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A dispersion minimizing finite difference scheme and preconditioned solver for the 3D Helmholtz equation ☆

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A B S T R A C T

In this paper, a new 27-point finite difference method is presented for solving the 3D Helmholtz equation with perfectly matched layer (PML), which is a second order scheme and pointwise consistent with the equation. An error analysis is made between the numerical wavenumber and the exact wavenumber, and a refined choice strategy based on minimizing the numerical dispersion is proposed for choosing weight parameters. A full-coarsening multigrid-based preconditioned Bi-CGSTAB method is developed for solving the linear system stemming from the Helmholtz equation with PML by the finite difference scheme. The shifted-Laplacian is extended to precondition the 3D Helmholtz equation, and a spectral analysis is given. The discrete preconditioned system is solved by the Bi-CGSTAB method, with a multigrid method used to invert the preconditioner approximately. Full-coarsening multigrid is employed, and a new matrix-based prolongation operator is constructed accordingly. Numerical results are presented to demonstrate the efficiency of both the new 27-point finite difference scheme with refined parameters, and the preconditioned Bi-CGSTAB method with the 3D full-coarsening multigrid.

1. Introduction

The wave equation has numerous important applications in sciences and engineering, for instance, in geophysics, aeronautics, marine technology. Applying the Fourier transform with respect to time to the wave equation, we obtain the frequency domain wave equation, which is the well-known Helmholtz equation. The Helmholtz equation is so important that its numerical simulation has stimulated significant research. To solve the Helmholtz equation numerically, artificial boundary conditions are often employed so that we can truncate the infinite computing domain into a finite one. The perfectly matched layer (PML, cf. [8,30,40]) proposed by Bérenger is a popular artificial absorbing boundary condition, which is used to gradually damp the outgoing waves and eliminate boundary reflections. For convenience, we call the Helmholtz equation with PML the Helmholtz-PML equation, which is considered in this paper.

To discretize the Helmholtz equation, we mainly have finite difference methods (cf. [11,19,22,30,31,33,34,43]) and finite element methods (cf. [2,3,10,13,16,20]). Finite difference methods are commonly used in engineering field such as geophysics. In scientific computing, solving the Helmholtz equation numerically with high wavenumbers still remains as one of the most difficult tasks. Due to the pollution effect of high wavenumbers, the wavenumber of the numerical solution is different

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from the wavenumber of the exact solution, which is known as "numerical dispersion" (cf. [20,21]). The conventional 2D 5-point and 3D 7-point finite difference schemes lead to serious numerical dispersion, polluting the numerical accuracy. To reduce the numerical dispersion, some weighted transformed-based finite difference schemes have been constructed (cf. [19,22,24,25,28,32]), which need less grids per wavelength, while maintaining a comparable accuracy. For the 3D Helmholtz equation, the weighted transformed-based finite difference schemes are very complicated. For instance, in [25], seven rotated coordinate systems were employed to construct a 3D 27-point difference scheme.

In this paper, we shall propose an alternative finite difference scheme for the 3D Helmholtz equation, which is an extension of our previous work for the 2D case in [11]. This new scheme remains weighted, but is rotation-free. We call it a dispersion minimizing finite difference scheme, since the weight parameters are obtained by minimizing the numerical dispersion. The dispersion minimizing finite difference scheme is of second order and pointwise consistent. Its construction is much simple without rotating the coordinate system in 3D space, compared with the staggered-grid 27-point formulation, which was originally proposed for the wave equation in [24], and was further developed to the 3D Helmholtz equation in [25]. Interestingly, we shall present that our scheme is equivalent to the scheme in [25] under certain conditions. Moreover, weight parameters of our scheme are chosen by refining parameter intervals, which is called as the refined choice strategy. We shall give an error analysis between the numerical wavenumber and exact wavenumber, and numerical experiments show that the new scheme with the refined strategy outperforms the staggered-grid scheme in reducing the numerical dispersion.

For the Helmholtz equation, high-order finite difference schemes (cf. [4,31,34]) are also constructed to improve the numerical accuracy. For instance, in [34], compact finite difference schemes of sixth order are proposed for the 3D Helmholtz equation. These sixth order schemes perform pretty well for small constant wavenumbers. Theoretically, sixth order schemes are more competitive, so long as the step size is small enough. However, grids per wavelength can not be too much in practical, that is, the step size can not be too small. Also, the pollution analysis of error shows that the accuracy not only depends on the convergence order, but also the wavenumber. Then, though the sixth order scheme has a higher convergence order, it does not always means a higher accuracy. For certain step size and large wavenumbers, the new second order scheme may compete with the sixth order scheme, since it minimizes the numerical dispersion. In this paper, we shall compare the new second order scheme with the 3D sixth order compact scheme in [34], and numerical examples show that the new second order scheme performs better for certain step sizes and large wavenumber. Moreover, we specially point out that sixth order schemes are more demanding, since they require the solution and source term be continuously differentiable of sixth and fourth order, respectively. They also require the wavenumber be constant and the step sizes be equal in three directions. However, these requirements may not be met in practice. For example, in geophysical applications, we have to deal with the Helmholtz equation with varying wavenumbers in heterogeneous medium, and the step size in the third direction may differ from others. In addition, high order schemes may have difficulties in dealing with boundary conditions, and a high convergence order may not be obtained if the boundary condition is not dealt properly.

After discretization of the Helmholtz equation, the preconditioned Bi-CGSTAB method is employed to solve the large indefinite linear system, and the shifted-Laplacian (cf. [14,15,23]) is considered as the preconditioner. The shifted-Laplacian preconditioner is an extension of the Laplacian preconditioner, which was originally proposed in [5,6] for the 2D case. In this paper, for the 3D Helmholtz-PML equation, the corresponding preconditioner we employ is the 3D complex shifted-Laplacian-PML. We specially analyze the spectral distribution of the linear system from the perspective of linear fractal mapping in complex variable functions. We propose a new prolongation operator for the 3D full-coarsening multigrid, which is used to invert the preconditioner approximately. With the same number of iterations, it is expected that the full-coarsening multigrid shall consume less CPU time than the semi-coarsening case, which decreases more gradually in grid size. Numerical results are presented to illustrate that the 3D full-coarsening multigrid with the new prolongation operator gives a better performance, reducing both the number of iterations and the total CPU time needed for convergence. In the experiment, wavenumbers range from constant in homogeneous medium to greatly varying ones in heterogeneous medium. For the case of constant wavenumber, the dimensionless wavenumber (cf. [21]) we compute in our experiment is as large as 220. We specially point out that the number of iterations scales roughly linearly with the wavenumber, which seems to be a classical problem for iterative solutions of the Helmholtz equation. We have not solved this problem.

In this paper, we aims at solving the 3D Helmholtz-PML equation related with geophysical applications, and focuses on both the discretization of the operator equation and iterative method of the discrete linear system. The remainder of this paper is organized as follows. In Section 2, a new 27-point finite difference scheme is developed and analyzed. In Section 3, an error analysis is presented between the numerical wavenumber and exact wavenumber. In Section 4, a refined choice strategy is given to choose weighted parameters of the new scheme. In Section 5, we discuss the 3D complex shifted-Laplacian preconditioning, and make some spectral analysis. In Section 6, we propose a new prolongation operator for the full-coarsening multigrid. In Section 7, some numerical experiments are presented. Finally, in Section 8, some conclusions are drawn.

2. A consistent 27-point finite difference scheme for the 3D Helmholtz-PML equation

In this section, we formulate a new 27-point finite difference scheme for the 3D Helmholtz-PML equation, based on the idea of weighted average (cf. [30]). This scheme is pointwise consistent with the equation and of second order. Compared