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A 4th-order Implicit Procedure for the Simulation of Acoustics

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Abstract: This article is concerned with a new fourth-order *implicit* time-stepping scheme for the simulation of acoustic waves. For an enhanced efficiency, the new scheme is incorporated with a locally one-dimensional (LOD) procedure. Its stability and accuracy are analyzed and compared with those of the standard explicit fourth-order scheme. It has been observed from various experiments that the computational cost of the implicit LOD algorithm is only about 40% higher than that of the explicit method, for the problems of the same size in two space variables; the implicit procedure produces less dispersive solutions in heterogeneous media.

Key-Words: Acoustic wave, high-order method, locally one-dimensional (LOD) method, numerical dispersion.

1. Introduction

Let $\Omega \subset \mathbb{R}^m$, $1 \le m \le 3$, be a bounded domain with its boundary $\Gamma = \partial\Omega$ and $J = (0, T]$, $T > 0$. Consider the following acoustic wave equation

$$\begin{array}{ll} \text{(a)} & \frac{1}{c^2} u_{tt} - \Delta u = S(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times J, \\ \text{(b)} & \frac{1}{c} u_t + u_\nu = 0, \quad (\mathbf{x}, t) \in \Gamma \times J, \\ \text{(c)} & u(\mathbf{x}, 0) = g_0(\mathbf{x}),\ u_t(\mathbf{x}, 0) = g_1(\mathbf{x}),\ \mathbf{x} \in \Omega, \end{array} \tag{1}$$

where $c = c(\mathbf{x}) > 0$ denotes the normal velocity of the wavefront, S is the wave source/sink, ν denote the unit outer normal from Γ, and g_0 and g_1 are initial data. Equation (1.b) is popular as a simple-but-effective absorbing boundary condition (ABC), since introduced by Clayton and Engquist [3].

Equation (1) has been extensively studied as a model problem for second-order hyperbolic problems; see e.g. [1, 2, 5, 10, 12]. It is often the case that the source is given in the following form

$$S(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{x}_s) f(t),$$

where $\mathbf{x}_s \in \Omega$ is the source point. For the function f, the Ricker wavelet of frequency λ can be chosen, i.e.,

$$f(t) = \pi^2\lambda^2 \,(1 - 2\pi^2\lambda^2 t^2)\, e^{-\pi^2\lambda^2 t^2}.$$

In Geophysical applications, the wave equation (1) is often solved by explicit time-stepping schemes, which require to choose the time step size sufficiently small to satisfy the stability condition and to reduce numerical dispersion as well. An alternative conventional approach for solving wave equations introduces an auxiliary variable to rewrite the equation as a first-order hyperbolic system. With the approach one introduces a new unknown, which results in an increase in the number of variables in the discrete problems. Thus, there are good reasons to try to keep the formulation involving the second time-derivative and a scalar unknown. However, it has been known that with this formulation it is hard to construct numerical methods having desirable properties in both stability and high-order accuracy [9]. In this paper we shall introduce a one-parameter family of three-level methods incorporating the LOD time-stepping procedure for an efficient simulation of (1). It is analyzed to be unconditionally stable for the parameter in a certain range.

2. Preliminaries

In this section, we review conventional methods for the numerical solution of (1). Let $\mathcal{A}$ denote an approximation of $-\Delta$ of order p, i.e.,

$$\mathcal{A}\, u \,\approx\, -\Delta u + \mathcal{O}(h^p),$$

where h is the grid size; in most cases, p is 2 or 4. Then, the semi-discrete equation for the acoustic wave equation reads

$$\frac{1}{c^2}\, v_{tt} + \mathcal{A} v = S. \tag{2}$$

Now, let Δt be the time step size and $t^n = n\Delta t$. Set $v^n(\mathbf{x}) = v(\mathbf{x}, t^n)$. For a simpler presentation, we define the following difference operator

$$\overline{\partial}_{tt} v^n := \frac{v^{n+1} - 2v^n + v^{n-1}}{\Delta t^2}.$$

2.1. Explicit schemes

Explicit methods are still popular in the simulation of waveforms. We begin with the second-order scheme (in time) formulated as

$$\frac{1}{c^2}\,\overline{\partial}_{tt} v^n + \mathcal{A} v^n = S^n. \tag{3}$$

As a stability constraint, the scheme requires to choose $\Delta t = \mathcal{O}(h)$. The scheme (3) works well for smooth solutions, but otherwise it can introduce severe nonphysical oscillations.

To formulate the fourth-order scheme, consider the Taylor expansion

$$v_{tt}(t^n) \approx \overline{\partial}_{tt} v^n - \frac{\Delta t^2}{12} v_{tttt}(t^n) + \mathcal{O}(\Delta t^4). \tag{4}$$

It follows from (2) that

$$\begin{aligned} v_{tttt}(t^n) &= c^2 (S^n_{tt} - \mathcal{A} v^n_{tt}) \\ &= c^2 [\, S^n_{tt} - \mathcal{A}(c^2(S^n - \mathcal{A} v^n))\,]. \end{aligned} \tag{5}$$

From (4) and (5), the explicit fourth-order algorithm can be formulated as

$$\begin{aligned} \frac{1}{c^2}\,\overline{\partial}_{tt} v^n + \mathcal{A}\Big(v^n - \frac{\Delta t^2}{12} c^2 \mathcal{A} v^n\Big) \\ = S^n + \frac{\Delta t^2}{12}(\overline{\partial}_{tt} S^n - \mathcal{A} c^2 S^n). \end{aligned} \tag{6}$$

See [4, 5, 13] for details.

2.2. Two-level implicit schemes

Rewrite the system (2) as

$$\eta_t + \mathcal{A} v = S, \quad \frac{1}{c^2} v_t - \eta = 0, \tag{7}$$

where η is an auxiliary variable. Then, the two-level implicit scheme can be formulated as follows [9]:

$$\begin{aligned} &\text{(a)} \quad \frac{\eta^{n+1} - \eta^n}{\Delta t} + \mathcal{A}[\alpha v^{n+1} + (1-\alpha) v^n] = S^{n+\alpha}, \\ &\text{(b)} \quad \frac{1}{c^2}\frac{v^{n+1} - v^n}{\Delta t} - [\beta \eta^{n+1} + (1-\beta)\eta^n] = 0, \end{aligned} \tag{8}$$

where α and β are algorithm parameters, $0 \le \alpha, \beta \le 1$, and $S^{n+\alpha} = \alpha S^{n+1} + (1-\alpha) S^n$. In the literature, the following is well known for the two-level algorithm (see e.g. [9, §9.11]):

- The algorithm (8) is unconditionally stable when $\alpha, \beta \ge 0.5$.
- It is second-order if $(\alpha, \beta) = (0.5, 0.5)$, for example.
- It coincides with the explicit second-order scheme (3) when $(\alpha, \beta) = (0, 1)$.

The case $(\alpha, \beta) = (0.5, 0.5)$ is particularly interesting, because it allows the algorithm to be both second-order accurate (in time) and unconditionally stable. For an efficient implementation, (8) can be reformulated as follows. Multiply (8.a) and (8.b) by $\beta\Delta t^2$ and Δt, respectively, and add the resulting equations to have

$$\begin{aligned} \Big(\frac{1}{c^2} + \alpha\beta\Delta t^2 \mathcal{A}\Big) v^{n+1} = \Big(\frac{1}{c^2} - (1-\alpha)\beta\Delta t^2 \mathcal{A}\Big) v^n \\ + \Delta t\, \eta^n + \beta \Delta t^2 S^{n+\alpha}. \end{aligned} \tag{9}$$

Along with (8.b) and $\eta^0 = v^0_t / c^2 = g_1 / c^2$, the above equation solves the problem.

For a purpose of comparison with the three-level algorithms to be presented in Section 3, we reformulate (8), by eliminating η, as follows: for $n \ge 1$,

$$\begin{aligned} \frac{1}{c^2}\overline{\partial}_{tt} v^n + \mathcal{A}[\alpha\beta v^{n+1} + (\alpha + \beta - 2\alpha\beta) v^n \\ + (1-\alpha)(1-\beta) v^{n-1}] \\ = \beta S^{n+\alpha} + (1-\beta) S^{n-1+\alpha}. \end{aligned} \tag{10}$$

3. New Approaches

This section introduces one-parameter family of three-level implicit schemes for (1) and its LOD procedure. We will close the section with a certain parameter which makes the algorithm a fourth-order accuracy in time.

3.1. A three-level implicit method

We suggest a three-level implicit time-stepping algorithm for the acoustic wave equation (1) as follows: Given $v^0, \cdots, v^n$, $n \ge 1$, find v^{n+1} by solving

$$\begin{aligned} \frac{1}{c^2}\,\overline{\partial}_{tt} v^n + \mathcal{A}\left(\theta v^{n+1} + (1-2\theta) v^n + \theta v^{n-1}\right) \\ = S^n + \theta \Delta t^2 \overline{\partial}_{tt} S^n, \end{aligned} \tag{11}$$

where θ is an algorithm parameter to be selected in $[0, 0.5]$. One can verify the following:

- The truncation error of (11) is $\mathcal{O}(\Delta t^2 + h^p)$ for $\theta \in [0, 0.5]$.
- When $\theta = 0$, (11) turns out to be the second-order explicit scheme (3).

- When $\theta = 1/12$, the truncation error of (11) becomes $\mathcal{O}(\Delta t^4 + h^p)$. (See §3.3 below.)
- The algorithm is unconditionally stable when $\theta \in [0.25, 0.5]$. (See Theorem 1 below.)
- From a comparison between (10) and (11), we can see that the two-level and three-level implicit algorithms are equivalent to each other, when $\alpha = \beta = 0.5$ and $\theta = 0.25$.
- They are also equivalent when $\alpha = r_1$, $\beta = r_2$, and $\theta = 1/12$, where r_1 and r_2 are the two zeros of $x^2 - x + 1/12 = 0$. With these parameters, the algorithms are fourth-order accurate in time.

The implicit method (11) requires an appropriate initialization for v^1. Recall the initial conditions given in (1.c) and the Taylor series expansion

$$\begin{aligned} u^1 = u^0 + \Delta t u_t^0 + \frac{\Delta t^2}{2} u_{tt}^0 + \frac{\Delta t^3}{3!} u_{ttt}^0 \\ + \frac{\Delta t^4}{4!} u_{tttt}^0 + \mathcal{O}(\Delta t^5). \end{aligned} \tag{12}$$

Consider the equalities

$$\begin{aligned} u_t^0 &= g_1, \\ u_{tt}^0 &= c^2(S^0 - \mathcal{A}g_0), \\ u_{ttt}^0 &= c^2(S_t^0 - \mathcal{A}g_1), \\ u_{tttt}^0 &= c^2[S_{tt}^0 - \mathcal{A}(c^2(S^0 - \mathcal{A}g_0))], \end{aligned} \tag{13}$$

and approximations

$$\begin{aligned} S_t^0 &\approx \frac{-3S^0 + 4S^1 - S^2}{2\Delta t} + \mathcal{O}(\Delta t^2), \\ S_{tt}^0 &\approx \frac{S^0 - 2S^1 + S^2}{\Delta t^2} + \mathcal{O}(\Delta t). \end{aligned} \tag{14}$$

Then, it follows from (12)-(14) that

$$\begin{aligned} &\text{(a)} \quad v^1 \approx g_0 + \Delta t g_1 + \frac{\Delta t^2 c^2}{2}(S^0 - \mathcal{A}g_0) \\ &\qquad\qquad + \mathcal{O}(\Delta t^3), \\ &\text{(b)} \quad v^1 \approx g_0 + \Delta t g_1 + \frac{\Delta t^2 c^2}{2}\Big[\frac{7S^0 + 6S^1 - S^2}{12} \\ &\qquad - \mathcal{A}\Big(g_0 + \frac{\Delta t}{3} g_1 + \frac{\Delta t^2 c^2}{12}(S^0 - \mathcal{A}g_0)\Big)\Big] \\ &\qquad\qquad + \mathcal{O}(\Delta t^5). \end{aligned} \tag{15}$$

The initial values in (15.a) and (15.b) can be adopted respectively for the second- and fourth-order methods in time.

3.2. The LOD procedure

In many applications including Geophysical ones, the domain is rectangular or cubic. To solve the implicit algorithm (11) efficiently in these regular domains, we can adopt a locally one-dimensional (LOD) method, in particular, the alternating direction implicit (ADI) method [6, 7, 8, 11]. We will formulate the LOD procedure for 3D problems. Decompose $\mathcal{A}$ into the three directional operators $\mathcal{A}_\ell$, $\ell = 1, 2, 3$, i.e.,

$$\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3,$$

where $\mathcal{A}_\ell$ is the pth-order finite difference (FD) approximation of $-\partial_{x_\ell x_\ell}$. Then, an LOD time-stepping procedure for (11) can be constructed as follows. Given $w^0, \cdots, w^n$, we first approximate the solution at t^{n+1} by the explicit scheme:

$$\frac{1}{c^2}\frac{w^{n+1,0} - 2w^n + w^{n-1}}{\Delta t^2} + \mathcal{A}w^n = S^n + \theta\Delta t^2 \overline{\partial}_{tt} S^n, \tag{16}$$

and then apply the implicit directional sweeps

$$\begin{aligned} \frac{1}{c^2}\frac{w^{n+1,1} - w^{n+1,0}}{\Delta t^2} + \theta\, \mathcal{A}_1 \left(w^{n+1,1} - \widetilde{w}^n\right) = 0, \\ \frac{1}{c^2}\frac{w^{n+1,2} - w^{n+1,1}}{\Delta t^2} + \theta\, \mathcal{A}_2 \left(w^{n+1,2} - \widetilde{w}^n\right) = 0, \\ \frac{1}{c^2}\frac{w^{n+1} - w^{n+1,2}}{\Delta t^2} + \theta\, \mathcal{A}_3 \left(w^{n+1,3} - \widetilde{w}^n\right) = 0, \end{aligned} \tag{17}$$

where $\widetilde{w}^n = 2w^n - w^{n-1}$.

To find the splitting error involved during the LOD perturbation, we will eliminate the intermediate values in (16)-(17). Adding the four equations in (16)-(17), followed by some algebra, reads

$$\begin{aligned} \frac{1}{c^2}\,\overline{\partial}_{tt} w^n + \mathcal{A}\Big(\theta w^{n+1} + (1-2\theta)w^n + \theta w^{n-1}\Big) \\ + \mathcal{B}_\theta(w^{n+1} - 2w^n + w^{n-1}) = S^n + \theta\Delta t^2 \overline{\partial}_{tt} S^n, \end{aligned} \tag{18}$$

where

$$\begin{aligned} \mathcal{B}_\theta = \theta^2 \Delta t^2 c^2 (\mathcal{A}_1\mathcal{A}_2 + \mathcal{A}_1\mathcal{A}_3 + \mathcal{A}_2\mathcal{A}_3) \\ + \theta^3 (\Delta t^2 c^2)^2\, \mathcal{A}_1\mathcal{A}_2\mathcal{A}_3. \end{aligned}$$

Compared with (11), the LOD algorithm (16)-(17) incorporates an extra term $\mathcal{B}_\theta(w^{n+1} - 2w^n + w^{n-1})$, which is the splitting error. Since $(w^{n+1} - 2w^n + w^{n-1}) = \mathcal{O}(\Delta t^2)$ for sufficiently smooth solutions, the splitting error turns out to be fourth-order in time, i.e.,

$$\mathcal{B}_\theta(w^{n+1} - 2w^n + w^{n-1}) = \mathcal{O}(\Delta t^4). \tag{19}$$

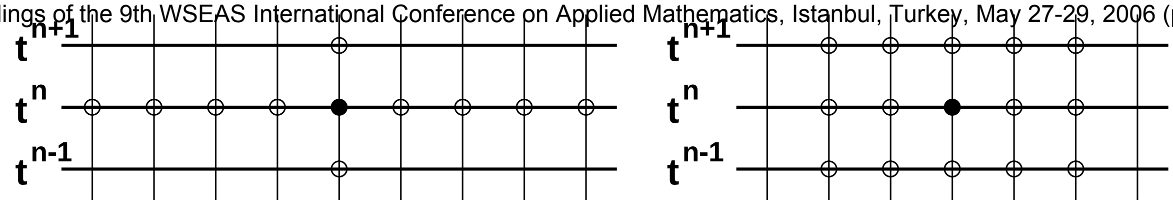

Fig. 1. The FD stencils, depicted in one space variable, for the fourth-order explicit scheme (left) and the fourth-order implicit scheme (right).

Thus the LOD algorithm (16)-(17) solves the three-level implicit FD equation (11) accurately, with an extra error (splitting error) in $\mathcal{O}(\Delta t^4)$. For 2D problems, the last sweep in (17) must be omitted and $w^{n+1,2}$ becomes the solution in the new time level, i.e., $w^{n+1} = w^{n+1,2}$.

The LOD algorithm presented in (16)-(17) can be implemented as follows:

$$\begin{aligned}
&\widetilde{w}^n = 2w^n - w^{n-1},\\
&w^{n+1,0} = \widetilde{w}^n + \Delta t^2 c^2 (S^n + \theta \Delta t^2 \overline{\partial}_{tt} S^n - \mathcal{A} w^n),\\
&(I + \theta \Delta t^2 c^2 \mathcal{A}_1) w^{n+1,1} = w^{n+1,0} + \theta \Delta t^2 c^2 \mathcal{A}_1 \widetilde{w}^n,\\
&(I + \theta \Delta t^2 c^2 \mathcal{A}_2) w^{n+1,2} = w^{n+1,1} + \theta \Delta t^2 c^2 \mathcal{A}_2 \widetilde{w}^n,\\
&(I + \theta \Delta t^2 c^2 \mathcal{A}_3) w^{n+1} \;\;= w^{n+1,2} + \theta \Delta t^2 c^2 \mathcal{A}_3 \widetilde{w}^n.
\end{aligned} \tag{20}$$

The three-level implicit algorithm (11) and its LOD procedure (16)-(17) can be analyzed for stability. We present a stability analysis; the proof will appear elsewhere.

Theorem 1. *Let* $\theta \in [0.25, 0.5]$. *Then* (11) *and its LOD procedure* (16)-(17) *are unconditionally stable.*

3.3. Fourth-order accuracy in time ($\theta = 1/12$)

When $\theta = 1/12$, the algorithms (11) and (16)-(17) become fourth-order in time. To see this, recall the Taylor expansion for $v_{tt}(t^n)$ in (4). Utilize

$$v_{tttt}(t^n) \;=\; c^2 (S^n_{tt} - \mathcal{A} v^n_{tt}) \tag{21}$$

to rewrite (4) as

$$\begin{aligned}
v_{tt}(t^n) \;&\approx\; \overline{\partial}_{tt} v^n - \frac{\Delta t^2}{12} c^2 (S^n_{tt} - \mathcal{A} v^n_{tt}) + \mathcal{O}(\Delta t^4)\\
&\approx\; \overline{\partial}_{tt} v^n - \frac{\Delta t^2}{12} c^2\, \overline{\partial}_{tt} S^n\\
&\quad + \frac{c^2}{12}\, \mathcal{A}(v^{n+1} - 2v^n + v^{n-1}) + \mathcal{O}(\Delta t^4),
\end{aligned} \tag{22}$$

where the central second-order approximations are applied for S^n_{tt} and v^n_{tt}. Thus a fourth-order time-stepping algorithm can be formulated as

$$\begin{aligned}
\frac{1}{c^2}\, \overline{\partial}_{tt} v^n + \frac{1}{12}\, \mathcal{A}(v^{n+1} - 2v^n + v^{n-1}) + \mathcal{A} v^n&\\
= S^n + \frac{\Delta t^2}{12}\, \overline{\partial}_{tt} S^n&,
\end{aligned} \tag{23}$$

which is identical to (11) when $\theta = 1/12$. The LOD variant of (23) clearly reads

$$\begin{aligned}
&\frac{1}{c^2}\, \overline{\partial}_{tt} v^n + \frac{1}{12}\, \mathcal{A}(v^{n+1} - 2v^n + v^{n-1}) + \mathcal{A} v^n\\
&\quad + \mathcal{B}_{1/12}(v^{n+1} - 2v^n + v^{n-1}) = S^n + \frac{\Delta t^2}{12}\, \overline{\partial}_{tt} S^n,
\end{aligned} \tag{24}$$

which is equivalent to (16)-(17) when $\theta = 1/12$. $\square$

Remark. The fourth-order explicit scheme utilizes the identity (5) for the approximation of v_{tttt}, while the new implicit method employs (21). As a result, the new implicit method adopts a more compact set of grid points in the FD approximation. See Figure 1, where the FD stencils are depicted for the fourth-order explicit scheme (left) and the fourth-order implicit scheme (right), in one space variable.

4. Numerical Experiments

The fourth-order explicit method (6) and the LOD algorithm (20) are implemented for the acoustic wave equation in two space variables. For the spatial derivatives, the fourth-order FD scheme is adopted for both algorithms.

Figure 2 presents a vertical section of a real velocity in the Gulf of Mexico (left), provided from Shell Offshore Inc., and the snapshots of the numerical solution at $t = 2.2$ for the fourth-order explicit method (center) and the fourth-order LOD (right). For the point source, a Ricker wavelet of 10Hz ($\lambda = 10$) is located at the center of the top edge ($\mathbf{x}_s = (4.57, 0)$). Since the velocity $c(\mathbf{x}) \in [1.50, 4.42]$ (Km/sec), the wavelength ($:= c/\lambda$) varies between 150 and 442 meters. The velocity model contains 240×160 cells of the edge length 38.1 meters ($h = 38.1$). Thus the *grid frequency* G_f (the number of grid points per wavelength)

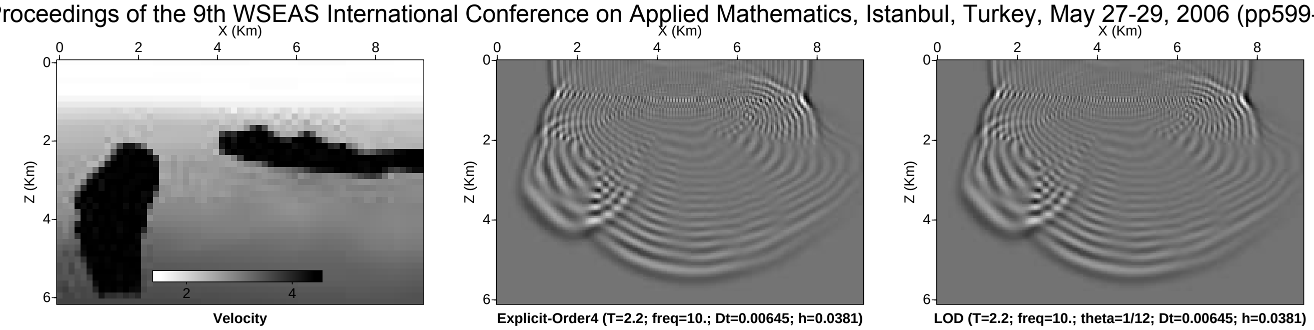

Fig. 2. The velocity (left) and the snapshots at $t = 2.2$ for the fourth-order explicit method (center), and the fourth-order LOD ($\theta = 1/12$) (right). The fourth-order central FD scheme is applied for the spatial derivatives for all cases.

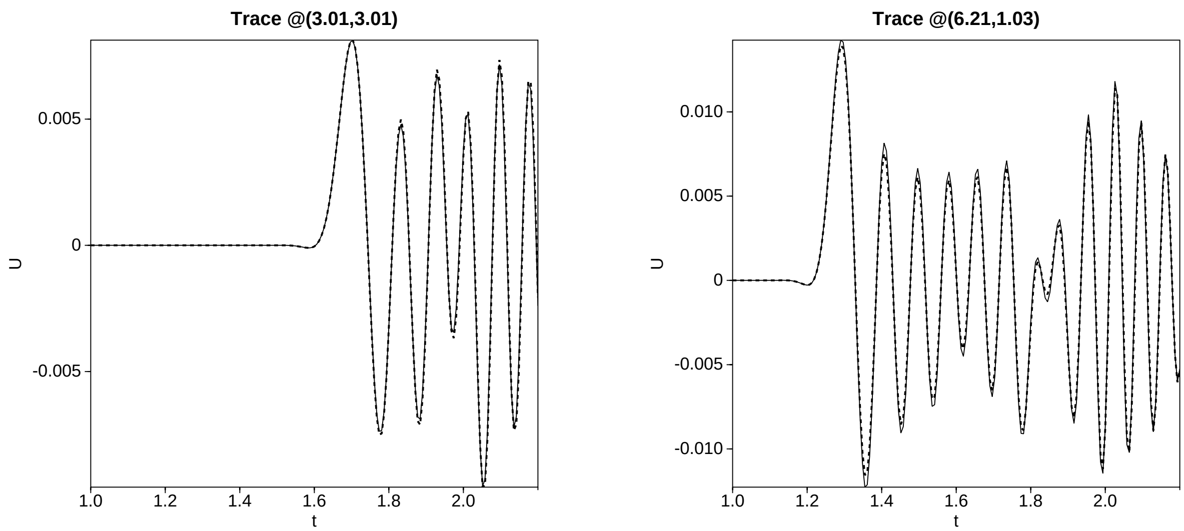

Fig. 3. The traces seen at $\mathbf{x} = (3.01, 3.01)$ (left) and $\mathbf{x} = (6.21, 1.03)$ (right). The solid and dashed curves correspond to LOD($\theta = 1/12$) and the fourth-order explicit methods, respectively.

becomes $3.94 \sim 11.60$. The time step size Δt is selected for the Courant number σ near to 0.75 such that 2.2 is an integer multiple of Δt, i.e.,

$$\sigma := \frac{\Delta t\, \|c\|_\infty}{h} \approx 0.75,$$

where $\|c\|_\infty$ denotes the maximum of the velocity c. (The total number of timesteps is 341.)

The solutions from the fourth-order methods hardly differ from each other; the implicit LOD ($\theta = 1/12$) method seems producing a slightly sharper solution than the fourth-order explicit method.

To see the differences in detail, the traces are observed and compared at a few points. Figure 3 contains the traces recorded at $\mathbf{x} = (3.01, 3.01)$ (left) and $\mathbf{x} = (6.21, 1.03)$ (right), where the waveform is expected to oscillate a lot due to sudden changes in velocity and therefore strong reflections. The solid and dashed curves correspond to LOD($\theta = 1/12$) and the fourth-order explicit methods, respectively. As one can see from the figure, the solutions obtained from the two fourth-order methods match each other quite well. It has been observed from various experiments (not presented here) that

- The implicit method shows a similar numerical stability as the explicit scheme. That is, instability has been observed for a similarly large Δt for both methods. Thus the implicit method may not gain efficiency over the explicit method by choosing a larger time step size. They have been stable for most cases when the Courant number $\sigma \le 0.7 \sim 1.0$.
- The implicit method takes about 40% more computation time than the explicit method for 2D problems of the same size, in practice.
- The fourth-order LOD method is less dispersive; it often produces a solution of less nonphysical

oscillation than the fourth-order explicit scheme. It can be advantageous for the numerical solution in very oscillatory media.

- Second-order methods (in time) produce more dissipative solutions than fourth-order methods. Thus second-order methods are less attractive, although they can be unconditionally stable. A sharp resolution of wavefronts is often very important in wave simulation.

5. Conclusions

We have introduced one-parameter family of three-level implicit FD schemes for the numerical solution of the acoustic wave equation. For an efficient simulation, a locally one-dimensional (LOD) procedure, having the splitting error in $\mathcal{O}(\Delta t^4)$, has been adopted. It has been analyzed to be unconditionally stable (but second-order in time) when the parameter is in a certain range ($\theta \in [0.25, 0.5]$). Also we have seen that the algorithm is fourth-order in time when $\theta = 1/12$. The new algorithm is compared with the conventional two-level implicit methods; parameters are found such that the methods are equivalent to each other with either second- or fourth-order accuracy in time. The three-level fourth-order implicit method is compared with the standard (three-level) explicit method in numerical stability, accuracy, and efficiency:

- The implicit method shows a similar stability condition as the explicit scheme, in practice.
- The implicit method turns out to be 40% more expensive than the explicit method for 2D problems of the same size.
- The implicit method introduces a less nonphysical oscillation (dispersion). Due to this property, the implicit scheme can be advantageous over the explicit scheme for the waveform simulation in very oscillatory media.

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