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On the stability and efficiency of high-order parallel algorithms for 3D wave problems

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Abstract. In this work, we investigate the stability conditions for four new high-order ADI type schemes proposed to solve 3D wave equations with a non-constant sound speed coefficient. This analysis is mainly based on the spectral method, therefore a basic benchmark problem is formulated with a constant sound speed coefficient. For a case of general non-constant coefficient the stability analysis is done by using the energy method. Our main conclusion states that the selected ADI type schemes use different factorization operators (mainly due to the need to approximate the artificial boundary conditions on the split time levels), but the general structure of the stability factors are similar for all schemes and thus the obtained CFL conditions are also very similar.
The second goal is to compare the accuracy and efficiency of the selected ADI solvers. This analysis also includes parallel versions of these schemes. Two schemes are selected as the most effective and accurate.

Keywords: ADI discrete schemes; 3D wave problem; stability; parallel algorithms.

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1 Introduction

We are interested in solving the following Cauchy problem for the 3D wave equation for function $u = u(x, y, z, t)$, namely

$$\frac{\partial^2 u}{\partial t^2} = c^2(X)\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + f(X,t), \tag{1.1}$$

$$u(X,0) = u_0(X), \qquad \partial_t u|_{t=0} = u_1(X), \qquad u|_{\partial\Omega} = g(X,t),$$
$$t \in (0,T], \qquad X := (x,y,z) \in \Omega, \qquad \Omega = (0,L)^3. \tag{1.2}$$

Here $c(X)$ is the variable sound velocity, we assume that

$$0 < c_m \le c(X) \le c_M, \quad \text{for } X \in \Omega.$$

Before proceeding, it is important to make the following remarks.

1. The importance of the topic is emphasized by the fact that a number of different theoretical approaches have been proposed to construct high-order compact schemes for solving the 3D wave equations (see below).

2. This study does not consider the case of a non-stationary sound velocity coefficient $c(X, t)$, we restrict ourselves with $c(X)$.

3. Compact approximations are defined as approximations of the Laplace operator on three-point space mesh stencils in each dimension. Therefore, we deal with tridiagonal matrices, which is very convenient for the efficient implementation of the algorithms.

4. Integration in time is also done using high-order integration schemes. They are based on factorized operators of the ADI (Alternating Direction Implicit) and LOD (Locally One-Dimensional) types.

In order to reduce the linear algebra part of the time integration scheme to solution of systems with tridiagonal matrices, the factorization methods should be supplemented with special boundary conditions at all splitting steps. We prefer schemes where these boundary conditions are defined on the same compact mesh stencil and the additional equations follow from the basic discrete equations. Another popular approach, which employs one-sided high-order approximation techniques to resolve the challenge of artificial boundary conditions, is beyond the scope of this paper.

5. One of our goals is to compare the stability factors of the evolution matrices of the selected compact high-order schemes.

6. 3D problems require the use of discrete approximations on meshes with a very large number of discrete points and unknowns defined on these points. Therefore, the efficiency of parallel versions of these schemes is also analyzed.

Next, we give a brief overview of the main scientific results recently achieved in this direction. We limit ourselves to the most important works that have a direct relation to the discrete schemes chosen as the basic sources of our analysis.

Compact schemes of the ADI type are constructed in [2]. This article focuses on the analysis of high-order compact ADI method for solving 2D coupled sine-Gordon equations. The classical Crank-Nicolson method is used for the time discretization. It is important to note that not only the spectral method but also the energy method is used for the stability analysis.

A family of high-order LOD schemes for the 3D elastic wave equation is constructed and analyzed in [11]. We note that the same restrictions on the velocity coefficient $c(X)$ and on boundary conditions can be found in the earlier paper [12].

For 2D wave equations the analysis of fourth-order accurate compact finite difference schemes in both space and time, was started in [1]. The discrete schemes have also been constructed for models with variable sound speed. Although these schemes are implicit and only conditionally stable, they are more efficient than the lower-order schemes. Fast time marching of the implicit schemes is achieved by iterative methods such as conjugate gradient and multigrid. Stability is investigated using techniques based on the energy method, as previously applied to nonstationary advection-diffusion problems.

The solutions of acoustic problems can have singularities in some parts of the domain and adaptive/nonuniform meshes can be recommended in such situations. Still we want to note that high-order schemes of the type given in this paper can't be constructed on adaptive meshes. Thus we needed to chose one or another way to solve such problems. In this paper we consider the case of uniform meshes and high order approximations. The case of non-uniform schemes will be considered in a separate paper.

Stability and accuracy analysis of 4th order finite-difference schemes for the wave equation is performed in [15]. An important result of [15] is a new template of the discrete problems for which the stability estimates can be proved by using the energy method. This technique is then further applied to certain discrete schemes.

[14] can be considered as a continuation of [15]. One of the discrete schemes developed in [14] is selected as a benchmark for a new class of compact high-order ADI type schemes developed by using Numerov's approximation approach. Thereafter, general properties of such schemes are investigated for the wave equation with the variable sound speed coefficient.

A new family of LOD schemes with fourth-order accuracy in both space and time for the three-dimensional (3D) acoustic wave equation is proposed in [12]. Still only wave equations in a homogeneous media are investigated and boundary conditions are also homogeneous. This family of LOD schemes has a different stability factor in comparison with ADI type schemes, moreover, LOD scheme has a smaller CFL (Courant-Friedrichs-Lewy) constant.

A compact in space 4th order scheme is constructed in [5] by using the well known high-order approximation of the second derivative. The approximation error in time is $O(\tau^2)$. Both high-order approximations of the solution and its second derivative generate commuting operators. Therefore the same combined energy and spectral analysis as in [1] can be applied. The obtained CFL constant is a little bit worse than that obtained by the direct application of the spectral analysis for a constant sound speed coefficient. Here, the boundary conditions in all computational experiments are homogeneous.

Parallelization and convergence of ADI time integrators for 2D finite difference acoustic wave propagation are analyzed in [8]. Three parallel versions of each method are investigated. It is shown that parallel solvers based on compact finite difference solvers with tridiagonal matrices and CUDA kernels for a NVIDIA card give the highest performance.

The rest of the paper is organized as follows. In Section 2, the mathematical problem is formulated for a general 3D wave equation with a variable sound speed coefficient. We are interested to analyze state of the art compact high-order parallel finite-volume schemes.

Two different approaches are used.

First, the discretization is done by using the Padé approximation and application of the factorized implicit regularization operator (ADI type schemes).

Second, the Numerov type approximations are used. The time integration is implemented by using factorized operators and the important part consists in the formulation of artificial boundary conditions.

In Section 3, the stability analysis is performed for all constructed compact high-order discrete schemes of the ADI type. Both the spectral and energy methods are used. In order to directly compare the dynamic stability factors of discrete schemes, a simplified model problem is defined for which the sound speed is constant. Then, the spectral method is used to find and compare CFL stability factors. These factors are close to the stability conditions of classical symmetric explicit schemes.

The energy method is used for general coefficients $c(x, y, z)$. However, we note that no complete results are known for $c \neq \text{const}$. A partial stability result is obtained for a simplified compact scheme.

In Section 4, results of computational experiments are given. We consider two test problems and provide errors, experimental convergence rates, and CPU times for a sequence of time and space steps. It is shown that the EHOC scheme gives the most accurate approximations and is the most efficient in terms of CPU time. The results of the computational experiments confirm both the theoretical accuracy and the stability estimates.

The second set of the computational experiments deals with parallel computations. It is shown that parallel versions of compact factorized high-order ADI schemes can be implemented very efficiently. This property is important when simulating large-scale applied 3D wave propagation problems.

Finally, conclusions are given in Section 5.

2 High-order discrete schemes

The uniform time mesh $\bar{\omega}_\tau$ on $[0, T]$ with the discrete step $\tau = T/N$ is defined by

$$\bar{\omega}_\tau = \big\{t^n : t^n = n\tau, \quad n = 0, \dots, N\big\}.$$

In what follows, H_h denotes the Hilbert space of discrete functions on the uniform space mesh $\bar{\omega}_h$ on $\bar{\Omega}$, where h is the space discretization parameter and

$$\bar{\omega}_h = \big\{(x_i, y_j, z_k) : x_i = ih, \ y_j = jh, \ z_k = kh, \quad 0 \le i, j, k \le M\big\}.$$

For the sake of simplicity, h is assumed to be the same in all three directions. We define the discrete function

$$U^n_{ijk} = U(X_{ijk}, t^n), \quad X_{ijk} = (x_i, y_j, z_k), \quad (X_{ijk}, t^n) \in \omega_h \times \omega_\tau,$$

that approximates the exact solution $u(X_{ijk}, t^n)$.

First we formulate the benchmark problem, which is used to compare approximation errors and stability results for different compact high-order discrete schemes. The problem is obtained by applying the following assumptions for the mathematical problem (1.1)–(1.2):

$$c(X) := C, \quad f(X,t) = 0, \tag{2.1}$$

i.e., the velocity $c(X)$ is constant.

In [7] a rather general technique was used to construct the fourth-order compact approximation of the benchmark problem (1.1)–(2.1). This approach is based on the Padé approximation and the application of the factorized implicit operator to the discrete second-order time derivative

$$\begin{aligned}(1+\rho\delta_x^2)(1+\rho\delta_y^2)(1+\rho\delta_z^2)\delta_t^2 U^n &= r^2\Big[\delta_x^2\Big(1+\frac{1}{12}\delta_y^2\Big)\Big(1+\frac{1}{12}\delta_z^2\Big)\\ &+\delta_y^2\Big(1+\frac{1}{12}\delta_x^2\Big)\Big(1+\frac{1}{12}\delta_z^2\Big)+\delta_z^2\Big(1+\frac{1}{12}\delta_x^2\Big)\Big(1+\frac{1}{12}\delta_y^2\Big)\Big]U^n, \end{aligned}\tag{2.2}$$

where $r = C\tau/h$ and $\rho = (1-r^2)/12$. We use the standard notations

$$(\delta_t^2 U)^n = U^{n+1} - 2U^n + U^{n-1}, \qquad \begin{aligned}(\delta_x^2 U)_{ijk} &= U_{i+1,j,k} - 2U_{ijk} + U_{i-1,j,k},\\ (\delta_y^2 U)_{ijk} &= U_{i,j+1,k} - 2U_{ijk} + U_{i,j-1,k},\\ (\delta_z^2 U)_{ijk} &= U_{i,j,k+1} - 2U_{ijk} + U_{i,j,k-1}.\end{aligned}$$

The popularity of this and similar ADI schemes stems from the fact that they can be solved efficiently in three simple steps:

$$\begin{aligned}(1+\rho\delta_x^2)U^{n+1/3} &= r^2\Big[\delta_x^2\Big(1+\frac{1}{12}\delta_y^2\Big)\Big(1+\frac{1}{12}\delta_z^2\Big)\\ &+\delta_y^2\Big(1+\frac{1}{12}\delta_x^2\Big)\Big(1+\frac{1}{12}\delta_z^2\Big)+\delta_z^2\Big(1+\frac{1}{12}\delta_x^2\Big)\Big(1+\frac{1}{12}\delta_y^2\Big)\Big]U^n, \end{aligned}\tag{2.3}$$

$$\begin{aligned}(1+\rho\delta_y^2)U^{n+2/3} &= U^{n+1/3},\\ (1+\rho\delta_z^2)\delta_t^2 U^n &= U^{n+2/3}.\end{aligned}\tag{2.4}$$

It is clear that Equations (2.3)–(2.4) can be solved as a sequence of $3M^2$ tridiagonal linear systems with $M \times M$ matrices.

An important note needs to be considered here. Such an ADI-type implementation preserves the $O(\tau^4 + h^4)$ accuracy when special boundary conditions are used [3, 9]. A set of boundary conditions consistent with the discrete equation (2.2) is the following [7]:

$$\begin{aligned}U^{n+1/3}\big|_{\partial\omega_{hx}} &= (1+\rho\delta_y^2)(1+\rho\delta_z^2)\,\delta_t^2 U^n\big|_{\partial\omega_{hx}},\\ U^{n+2/3}\big|_{\partial\omega_{hy}} &= (1+\rho\delta_z^2)\,\delta_t^2 U^n\big|_{\partial\omega_{hy}}.\end{aligned}$$

Since the scheme (2.2) is a three-level scheme, it requires the initial condition for U^1. To construct the fourth-order approximation the standard method of Taylor series can be used. The detailed definition of this condition is not important for what follows (see [7] for all details).

Next, we consider the explicit high-order compact scheme (EHOC) constructed in [4]. In the following, the discrete functions V_x^n, V_y^n and V_z^n approximate the second-order derivatives $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^2 u}{\partial y^2}$ and $\frac{\partial^2 u}{\partial z^2}$, respectively. Fourth-order Padé approximation is used to compute the values of these functions:

$$V^n_{x,\,i+1,jk} + 10V^n_{x,\,ijk} + V^n_{x,\,i-1,jk} = 12\,\frac{(\delta_x^2 U)^n_{ijk}}{h^2}, \qquad \begin{array}{r} 1 \le i < M, \\ 0 \le j,k \le M, \end{array} \tag{2.5}$$

$$V^n_{y,\,i,j+1,k} + 10V^n_{y,\,ijk} + V^n_{y,\,i,j-1,k} = 12\,\frac{(\delta_y^2 U)^n_{ijk}}{h^2}, \qquad \begin{array}{r} 1 \le j < M, \\ 0 \le i,k \le M, \end{array}$$

$$V^n_{z,\,ij,k+1} + 10V^n_{z,\,ijk} + V^n_{z,\,ij,k-1} = 12\,\frac{(\delta_z^2 U)^n_{ijk}}{h^2}, \qquad \begin{array}{r} 1 \le k < M, \\ 0 \le i,j \le M. \end{array} \tag{2.6}$$

An important advantage of this scheme is that the boundary conditions for the functions V_ξ^n, $\xi = x, y, z$ follow directly from the exact boundary conditions of the differential mathematical model (1.1)–(1.2). For the sake of brevity, we only give the boundary conditions in the x direction:

$$V^n_{x,\,Ijk} = \left[\frac{1}{c^2(X)}\left(\frac{\partial^2 g(X,t)}{\partial t^2} - f(X,t)\right) - \frac{\partial^2 g(X,t)}{\partial y^2} - \frac{\partial^2 g(X,t)}{\partial z^2}\right]_{\substack{t=t^n,\\ X=X_{Ijk}}},$$

$$I = 0, M, \quad 0 \le j,k \le M, \quad n > 0. \tag{2.7}$$

Note that the coefficient matrices in the system (2.5)–(2.7) are tridiagonal, so the standard Thomas algorithm [3] can be used to solve these linear systems efficiently.

The temporal part of the scheme is constructed applying the Taylor series in time:

$$\begin{aligned} U^{n+1}_{ijk} &= 2U^n_{ijk} - U^{n-1}_{ijk} + \frac{c^2_{ijk}\tau^2\lambda^2}{12} \\ &\quad \times \Big\{ F^n_{i-1,jk} + F^n_{i+1,jk} + F^n_{i,j-1,k} + F^n_{i,j+1,k} + F^n_{ij,k-1} + F^n_{ij,k+1} \\ &\qquad + c^2_{i-1,jk}\big[V^n_{x,\,i-1,jk} + V^n_{y,\,i-1,jk} + V^n_{z,\,i-1,jk}\big] \\ &\qquad + c^2_{i+1,jk}\big[V^n_{x,\,i+1,jk} + V^n_{y,\,i+1,jk} + V^n_{z,\,i+1,jk}\big] \\ &\qquad + c^2_{i,j-1,k}\big[V^n_{x,\,i,j-1,k} + V^n_{y,\,i,j-1,k} + V^n_{z,\,i,j-1,k}\big] \\ &\qquad + c^2_{i,j+1,k}\big[V^n_{x,\,i,j+1,k} + V^n_{y,\,i,j+1,k} + V^n_{z,\,i,j+1,k}\big] \\ &\qquad + c^2_{ij,k-1}\big[V^n_{x,\,ij,k-1} + V^n_{y,\,ij,k-1} + V^n_{z,\,ij,k-1}\big] \\ &\qquad + c^2_{ij,k+1}\big[V^n_{x,\,ij,k+1} + V^n_{y,\,ij,k+1} + V^n_{z,\,ij,k+1}\big]\Big\} \\ &\quad + \tau^2\Big(1 - 0.5c^2_{ijk}\lambda^2\Big)\Big(F^n_{ijk} + c^2_{ijk}\big[V^n_{x,\,ijk} + V^n_{y,\,ijk} + V^n_{z,\,ijk}\big]\Big) \\ &\quad + \frac{\tau^4}{12}\left(\frac{\partial^2 F^n}{\partial t^2}\right)_{ijk}, \end{aligned} \tag{2.8}$$

where $\lambda = \tau/h$.

In [13] the following compact ADI scheme is introduced

$$B_{c,h}\left(\frac{1}{c^2}\delta_t\delta_{\bar{t}}U\right)+A_hU=\frac{1}{c^2}F_h \quad \text{on} \quad \omega_h\times\omega_\tau, \tag{2.9}$$
$$B_{c,h}\left(\frac{1}{c^2}\delta_tU^0\right)+0.5\tau A_hU^0=u_1(t^n)+0.5\tau F^0 \quad \text{on} \quad \omega_h,$$
$$U^n\big|_{\partial\omega_h}=g(t^n),$$

where the discrete derivative time operators are defined by

$$\delta_tU^n=\frac{U^{n+1}-U^n}{\tau}, \quad \delta_{\bar{t}}U^n=\frac{U^n-U^{n-1}}{\tau}.$$

The splitting operator $B_{c,h}$ is defined as the product of 1D operators defined on a three-point mesh stencil

$$B_{c,h}:=B_{x,ch}B_{y,ch}B_{z,ch}, \quad B_{\xi,ch}:=I_h+\frac{h^2(h^2-\tau^2c^2)}{12}\Lambda_{\xi h}, \quad \xi=x,y,z,$$

where I_h is the discrete identity operator and the operators $\Lambda_{\xi h}$ are defined as

$$\Lambda_{xh}V=\frac{(\delta_x^2V)_{ijk}}{h^2}, \quad \Lambda_{yh}V=\frac{(\delta_y^2V)_{ijk}}{h^2}, \quad \Lambda_{zh}V=\frac{(\delta_z^2V)_{ijk}}{h^2}.$$

3 Stability analysis

We recall that we consider two PDE benchmark problems. In the first one, the sound speed in (1.1)–(1.2) is a general stationary function $c(x,y,z)$. Stability analysis for discrete schemes that approximate this problem is usually based on various versions of the energy method.

In the second simplified benchmark problem for (1.1)–(1.2), (2.1) the coefficient c is constant. This assumption allows the use of spectral stability analysis. Exactly this technique allows us to compare the stability properties of the high-order discrete schemes constructed in the previous section.

We approximate the problem (1.1)–(1.2), (2.1) by the explicit symmetric scheme [3, 9]

$$\delta_t^2U^n=r^2(\delta_x^2+\delta_y^2+\delta_z^2)U^n, \quad 1\le n<N, \tag{3.1}$$

where we recall that $r=C\tau/h$. The eigenvectors and eigenvalues of the discrete space operator δ_x^2 are defined by

$$-\delta_x^2\varphi^l(x_i)=\lambda_l\varphi^l(x_i), \quad l=1,\dots,M-1, \quad x_i\in\omega_h,$$

the eigenvectors and eigenvalues for the operators δ_y^2 and δ_y^2 are defined in a similar way. For the following stability analysis it is very convenient that the set of eigenvalues can be written in an explicit form (see, e.g. [9])

$$\lambda_l=4\sin^2\left(\frac{l\pi h}{2}\right), \quad l=1,\dots,M-1, \quad 0<\lambda_1<\ldots<\lambda_{M-1}<4.$$

Since the eigenvectors $\{\varphi^l, l = 1, \dots, M-1\}$ define a complete orthonormal set of basis functions, we can write the solution U^n in the form

$$U_{ijk}^n = \sum_{l,m,r=1}^{M-1} c_{lmr} q_{lmr}^n \varphi^l(x_i)\varphi^m(y_j)\varphi^r(z_k), \tag{3.2}$$

where the coefficients c_{lmr} define the initial vector, q_{lmr} are real numbers and define the stability factors of the discrete scheme, the dynamics of the solution is computed as $q_{lmr}^n = (q_{lmr})^n$. The stability factors q_{lmr} are defined for each discrete scheme and depend on eigenvalues of basic eigenvectors. We are interested in partial solutions in which the indices l, m, r are fixed. The discrete scheme (3.1) is stable if the following condition for the stability factor q_{lmr}

$$|q_{lmr}| \le 1, \quad 1 \le l, m, r \le M-1,$$

holds.

Substituting (3.2) into the discrete scheme (3.1) and using the orthonormality of the basis functions (eigenvectors), we obtain the following second order equations for the coefficients q_{lmr}

$$q_{lmr}^2 - [2 - r^2(\lambda_l + \lambda_m + \lambda_r)]q_{lmr} + 1 = 0.$$

It follows from the Hurwitz criterion that $|q_{lmr}| \le 1$ if

$$|2 - r^2(\lambda_l + \lambda_m + \lambda_r)| \le 2 \quad \Rightarrow \quad 0 \le r^2(\lambda_l + \lambda_m + \lambda_r) \le 4.$$

The most restrictive condition is obtained for the highest spectral component

$$3r^2\lambda_{M-1} \le 4 \quad \Rightarrow \quad 3r^2 \le 1.$$

Thus we get the following stability result (in fact, this result is quite well known):

Lemma 1. *The three-level symmetric discrete scheme* (3.1) *is stable if the time and space steps satisfy the estimate*

$$\tau \le \frac{1}{C}\frac{\sqrt{3}}{3}h. \tag{3.3}$$

For our stability analysis of high-order discrete schemes, this conditional stability estimate defines the benchmark stability condition for explicit classical discrete schemes.

Now we consider the stability of the explicit symmetric scheme for a problem with a non-constant sound speed c

$$\frac{1}{c^2(x,y,x)}\frac{1}{\tau^2}\delta_t^2 U^n = \frac{1}{h^2}(\delta_x^2 + \delta_y^2 + \delta_z^2)U^n, \quad 1 \le n < N, \tag{3.4}$$

using the energy method. Consider one of the canonical forms of three-layer schemes (see [9]):

$$D_h\Big(\frac{1}{\tau^2}\delta_t^2\Big)U^n + A_h U^n = 0, \tag{3.5}$$

where D_h, A_h are constant in time self-adjoint positive operators

$$A_h = A_h^*, \quad A_h > 0, \quad D_h = D_h^*, \quad D_h > 0. \tag{3.6}$$

For discrete functions $V := \{V_{ijk} := V(x_i, y_j, z_k),\ X \in \bar{\omega}_h\}$ in H_h we define the standard inner product $(\cdot,\cdot)$ and the corresponding norm $\|\cdot\|$. We will use the following stability result [9]:

Theorem 1. *The discrete scheme* (3.5) *under conditions* (3.6) *and the additional constraint*

$$D_h \geq \frac{\tau^2}{4} A_h, \tag{3.7}$$

is stable with respect to the initial data.

Example. Let us consider the explicit symmetric scheme (3.4) when the sound speed c is constant. Then we have the operators

$$D_h = \frac{1}{c^2} I_h, \quad A_h = -\frac{1}{h^2}(\delta_x^2 + \delta_y^2 + \delta_z^2).$$

It is easy to prove that

$$(D_h V, V) = \frac{1}{c^2}(V, V), \quad (A_h V, V) < \frac{12}{h^2}(V, V),$$

and the stability condition (3.7) is satisfied if

$$\frac{\tau^2}{4} A_h \leq \frac{3\tau^2}{h^2} I_h \leq \frac{1}{c^2} I_h \quad \Longrightarrow \quad \tau \leq \frac{1}{c}\frac{\sqrt{3}}{3} h.$$

The latter condition coincides with the estimate (3.3) derived by using the spectral method.

Example. Let us consider the explicit symmetric scheme (3.4) when the sound speed $c(x, y, z)$ is non-constant. We then deal with the diagonal matrix and the Laplace operator

$$D_h = \text{diag}\left(\frac{1}{c_{ijk}^2}\right), \quad A_h = -\frac{1}{h^2}(\delta_x^2 + \delta_y^2 + \delta_z^2).$$

By calculating scalar products

$$(D_h V, V) = \sum_{i,j,k=1}^{M-1} \frac{1}{c_{ijk}^2} v_{ijk}^2 \geq \frac{1}{c_{\max}^2}(V, V), \quad (A_h V, V) < \frac{12}{h^2}(V, V)$$

we obtain

$$D_h \geq \frac{1}{c_{\max}^2} I_h \geq \frac{3\tau^2}{h^2} I_h \geq \frac{\tau^2}{4} A_h.$$

So the stability condition (3.7) is satisfied if

$$\tau \leq \frac{1}{c_{\max}} \frac{\sqrt{3}}{3} h.$$

Stability of the high-order discrete scheme (2.2). The sound speed is constant C in this problem, so the spectral stability method can be used. The solution U^n is written as

$$U^n_{ijk} = \sum_{l,m,p=1}^{M-1} u^n_{lmp} \varphi^l(x_i)\varphi^m(y_j)\varphi^p(z_k).$$

We restrict our analysis to the critical high eigenvector:

$$l = m = p = M-1 \quad \text{with} \quad u^n_{M-1,M-1,M-1} = (q)^n.$$

Substituting the above U^n into the discrete equation (2.2) we get an equation for the stability factor q

$$(1-\rho\lambda_{M-1})^3(q^2-2q+1) + 3r^2\lambda_{M-1}(1-\lambda_{M-1}/12)^2 q = 0.$$

Taking into account that $r = C\tau/h$ and $\rho = (1-r^2)/12$, the following quadratic equation is obtained

$$q^2 - (2-\gamma)q + 1 = 0, \quad \gamma = \frac{3r^2\lambda_{M-1}(1-\lambda_{M-1}/12)^2}{\big(1-\lambda_{M-1}(1-r^2)/12\big)^3}, \tag{3.8}$$

where $\lambda_{M-1} < 4$. It follows from the Hurwitz criterion that discrete scheme (2.2) is stable if $0 \le \gamma \le 4$. By solving the inequality we get that the stability condition is satisfied for

$$C\tau < 0.607935083\, h.$$

This CFL estimate agrees well with results provided in [7]. We see that the stability constant of this splitting scheme is a little bit larger than the CFL stability constant for the the standard second-order explicit difference scheme (3.4) for which $C\tau < 0.5773502693\, h$.

Stability of the EHOC high-order discrete scheme (2.9). The non-constant sound speed is limited by the "frozen" constant $C = \max|c(x,y,z)|$. Therefore, the spectral stability method will be used to analyze the stability of the modified discrete scheme.

The discrete solutions U^n, V^n are written as

$$U^n_{ijk} = \sum_{l,m,p=1}^{M-1} u^n_{lmp} \varphi^l(x_i)\varphi^m(y_j)\varphi^p(z_k),$$

$$V^n_{\xi,ijk} = \sum_{l,m,p=1}^{M-1} v^n_{\xi,lmp} \varphi^l(x_i)\varphi^m(y_j)\varphi^p(z_k), \quad \xi = x, y, z.$$

As in the previous case, we restrict our analysis to the critical high eigenvector with $l = m = p = M-1$ and set

$$u^n_{M-1,M-1,M-1} = (q)^n, \quad v^n_{\xi,M-1,M-1,M-1} = (v_\xi)^n, \quad \xi = x, y, z.$$

Substituting these expressions into the discrete equations (2.5)–(2.6) we get the following relation for the stability factor q

$$(12-\lambda_{M-1})(v_\xi)^n = -12\frac{\lambda_{M-1}}{h^2}(q)^n, \quad \xi = x,y,z. \tag{3.9}$$

Next, using the temporal part of the EHOC scheme (2.8) and relations (3.9), we get

$$\begin{aligned} q^{n+1} - 2q^n + q^{n-1} &= C^2\tau^2\Big(1 - \frac{C^2\tau^2}{4h^2}\,\lambda_{M-1}\Big)\big(v_x^n + v_y^n + v_z^n\big) \\ &= -\frac{36\lambda_{M-1}}{12-\lambda_{M-1}}\frac{C^2\tau^2}{h^2}\Big(1 - \frac{C^2\tau^2}{4h^2}\,\lambda_{M-1}\Big)\,q^n. \end{aligned}$$

The latter equation can be written in the following standard form

$$q^2 - (2-\gamma)q + 1 = 0, \quad \gamma = \frac{36\lambda_{M-1}}{12-\lambda_{M-1}}\,r^2\Big(1 - \frac{r^2}{4}\,\lambda_{M-1}\Big),$$

where $r = C\tau/h$. It follows from the Hurwitz criterion that EHOC scheme is stable if

$$\gamma \le 4 \quad \Longrightarrow \quad C\tau \le 0.5773502693\,h.$$

Thus, the CFL stability condition is the same as for the standard second-order explicit difference scheme (3.4).

The spectral stability analysis for a compact ADI scheme with variable sound speed coefficient. In [6] a compact-higher order ADI scheme is proposed

$$\begin{aligned} &\Big(1 - \frac{c_{ijk}^2}{12}\,\frac{\nu\delta_x^2}{1+\delta_x^2/12}\Big)\Big(1 - \frac{c_{ijk}^2}{12}\,\frac{\nu\delta_y^2}{1+\delta_y^2/12}\Big)\Big(1 - \frac{c_{ijk}^2}{12}\,\frac{\nu\delta_z^2}{1+\delta_z^2/12}\Big)\big(\delta_t^2 U^n\big)_{ijk} \\ &\quad = c_{ijk}^2\Big(\frac{\nu\delta_x^2}{1+\delta_x^2/12} + \frac{\nu\delta_y^2}{1+\delta_y^2/12} + \frac{\nu\delta_z^2}{1+\delta_z^2/12}\Big)(U^n)_{ijk}, \end{aligned} \tag{3.10}$$

for the 3D acoustic wave equation with variable sound speed coefficient. Here $\nu = \tau/h$.

We will not consider a full convergence and stability analysis of this scheme, since its implementation is based on an extended space mesh stencil and the one-sided approximations are used to formulate additional boundary conditions. These details of the discrete scheme are not included in the stability analysis, presented in [6]. The authors restrict themselves to the stability analysis of the simplified (unfactorized) discrete equation

$$\frac{\delta_t^2}{1+\delta_t^2/12}\big(U^n\big)_{ijk} = c_{ijk}^2\Big(\frac{\nu\delta_x^2}{1+\delta_x^2/12} + \frac{\nu\delta_y^2}{1+\delta_y^2/12} + \frac{\nu\delta_z^2}{1+\delta_z^2/12}\Big)\big(U^n\big)_{ijk}.$$

The stability analysis is based on the standard energy method, the well-known estimate for the spectrum of a self-adjoint operator A and a mapping of a real valued measurable function [10]:

$$\sigma\big(f(A)\big) \subseteq \overline{f\big(\sigma(A)\big)},$$

where $\sigma(A)$ is the spectrum of A and $\overline{f\big(\sigma(A)\big)}$ is the closure of the set $f\big(\sigma(A)\big)$.

The following stability condition

$$\max_{ijk} |c_{ijk}|\tau < \frac{h}{\sqrt{3}}.$$

is proved in [6]. The latter equation is identical to the stability condition we have proved above for the standard explicit second-order difference scheme (3.4).

In order to test the proposed stability analysis technique, we consider the scheme (3.10) in the case of constant C. Applying the spectral form of the solution, the following quadratic equation is derived for the stability factor:

$$q^2 - (2-\gamma)q + 1 = 0, \quad \gamma = \left(\frac{3r^2\lambda_{M-1}}{1-\lambda_{M-1}/12}\right) \Big/ \left(1 + \frac{r^2\lambda_{M-1}}{1-\lambda_{M-1}/12}\right)^3,$$

where $r = C\tau/h$. After simple transformations we get that parameter γ is equal to this parameter in the stability equation of scheme (2.2). Thus ADI scheme (3.10) is stable if the CFL condition

$$C\tau < 0.607935083\, h$$

is satisfied. Clearly, this result is obtained for the constant sound speed C.

Stability of compact ADI scheme (2.9). Now we consider stability of high-order compact ADI scheme (2.9). This scheme solves the 3D acoustic wave equation with a non-constant sound speed coefficient $c(x, y, z)$.

First, we examine the stability of this scheme when the basic technique of spectral stability analysis can be applied, i.e., for the constant coefficient C. Here the stability factor q satisfies the same quadratic equation (3.8) as for the discrete scheme (2.2). Therefore the discrete scheme (2.9) is stable for the constant speed of sound C, if again $C\tau < 0.607935083\, h$. For the general case of a varying sound speed coefficient $c(x, y, z)$, the stability analysis cannot be based on Theorem 1. Therefore a different three-level in t template is proposed in [13]:

$$B_h D_h \delta_t \delta_{\bar{t}} V + \sigma h_t^2 A_h \delta_t \delta_{\bar{t}} V + A_h V = F \quad \text{in} \quad H_h \quad \text{on} \quad \omega_\tau,$$

and the following sufficient stability conditions are formulated

$$\begin{aligned} &A_h = A_h^* > 0, \quad B_h = B_h^* > 0, \quad D_h = D_h^* > 0, \\ &A_h B_h = B_h A_h, \\ &(1/4 - \sigma)\tau^2 B_h^{-1} A_h \le D_h. \end{aligned}$$

This template cannot be used for the ADI scheme (2.9). However, one can construct a modified ADI scheme for which the template easily gives the stability results. Let us consider the following factorized ADI scheme [13]

$$\bar{B}_{\sigma,h}\left(\frac{1}{c^2}\delta_t\delta_{\bar{t}}U\right) + \bar{A}_h U = 0 \quad \text{on} \quad \omega_h \times \omega_\tau,$$

The splitting operator $\bar{B}_{\sigma,h}$ is defined as the product of 1D operators defined on a three-point mesh stencil

$$\bar{A}_h := -\big(\bar{s}_{h,y}\bar{s}_{h,z}\Lambda_x + \bar{s}_{h,x}\bar{s}_{h,z}\Lambda_y + \bar{s}_{h,x}\bar{s}_{h,y}\Lambda_z\big), \quad \bar{s}_{h,\xi} := I_h + \frac{h^2}{12}\Lambda_\xi,$$

$$\bar{B}_{\sigma,h} := \bar{B}_{x,\sigma h}\bar{B}_{y,\sigma h}\bar{B}_{z,\sigma h}, \quad \bar{B}_{\xi,\sigma h} := I_h + \frac{h^2(h^2-\sigma\tau^2 c_{\max}^2)}{12}\Lambda_\xi, \quad \xi = x, y, z.$$

The stability of this scheme follows directly from general estimates for the template scheme under the conditions of CFL type. This nice stability property is obtained at some cost, as the approximation order is reduced to $O(\tau^2 + h^4)$.

4 Results of computational experiments

4.1 Experimental estimates of convergence rate and CPU time.

In this section, we provide a number of numerical experiments conducted in order to demonstrate the accuracy and efficiency of the proposed higher-order compact ADI schemes for solving 3D acoustic wave equations. All simulations are implemented using C++ language on the computer with Intel(R) Core(TM) i7-12700 processors with 16 GB RAM.

First we solve the 3D test problem (1.1) with coefficients:

$$c(x, y, z) = 1, \quad 0 \le x, y, z \le \pi, \quad T = 1.$$

Initial and boundary data are defined according to the the exact solution

$$u(x, y, z, t) = \cos\left(\sqrt{3}t\right)\cos(x)\cos(y)\cos(z).$$

Errors $e(\tau)$, experimental convergence rates $\rho(\tau)$ and CPU times for the discrete solutions of ADI scheme (2.2), EHOC scheme and ADI scheme (2.9) for a sequence of time and space steps $\tau = T/N, h = \pi/M$, $e_2(N) = e_0(N)$ are presented in Table 1. It follows from computational results that errors for two ADI schemes (2.2) and (2.9) are equal for this test problem.

Table 1. Errors $e(\tau)$, experimental convergence rates $\rho(\tau)$ and CPU times for the discrete solutions of ADI scheme (2.2), EHOC scheme and ADI scheme (2.9) for a sequence of time and space steps $\tau = T/N, h = \pi/M$, $e_2(N) = e_0(N)$.

(N, M)	$e_0(N)$	$\rho_0(N)$	$T_0(N)$	$e_1(N)$	$\rho_1(N)$	$T_1(N)$	$T_2(N)$
(40, 32)	$8.0 \cdot 10^{-8}$	—	0.044	$5.7 \cdot 10^{-8}$	—	0.042	0.04
(80, 64)	$4.9 \cdot 10^{-9}$	4.02	0.743	$3.5 \cdot 10^{-9}$	4.02	0.635	0.72
(160, 128)	$3.1 \cdot 10^{-10}$	4.00	15.34	$2.2 \cdot 10^{-10}$	3.99	10.45	13.0
(320, 256)	$1.9 \cdot 10^{-11}$	4.00	268.3	$1.4 \cdot 10^{-11}$	4.00	177.0	221

It follows from the presented results that the convergence rates of all three discrete schemes are equal to four. The CPU time for the EHOC scheme is the smallest one.

As the second example we solve 3D test problem (1.1) with coefficients:

$$c(x,y,z)=1,\quad 0\le x,y,z\le \pi,\quad T=1,$$
$$f(x,y,z,t)=4\exp(-t)\cos(x)\cos(y)\cos(z).$$

Initial and boundary data are defined according to the the exact solution

$$u(x,y,z,t)=\exp(-t)\cos(x)\cos(y)\cos(z).$$

Errors $e(\tau)$, experimental convergence rates $\rho(\tau)$ and CPU times for the discrete solutions of EHOC scheme and ADI scheme (2.9) for a sequence of time and space steps $\tau = T/N, h = \pi/M$ are presented in Table 2. It follows from

Table 2. Errors $e(\tau)$, experimental convergence rates $\rho(\tau)$ and CPU times for the discrete solutions of EHOC scheme and ADI scheme (2.9) for a sequence of time and space steps $\tau = T/N, h = \pi/M$.

(N, M)	$e_1(N)$	$\rho_1(N)$	$T_1(N)$	$e_2(N)$	$\rho_2(N)$	$T_2(N)$
(40, 32)	$3.12\cdot 10^{-8}$	—	0.169	$1.36\cdot 10^{-7}$	—	0.233
(80, 64)	$2.08\cdot 10^{-9}$	3.91	2.718	$9.02\cdot 10^{-9}$	3.92	3.808
(160, 128)	$1.33\cdot 10^{-10}$	3.96	44.58	$5.77\cdot 10^{-10}$	3.97	62.55
(320, 256)	$8.45\cdot 10^{-12}$	3.98	727.7	$3.65\cdot 10^{-11}$	3.99	1052

the presented results that in the case of variable sound speed coefficients the convergence rates of both discrete schemes again are equal to four. The CPU time for the EHOC scheme is minimal also for this test problem.

4.2 Results of parallel computational experiments

We solved the second test problem. First, in order to test the efficiency of the parallel computers used in all computational experiments we solved this problem by using the parallel version of classical explicit symmetric second order accurate discrete scheme

$$\delta_t^2 U^n = c^2\big(\delta_x^2+\delta_y^2+\delta_z^2\big)U^n + F^n,\quad (x,y,z)\in\omega_h. \tag{4.1}$$

Since a computational part of the algorithm (4.1) is reduced in comparison with high-order ADI type schemes, this parallel solver can be used as a benchmark problem to test the efficiency of the communication part of all parallel discrete schemes constructed in this paper.

Results for the symmetric second order accurate scheme (4.1) are calculated by using one computational node and a different number of cores $p=1,2,4,8$.

These results are presented in Table 3, here CPU time is denoted by T_p, speed up $S_p = T_1/T_p$ and efficiency $E_p = S_p/p$. Results are presented for problems of two different sizes: a small size problem $N = 160$, $M = 128$ and a large size problem $N = 320$, $M = 256$, where this information is denoted as $\widetilde{T}_p$, $\widetilde{S}_p$ and $\widetilde{E}_p$.

The space mesh ω_h is split into $1\times1\times2$, $1\times2\times2$ and $2\times2\times2$ sub-meshes. Each process is responsible for computations at all discrete points of its mesh part. The obtained results agree well with the well-known theoretical complexity estimates of this parallel algorithm. Still we remark on one interesting point, that in the case of the large size problem the usage of the memory is not so effective as for the small size problem. This effect is explained by the fact that we increase a number of cores but the size of the total memory remains unchanged.

Table 3. Results for the symmetric second order accurate scheme (4.1), one node with a different number of cores $p = 1, 2, 4, 8$ is used. Here notation of CPU time T_p, speed up S_p and efficiency E_p are introduced for a small size problem $N = 160$, $M = 128$ and $\widetilde{T}_p$, $\widetilde{S}_p$, $\widetilde{E}_p$ for a large size problem $N = 320$, $M = 256$.

p	T_p	S_p	E_p	$\widetilde{T}_p$	$\widetilde{S}_p$	$\widetilde{E}_p$
1	10.206	1	1	165.9	1	1
2	5.278	1.934	0.967	87.26	1.901	0.951
4	2.831	3.608	0.901	47.68	3.479	0.870
8	1.588	6.429	0.804	27.44	6.046	0.756

Results of similar experiments for the parallel version of EHOC scheme are are given in Table 4. The main new part of the parallel algorithm deals with a parallel solution of split systems with tridiagonal matrices. It is implemented as a modification of the classical factorization algorithm when two processes solve their parts of the system by moving in different directions from the left and right sides of the system. They exchange information at the middle point of 1D mesh and continue calculation in the backward direction. Thus the total amount of arithmetical operations is not increased and it is optimally distributed among different cores. It follows from the given results of experiments, that the efficiency E_p of the parallel EHOC version is better than for the explicit symmetrical discrete scheme (4.1).

The second remark confirms the conclusion that for one node with different numbers of cores the efficiency of memory usage is decreased for the large size problem.

Results of similar experiments for the parallel version of the ADI scheme (2.9) are given in Table 5. The main new part of the parallel algorithm deals with a parallel solution of split systems with tridiagonal matrix. It is implemented as it was done in EHOC parallel algorithm.

All conclusions are the same as for the parallel EHOC algorithm.

Table 4. Results for the EHOC scheme where one node with a different number of cores $p = 1, 2, 4, 8$ is used. Here notation of CPU time T_p, speed up S_p and efficiency E_p are introduced for a small size problem $N = 160$, $M = 128$ and $\widetilde{T}_p$, $\widetilde{S}_p$, $\widetilde{E}_p$ for a large size problem $N = 320$, $M = 256$.

p	T_p	S_p	E_p	$\widetilde{T}_p$	$\widetilde{S}_p$	$\widetilde{E}_p$
1	44.541	1	1	727.7	1	1
2	22.437	1.985	0.993	366.9	1.983	0.991
4	11.672	3.816	0.954	192.4	3.781	0.945
8	6.571	6.778	0.847	109.8	6.630	0.829

Table 5. Results for the ADI scheme (2.9) where one node with a different number of cores $p = 1, 2, 4, 8$ is used. Here notation of CPU time T_p, speed up S_p and efficiency E_p are introduced for a small size problem $N = 160$, $M = 128$ and $\widetilde{T}_p$, $\widetilde{S}_p$, $\widetilde{E}_p$ for a large size problem $N = 320$, $M = 256$.

p	T_p	S_p	E_p	$\widetilde{T}_p$	$\widetilde{S}_p$	$\widetilde{E}_p$
1	62.550	1	1	1052.4	1	1
2	31.729	1.971	0.986	575.03	1.830	0.915
4	17.025	3.674	0.919	287.53	3.660	0.915
8	9.736	6.425	0.803	169.36	6.214	0.776

In order to investigate a possibility to distribute the computational mesh among different nodes (and cores of these nodes), we made computational experiments with a fixed total number of cores $p = 8$ distributed on different numbers of nodes. The following CPU times are obtained, where $T_8(n)$ denotes CPU time

$$T_8(1) = 169.36, \quad T_8(2) = 150.76, \quad T_8(4) = 143.37, \quad T_8(8) = 153.01,$$

for the case of 8 cores distributed among n nodes. These results show the influence of the size of computer memory on a CPU time. This trend is even more important for larger 3D problems and their CPU time is memory depended in many applications.

5 Conclusions

In summary, we have studied two main issues on the construction and analysis of high-order ADI-type discrete schemes for solving 3D acoustic problem with variable sound speed coefficient. First, we studied the stability of popular discrete schemes. The conclusion reached is that all the schemes studied in this paper are stable under very similar CFL conditions. Note that this result was obtained for the simplified benchmark problem when the coefficient $c(x, y, z)$ was approximated by the constant coefficient C. The challenge of developing efficient stability analysis techniques based on the energy method remains unresolved.

The important point of our analysis is that for the selected ADI schemes artificial boundary conditions are defined on the same stencil of space meshes. Only for one scheme the boundary conditions for sub-steps are constructed by using larger stencils and one-sided approximations. There are no rigorous theoretical results on the stability of this particular ADI scheme with respect to such boundary conditions.

The second part of this work was devoted to comparing the accuracy of new ADI-type schemes and the efficiency of parallel versions of the solvers. The latter point is really important for solving 3D problems. It is shown that for the selected test problems the EHOC schemes are the most accurate and efficient. On the other hand, the parallel efficiency of all schemes is similar. It is planned to test the efficiency of parallel solvers when more than 2 processes are used in one dimension. For example Wang's parallel algorithm can be used to solve systems with tridiagonal matrices.

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