuous and discretised domains, and we hope this is not confusing for the readers.) Accordingly, the excitation pulse in the discretised domain is defined by $s(X, n)$.

In this manuscript, compared to the k-Wave [3][4][10], two corrections are applied for including the source in the wave equation. At first, by ignoring the dependence on time, in an ideal case when a point source at position $x_0$ matches the point $X_0$ on the grid, the relation between the point source in the continuous and discretised domains satisfies

$$s(x) \delta(x - x_0) \equiv \frac{1}{(\Delta x)^d} s(X_0),$$

where $\Delta x$ is the grid spacing. This equation implies that a quantity on a sampled point on a homogeneous grid with voxels of volume $V$ is equivalent to an integration of the same quantity over the volume $V$ in the continuous domain.

In addition, using (3), the relation between the discretised directional components of the mass source and the discretised excitation pulse satisfies

$$s^\zeta_M(X, n) = \begin{cases} 0, & \text{if } n = 1 \\ \frac{\Delta t}{\rho_0} \sum_{n'=1}^{n-1} s(X, n'), & \text{if } n < 1 \leq N_s + 1. \end{cases}$$

A discretisation of the system of equations [2] on a grid staggered in space and time is outlined in the following algorithm.

**Algorithm 1** k-Wave iterations.

1. input: $c, \rho_0, \Delta t, \Lambda^\zeta (\zeta \in \{1, \ldots, d\}), s^\zeta_M(X, n + \frac{1}{2}) (n \in \{1, \ldots, N_T - 1\})$
2. initialise: $p(X, 1) = 0, \ u(X, 1) = 0, \ u\left(X, \frac{1}{2}\right) = 0, \ \forall X$  
   $\triangleright$ Set initial parameters
3. Start at iteration $n = 1$ and terminate at iteration $N_T - 1$  
   $\triangleright$ Iterate
4. $u^\zeta(X, n + \frac{1}{2}) \leftarrow \Lambda^\zeta \left[ \Lambda^\zeta u^\zeta(X, n - \frac{1}{2}) - \frac{\Delta t}{\rho_0} \partial_\zeta p(X, n) \right]$
5. $\rho^\zeta(X, n + 1) \leftarrow \Lambda^\zeta \left[ \Lambda^\zeta \rho^\zeta(X, n) - \Delta t \rho_0 \partial_\zeta u^\zeta(X, n + \frac{1}{2}) \right] + \Delta t s^\zeta_M(X, n + \frac{1}{2})$
6. $p(X, n + 1) \leftarrow c^2 \sum_{\zeta=1}^d \rho^\zeta(X, n)$

In Algorithm [1], the spatial derivatives are computed using a k-space pseudo-spectral method [3][10], and $s^\zeta_M(X, n + 1/2)$, which is a discretisation of the mass source shifted by $\Delta t/2$, can be computed by enforcing a k-space correction step [10]. Also, $\Lambda^\zeta$ is an operator representing the perfectly matched layers (PMLs) along the Cartesian coordinate $\zeta$. 
Remark 1. In the k-Wave solver, the relation between the discretised directional components of the mass source and the discretised excitation pulse \( s(X, n) \) (source.p) is defined by

\[
s'^\zeta_M(X, n) = \frac{s(X, n)}{c^2d} \frac{2c}{\Delta x}.
\]  

(cf. Eq. (2.19) in the k-Wave user manual [10], or Algorithm 1, line 5, the second term in the right-hand-side in [11].) However, Eq. (7), in which \( s \) has been assumed pressure in \( \text{kgm}^{-2} \text{s}^{-2} \text{(Pa)} \), has not been understood by the author. (cf. Table 3.3 in [10].)

2.3. Analytic solution to the wave equation. This section describes an analytic solution to the system of wave equations (2) using the Green’s function for homogeneous media. This approach will be used as the benchmark for measuring accuracy of the k-Wave solver for homogeneous media.

A frequency-domain version of (2) at a single angular frequency \( \omega \) can be described using a Helmholtz equation of the form

\[
\left( \frac{\omega}{c} \right)^2 + \nabla^2 p(\omega, x) = -s(\omega, x).
\]  

The analytic solution to Eq. (8) in terms of the Green’s function can be written in the form

\[
p(\omega, x; x') = \int g(\omega, x; x') s(\omega; x') \, dx',
\]  

where \( g(\omega, x; x') \) is the Green’s function at point \( x \) with respect to point \( x' \) at the single angular frequency \( \omega \). Eq. (9) is used for an emission element with finite volume. As \( s \) is a point source here, this equation becomes a scaling

\[
p(\omega, x; x_e) = g(\omega, x; x_e) s(\omega, x_e).
\]  

For a 2D homogeneous medium, the Green’s function is in the form [8]

\[
g_{0,2D}(\omega, x; x') \approx \frac{1}{(8\pi\phi_0(x; x'))^{1/2}} e^{i(\phi_0(x; x') + \pi/4)}.
\]  

For a 3D homogeneous medium, the Green’s function is in the form [8]

\[
g_{0,3D}(\omega, x; x') = \frac{1}{4\pi|x - x'|} e^{i\phi_0(x; x')},
\]  

where \( \phi_0(x; x') \) denotes the phase of the Green’s function, and satisfies for a homogeneous medium

\[
\phi_0(x; x') = k|x - x'|,
\]  

where \( k = \omega/c \), and is the wavenumber.

3. Numerical results

This section will describe numerical experiments demonstrating the accuracy of the k-Wave and its modified version, in which Eq. (7) has been replaced by Eqs. (5) and (6), as discussed in section 2.2. It must be reminded that the latter equation enforces a dimension-dependent scaling on the source to account for spatial sampling. For measuring accuracy of the k-Wave, an analytic solution to the wave equation using Eq. (9) is used as the benchmark.
3.1. 2D case. The k-Wave simulations were performed on a grid of size 0.4 mm. One emitter and 256 receivers were placed on a ring with a radius of 9.5 cm. The sound speed inside the ring was set 1500 m/s and homogeneous. The emitter was placed on the position $x_e = [0, -9.5]$ cm. Figure 1(a) shows the emitter (red circle) and receivers (blue circles). The interpolations between the position of the transducers and the grid points were performed using the k-Wave toolbox [6, 9].

The k-Wave simulations were performed using three different excitation pulses for a time $T = 163.26 \mu s$. Figures 2(a), 2(b) and 2(c) show the excitation pulses 1, 2 and 3, respectively. Here, a low-pass filter has been applied on each excitation pulse using the `filterTimeSeries.m` function in the k-Wave to ensure that the frequency spectrum of the pulse be smaller than the maximum frequency supported by the computational grid, and the maximum absolute amplitude of the excitation pulses has then been normalised. The maximum frequency supported by the grid for the k-Wave simulation can be determined by the Shannon-Nyquist limit [2]. For a homogeneous medium with sound speed $c$, the maximum supported frequency is

$$f_{\text{max}} = \frac{c}{2\Delta x}. \tag{14}$$

Here, $\Delta x$ is the grid spacing, and $c$ is the sound speed in water (1500 m/s), but here, the low-pass filter was chosen more conservatively using a lower sound speed (1470 m/s) in [14] for computing $f_{\text{max}}$. The computed $f_{\text{max}}$ was 1.84 MHz.

The simulation 1 was performed using a CFL number 0.1, which provides a time spacing $\Delta t = 25.25 \text{ ns}$, which is equivalent to a sampling rate of 39.6 MHz. The simulation 2 was performed using a CFL number 0.2, which gives a time spacing 50.51 ns, which is equivalent to a sampling rate of 19.80 MHz. The simulation 3 was performed using a CFL number 0.3, which is equivalent to a time spacing 75.76 ns and a sampling rate of 13.20 MHz. Figures 2(d), 2(e) and 2(f) show the amplitude and phase of the excitation pulse in the frequency domain for the simulations 1, 2 and 3, respectively.

For each simulation using the k-Wave and modified k-Wave, the pressure field was computed in time and was recorded on the receivers at the same discretised times as used for the k-Wave simulation. The recorded signal on each receiver was then decomposed into the frequency components.
(phase and amplitude) using a Fourier Transform operator. As a benchmark, the pressure field was also calculated analytically in the frequency domain using Eq. (10), in which the Green’s function is approximated using (11).

Figures 3(a), 3(b) and 3(c) show the amplitude of the pressure field induced by an excitation of the emitter (the red circle in figure 1(a)) and recorded on the receiver 100 (the green circle in figure 1(a)) as a function of frequency, when the excitation pulses 1, 2 and 3 were used, respectively. As shown in these figures, the amplitudes of the pressure field approximated using the modified k-Wave match the amplitudes analytically calculated using the Green’s function for all frequencies, but the amplitudes approximated using the k-Wave are different from the analytically calculated amplitudes. In the same way, figures 3(d), 3(e) and 3(f) show the phases of the pressure field recorded on the receiver 100, when the excitation pulses 1, 2 and 3 were used, respectively. The phases were wrapped to $[-\pi, \pi]$ rad. As shown in these figures, the phases approximated by the modified k-Wave and phases analytically calculated using the Green’s function match for all frequencies, but the phases approximated by the k-Wave are different from the analytically calculated phases.

Figures 4(a), 4(b) and 4(c) show the amplitudes of the pressure field recorded on all the receivers as a function of distance of receivers to the emitter, when the excitation pulses 1, 2 and 3 were used, respectively. In these figures, the amplitudes were computed at the single frequency $f_{\text{max}}/2 = 0.92$ MHz. As shown in these figures, for all the excitation pulses, the amplitudes computed using the modified k-Wave simulation (red plot) match the analytic solution to the wave equation using the Green’s function (green plot), but the amplitudes computed by the k-Wave (blue plot) are different from the analytically calculated amplitudes by almost the same factor.
In the same way, figures 4(d), 4(e) and 4(f) show the phase of the pressure field recorded on all the receivers, when the excitation pulses 1, 2 and 3 were used, respectively. The phases were wrapped to \([-\pi, \pi]\) rad. As shown in these figures, the phases approximated by the modified k-Wave match the analytically calculated phases on all the receivers, but the phases approximated using the k-Ware are different from the analytically calculated phases.

### 3.2. 3D case.

The k-Wave simulations were performed on a grid of size 0.5 mm. One emitter and 256 receivers were placed on a hemisphere with a radius of 12.35 cm, as shown in figure 1(b). The emitter was placed at the bottom of the hemisphere at position \(x_e = [1.54, 0, -12.25] \text{ cm}\). Figure 1(b) shows the emitter by the red colour and the receivers by the blue colour. The interpolations between the position of the transducers and the grid points were performed using the k-Wave toolbox [6, 9]. The sound speed inside the hemisphere was set 1500 ms\(^{-1}\) and homogeneous. The k-Wave simulations were performed using three excitation pulses for a time \(T = 212.2 \mu\text{s}\). Figure 5(a), 5(b) and 5(c) show the excitation pulses 1, 2 and 3 in the time domain, respectively. Here, a low-pass filter has been applied on each excitation pulse using the \texttt{filterTimeSeries.m} function in the k-Wave to ensure that the frequency spectrum of the pulse be smaller than the maximum frequency supported by the computational grid, and then the maximum absolute amplitude of the excitation pulses was normalised. The low pass filter was chosen conservatively using a sound speed of 1470 ms\(^{-1}\) for computing \(f_{\text{max}}\) in (14). The computed \(f_{\text{max}}\) was 1.47 MHz.

For the simulation using the excitation pulse 1, the CFL number was chosen 0.1, which is equivalent to a time spacing \(\Delta t = 31.57 \text{ ns}\) and a sampling rate of 31.68 MHz. The simulation
2D case. The pressure field at the single frequency $f_{\text{max}}/2$ on the receivers as a function of distance of the receivers to the emitter. Amplitude for simulations: a) 1, b) 2 and c) 3. Phase for simulations: d) 1, e) 2 and f) 3. The phases were wrapped to $[-\pi, \pi]$ rad.

2 was performed using the CFL number 0.2, which provides a time spacing 63.13 MHz, which is equivalent to a sampling rate 15.84 MHz. The simulation using the excitation pulse 3 was performed using the CFL number 0.3, which is equivalent to a time spacing 94.70 ns and a sampling rate of 10.56 MHz. Figures 5(d), 5(e) and 5(f) show the amplitude and phase of the excitation pulse in the frequency domain for the simulations 1, 2 and 3, respectively.

For each simulation using the k-Wave and modified k-Wave, the pressure field was computed in time and was recorded on the receivers at the same discretised times as used for the k-Wave simulation. The recorded signal on each receiver was then decomposed into the frequency components (phase and amplitude) using a Fourier Transform operator. The pressure field was also calculated analytically in the frequency domain using Eq. (10), in which the Green’s function is approximated using (12).

Figures 6(a), 6(b) and 6(c) show the amplitude of the pressure field recorded on receiver 100 (the green circle in figure 1(b)) after being produced by the emitter (the red circle in figure 1(b)) in the frequency domain for the simulation using the excitation pulse 1, 2 and 3, respectively. Because the amplitudes computed by the k-Wave (the blue plot) are much smaller than the amplitudes calculated using the Green’s function (green plot), a variant of the amplitudes which are enlarged by a factor 666.7 was also shown by the magenta colour for a better visualisation. As shown in these figures, the amplitudes approximated using the modified k-Wave match the amplitudes calculated analytically using the Green’s function for all frequencies. In addition, considering Eq. (12), the amplitude of the Green’s function in the 3D case depends only on distance, and is not changed with frequency. Note that for a nonabsorbing medium, the amplitude of the Green’s function represents
only geometrical attenuation. (cf. [7] and [8].) Therefore, the fact that the amplitude of the Green’s function in (12) is independent from frequency implies that the shape of the ultrasonic pulse should remain unchanged after propagation in the medium. A comparison between the amplitudes of the excitation pulse in figures 5(d), 5(e) and 5(f) and the approximated amplitudes of the pressure field on the receiver 100 in the respective figures 6(a), 6(b) and 6(c) show that the geometrical attenuation approximated by the k-Wave has changed with frequency, but the attenuation approximated using the modified k-Wave has remained unchanged with frequency. For example, for simulation 1, the maximum amplitude of the excitation pulse in the frequency domain, the amplitude analytically calculated using the Green’s function, and the amplitude approximated using the modified k-Wave in the frequency domain are all close to 0.6 MHz, but the maximum amplitude approximated using the k-Wave has been shifted to about 0.9 MHz, as shown in figure 6(a) by the magenta plot.

Figures 6(d), 6(e) and 6(f) show the phases of the pressure field recorded on the receiver 100, when the excitation pulses 1, 2 and 3 were used, respectively. The phases were wrapped to $[-\pi, \pi]$ rad. As shown in these figures, the phases approximated by the modified k-Wave and the phases calculated using the Green’s function match for all frequencies, but the phases approximated using the k-Wave are different.

Figures 7(a), 7(b) and 7(c) show the amplitudes of the pressure field recorded on all the receivers as a function of distances of receivers to the emitter, when the excitation pulses 1, 2 and 3 were used, respectively. In these figures, the amplitudes were computed at the single frequency $f_{\text{max}}/2 = 0.73$ MHz. Because the amplitudes computed by the k-Wave (blue plot) are much smaller than the Green’s function (green plot), they are also enlarged by a factor 666.7 for a better visualisation (magenta plot). As shown in these figures, using all the chosen excitation pulses, the amplitudes

Figure 5. 3D case. The excitation pulse in the time domain: a) 1, b) 2 and c) 3. The amplitude and phase of the excitation pulse in the frequency domain: d) 1, e) 2 and f) 3.
computed using the modified k-Wave (red plot) match the analytically calculated amplitudes (green plot), but the amplitudes computed by the k-Wave are different from the Green’s function by almost the same factor.

In the same way, figures 7(d), 7(e) and 7(f) show the phases, which have been wrapped to \([-\pi, \pi]\) rad. As shown in these figures, the phases approximated by the modified k-Wave match the analytically calculated phases for all the receivers, but the phases approximated using the k-Wave are different.

4. Discussion

This manuscript showed numerically that the k-space pseudo-spectral method proposed in [1, 2] for solving the three-coupled first order wave equations is almost exact for homogeneous media. A Matlab toolbox for a numerical implementation of this approach is available and was used in this study [3, 6, 10], but the approach taken for including source in the system of differential equations was revisited and modified. For measuring accuracy of this wave solver, an analytic solution to the second-order wave equation using the Green’s function was used as the benchmark. After applying the corrections discussed in section 2.2 for including the source in the equation of continuity (conservation of mass) in the system of three-coupled linearised wave equations, a good match between the wave solver and analytic solution to the wave equation was obtained.

In this study, the transducers were assumed points which are positioned off the grid and on the surface of a ring or hemisphere. Considering the match found between the Green’s function (Eq.
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Figure 7. 3D case. The pressure field at the single frequency $f_{\text{max}}/2$ on the receivers as a function of distance of the receivers to the emitter. Amplitude for simulations: a) 1, b) 2 and c) 3. Phase for simulations: d) 1, e) 2 and f) 3. The phases were wrapped to $[-\pi, \pi]$ rad.

...and Algorithm 1 (the wave solver) for a point source, it is clear that an approximation of the pressure field in 2D (resp. 3D) media using real transducers and with finite size requires an integration of the source over the area (resp. volume) of the transducers.

In general, acoustic sources can be time-varying or instant. This study was concentrated on including time-varying sources in the system of differential equations, but simulating propagation of instant acoustic sources are also widely used. One important application of instant sources is photo-acoustic tomography (PAT) [21, 22, 23]. The same comparisons can be done for simulating propagation of instant sources in homogeneous media.

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