A finite difference method with optimized dispersion correction for the Helmholtz equation

Pierre-Henri Cocquet, Martin J. Gander, Xueshuang Xiang

1 Introduction

We propose a new finite difference method (FDM) with optimized dispersion correction for the Helmholtz equation

$$L_k u := -\Delta u - k^2 u = f, \quad \text{in}\, \Omega \subset \mathbb{R}^2, \tag{1}$$

where Δ is the Laplacian, k is the wave number, and we assume boundary conditions such that the problem is well posed. The Helmholtz equation has important applications in many fields of science and engineering, e.g., acoustic and electromagnetic waves, and obtaining more accurate numerical discretizations has attracted significant research interest, see [2, 1, 8, 9, 12] and the references therein.

It is well known that all grid based numerical methods, e.g. finite element or finite difference methods, suffer from the so called *pollution effect*, which can not be eliminated [2], and the wave number of the numerical solution is different from that of the exact solution, leading to *numerical dispersion* [7, 6]. To keep the pollution effect and numerical dispersion under control, classical discretizations require a very fine mesh, which leads to very large discrete systems, especially when the frequency increases. To reduce the numerical dispersion of the standard 5-point finite difference scheme, a rotated 9-point FDM was proposed in [8] which minimizes the numerical dispersion, see also [3, 10, 13, 4] for more recent such approaches. Minimizing numerical dispersion is also important for effective coarse grid corrections in domain decomposition and for constructing efficient multigrid solvers: in 1D it is

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even possible to obtain perfect multigrid efficiency using dispersion correction [5], see also [11] for an approximation in higher dimensions.

We develop here a new dispersion minimizing FDM for the Helmholtz equation (1) using as a new idea a modified wave number. Compared with the finite difference scheme of [8] which minimizes already the numerical dispersion, our new scheme using the same stencil, but a modified wave number, has substantially less dispersion error and thus much more accurate phase speed. Our examples also indicate that for plane wave solutions, our new FDM is sixth-order accurate.

2 Dispersion correction for standard FDM

We first recall the definition of the dispersion relation and some notation. Given an operator P, e.g. the continuous operator L_k in (1) or any finite difference approximation for L_k, its symbol is

$$\sigma_P(\xi) := e^{-\mathbf{i}\xi\cdot x}(Pe^{\mathbf{i}\xi\cdot x}). \tag{2}$$

The dispersion relation of the operator P is then defined to be the set

$$\{\xi \in \mathbb{R}^2 | \sigma_P(\xi) = 0\}, \tag{3}$$

where $\xi = (\xi_1, \xi_2)$ denotes the wave vector. A direct computation using (2) gives for the continuous operator L_k in (1) the dispersion relation set $\{\xi \in \mathbb{R}^2 | \xi_1^2 + \xi_2^2 = k^2\}$.

For ξ such that $\sigma_P(\xi) = 0$, the number $\nu = \frac{k}{\|\xi\|}$ is called the (normalized) phase speed associated with a plane wave with angle θ given by $\tan\theta = \xi_2/\xi_1$. For the operator L_k in (1), the phase speed is equal to 1 for any angle. For any discretization scheme, we will consider the phase speed as a function of a dimensionless quantity, the *number of points per wavelength* $G = \frac{2\pi}{kh}$, or its inverse $1/G$.

For any discretization L_k^h of L_k, numerical dispersion can be defined as the difference between the dispersion relation of L_k and L_k^h. The numerical dispersion can also be evaluated by the difference of phase speed of L_k^h and 1 for different angles. A key idea for dispersion correction is to use a different numerical wave number $\hat{k}$ in the discretized operator $L_{\hat{k}}^h$ to minimize the numerical dispersion [5]. Take for example the 1D Helmholtz equation

$$-\frac{\partial^2 u}{\partial x^2} - k^2 u = f, \tag{4}$$

where the dispersion relation is $\{\xi \,|\, |\xi| = k\}$. The standard 3-point FDM of (4) is

$$(L_k^{h,fd3}u)_i = h^{-2}(2u_i - u_{i-1} - u_{i+1}) - k^2 u_i. \tag{5}$$

Using (2), the dispersion relation of $L_k^{h,fd3}$ is $\{\xi \in \mathbb{R} \,|\, 2h^{-2}(1-\cos(\xi h)) = k^2\}$, which is quite different from $\{\xi \,|\, |\xi| = k\}$. In order to make (5) have the same dis-

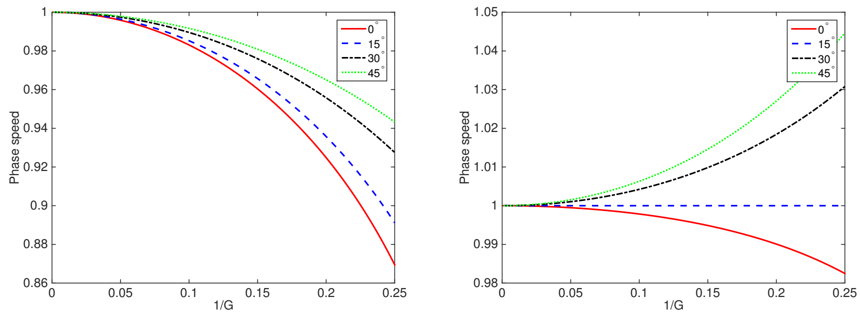

Fig. 1 Phase speed curves for 5-point FDM. Left: no dispersion correction. Right: dispersion correction for $\theta = 20°$.

persion as (4), it was proposed in [5] to use a different wave number in (5), denoted by $\hat{k}$. Choosing $\hat{k} = |\sqrt{2h^{-2}(1-\cos(kh))}|$ implies

$$\{\xi \in \mathbb{R} \,|\, 2h^{-2}(1-\cos(\xi h)) = \hat{k}^2\} = \{\xi \,|\, |\xi| = k\},$$

and hence there is no numerical dispersion!

We investigate now if a similar approach can be used for the 2D Helmholtz equation (1), whose standard 5-point FDM is given by

$$(L_k^{h,fd5}u)_{i,j} = h^{-2}(4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1}) - k^2 u_{i,j}, \tag{6}$$

Using (2), its dispersion relation of $L_k^{h,fd5}$ can readily be computed to be

$$\{\xi \in \mathbb{R}^2 | h^{-2}(4 - 2\cos(h\xi_1) - 2\cos(h\xi_2)) = k^2\}. \tag{7}$$

We show in Figure 1 (left) the phase speed v^{fd5} we computed using (7) for the angles $0°, 15°, 30°$ and $45°$ when $k = 10$. We can clearly see that the numerical dispersion increases as we decrease the number of points per wavelength G. Using the dispersion correction idea from the 1D Helmholtz equation, we can do dispersion correction as well, but only for a specific direction. Given an angle θ, for wave number k and mesh size h, we choose the numerical wave number to be

$$\hat{k}(\theta, k, h) = |\sqrt{h^{-2}(4 - 2\cos(kh\cos(\theta)) - 2\cos(kh\sin(\theta)))}|. \tag{8}$$

The 5-point FDM with dispersion correction is then given by

$$(L_{\hat{k}}^{h,fd5}u)_{i,j} = h^{-2}(4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1}) - \hat{k}^2 u_{i,j}, \tag{9}$$

and its dispersion relation is

$$\{\xi \in \mathbb{R}^2 | h^{-2}(4 - 2\cos(h\xi_1) - 2\cos(h\xi_2)) = \hat{k}^2\}. \tag{10}$$

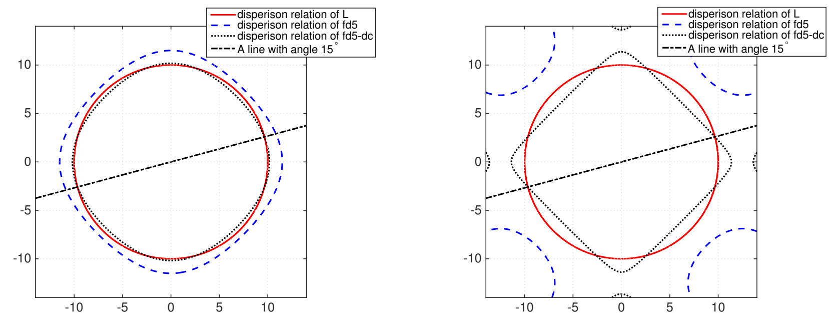

Fig. 2 Dispersion relation of operator L, fd5 and fd5-dc with dispersion correction for angle 15° and $G = 4$ (left) and $G = 2.5$ (right).

By the definition of $\hat{k}$ in (8), one can see that the dispersion correction is used to ensure that the phase speed $v^{fd5-dc} = 1$ for the specific angle θ, i.e. there is no dispersion error in that direction. However, for other angles, we still have numerical dispersion, as shown in Figure 1 (right), where we did dispersion correction for $\theta = 15°$, and then computed the phase speed v^{fd5-dc} for the angles $0°, 15°, 30°$ and $45°$ when $k = 10$. In Figure 2, we show the dispersion relation of L, $L_k^{h,fd5}$ and $L_{\hat{k}}^{h,fd5}$, where $\hat{k}$ is again the dispersion correction with $\theta = 15°$. We see that the discrete corrected dispersion relation is much closer to that of the continuous operator L_k than the uncorrected one. However, numerical dispersion still exists, it is not possible to make the phase speed $v^{fd5-dc} = 1$ for all angles using a modified wave number alone.

3 An optimized 9-point FDM with dispersion correction

To improve dispersion errors, a parametrized 9-point FDM was introduced in [8], where $-\Delta$ is discretized by a tensor product of a 1D mass matrix with stencil $[(1-a)/2, a, (1-a)/2]^T$ and the standard second order difference with stencil $[-h^{-2}, 2h^{-2}, -h^{-2}]^T$, and the the mass term $-k^2$ is discretized by the symmetric 9-point stencil

$$\begin{bmatrix} (1-b-c)/4 & c/4 & (1-b-c)/4 \\ c/4 & b & c/4 \\ (1-b-c)/4 & c/4 & (1-b-c)/4 \end{bmatrix}.$$

This leads with $\alpha = [a, b, c]$ and our numerical wave number $\hat{k}$ to the new 9-point FDM

$$\begin{aligned}(L_{\hat{k}}^{h,\alpha} u)_{i,j} = {} & (\tfrac{4a}{h^2} - \hat{k}^2 b) u_{i,j} + (\tfrac{1-2a}{h^2} - \tfrac{\hat{k}^2 c}{4})(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) \\ & -(\tfrac{1-a}{h^2} + \hat{k}^2 \tfrac{1-b-c}{4})(u_{i-1,j-1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i+1,j+1}).\end{aligned} \quad (11)$$

Computing its dispersion relation $\{\xi \in \mathbb{R}^2 | (e^{-\mathbf{i}\xi\cdot x})_{i,j}(L_{\hat{k}}^{h,\alpha} e^{\mathbf{i}\xi\cdot x})_{i,j} = 0\}$ gives

$$\begin{aligned}(4ah^{-2} - \hat{k}^2 b) + 2(\tfrac{1-2a}{h^2} - \tfrac{\hat{k}^2 c}{4})(\cos(h\xi_1) + \cos(h\xi_2))\\ -2(\tfrac{1-a}{h^2} + \hat{k}^2\tfrac{1-b-c}{4})(\cos(h(\xi_1+\xi_2)) + \cos(h(\xi_1-\xi_2))) = 0.\end{aligned} \tag{12}$$

For a vector ξ that satisfies the dispersion relation (12), we define

$$\eta_{\hat{k}}^{\alpha} := \|\xi\|, \tag{13}$$

which is a function that depends on θ. Then the phase speed of the operator $L_{\hat{k}}^{h,\alpha}$ is $v_{\hat{k}}^{\alpha} = \frac{k}{\eta_{\hat{k}}^{\alpha}}$. For the phase speed $v_{\hat{k}}^{\alpha}$ to be close to 1, we need that $\eta_{\hat{k}}^{\alpha}$ is close to k. We thus would need to solve the L^2 minimization problem[1]

$$\min_{\alpha,\hat{k}} \int_0^{2\pi} (\eta_{\hat{k}}^{\alpha}(\theta) - k)^2 d\theta. \tag{14}$$

Because we can not explicitly compute (13) from the transcendental relation (12), we propose a different minimization approach based on the reasonable

Assumption 3.1 *Given a mesh size h, there exist sets $\mathscr{K}$ and $\mathscr{P}$ such that*

- $\forall \hat{k} \in \mathscr{K}$, $\forall \alpha \in \mathscr{P}$, *the set of the dispersion relation* (12) *is not empty;*
- *Given $\alpha \in \mathscr{P}$, the mapping of $\mathscr{K}$ to $\{\eta_{\hat{k}}^{\alpha} | \hat{k} \in \mathscr{K}\}$ is injective.*

Let $\mathscr{F}^{h,\alpha} : p(\theta) \to q(\theta)$ be the operator which computes for given $p(\theta)$, $\theta \in [0, 2\pi]$ the solution $q(\theta)$ of

$$(e^{-\mathbf{i}[p(\theta)\cos(\theta),p(\theta)\sin(\theta)]^T\cdot x})_{i,j}(L_q^{h,\alpha} e^{\mathbf{i}[p(\theta)\cos(\theta),p(\theta)\sin(\theta)]^T\cdot x})_{i,j} = 0. \tag{15}$$

Since $\hat{k}^2$ appears only linearly in the 9-point FDM (11), $\mathscr{F}^{h,\alpha}$ is easy to compute numerically. In addition, by the definition of $\eta_{\hat{k}}^{\alpha}$ in (13) and Assumption 3.1, we have $\mathscr{F}^{h,\alpha}(\eta_{\hat{k}}^{\alpha}) = \hat{k}$. Thus, instead of solving (14), we solve $\min_{\alpha\in\mathscr{P},\hat{k}\in\mathscr{K}} \int_0^{2\pi}(\mathscr{F}^{h,\alpha}(\eta_{\hat{k}}^{\alpha}(\theta)) - \mathscr{F}^{h,\alpha}(k))^2 d\theta$, which, combined with $\mathscr{F}^{h,\alpha}(\eta_{\hat{k}}^{\alpha}) = \hat{k}$, yields

$$\min_{\alpha\in\mathscr{P},\hat{k}\in\mathscr{K}} \int_0^{2\pi} (\hat{k} - \mathscr{F}^{h,\alpha}(k))^2 d\theta, \tag{16}$$

where k can be interpreted as a constant function in θ. Using that $\hat{k}$ does not depend on θ, the objective function in (16) becomes by a direct calculation

$$\begin{aligned}\int_0^{2\pi} (\hat{k} - \mathscr{F}^{h,\alpha}(k))^2 d\theta = 2\pi \left(\hat{k} - \frac{1}{2\pi}\int_0^{2\pi} \mathscr{F}^{h,\alpha}(k) d\theta\right)^2 \\ + \int_0^{2\pi} \mathscr{F}^{h,\alpha}(k)^2 d\theta - \frac{1}{2\pi}\left(\int_0^{2\pi} \mathscr{F}^{h,\alpha}(k) d\theta\right)^2.\end{aligned}$$

[1] We could also use different norms leading to different optimized dispersion corrections.

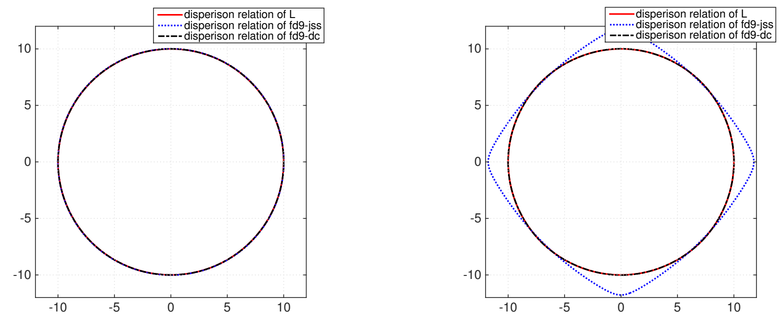

Fig. 3 Dispersion relation of L, fd9-jss and fd9-dc when $G = 4$ (left) and $G = 2.5$ (right).

For any fixed α, we can then take $\hat{k} = \frac{1}{2\pi}\int_0^{2\pi} \mathscr{F}^{h,\alpha}(k)d\theta$ to make the objective function reach its minimum, since the other terms do not depend on $\hat{k}$, and thus the minimization problem (16) is after a short calculation equivalent to minimizing the variance,

$$\min_{\alpha\in\mathscr{P}} \int_0^{2\pi} \left(\frac{1}{2\pi}\int_0^{2\pi} \mathscr{F}^{h,\alpha}(k)d\theta - \mathscr{F}^{h,\alpha}(k)\right)^2 d\theta. \tag{17}$$

This leads to the following algorithm to compute optimized α^* and $\hat{k}^*$:

Algorithm 3.1 *(Optimized parameters α^* and $\hat{k}^*$ for dispersion correction)*
1° *Input wave number k and mesh size h;*
2° *Construct operator $\mathscr{F}^{h,\alpha}$ in* (15)*;*
3° *Solve minimization problem* (17) *to obtain α^*;*
4° *Compute $\hat{k}^* = \frac{1}{2\pi}\int_0^{2\pi} \mathscr{F}^{h,\alpha^*}(k)d\theta$;*
5° *Output α^* and $\hat{k}^*$.*

4 Numerical examples

We use a Riemann sum, discretizing θ in Algorithm 3.1 from 0 to 2π with step size $\pi/100$, and solve (17) using Nelder Mead with initial guess $\alpha^0 = [1,1,0]$, which corresponds to the standard 5-point FDM. We denote our new 9-point FDM with dispersion correction by fd9-dc, and compare it to the the FDM of Jo, Shin and Suh in [8] denoted by fd9-jss. The parameters for fd9-jss do not depend on h and k and are given by $\alpha = [0.7731, 0.6248, 0.3752]$.

We first compare in Figure 3 the dispersion relation of fd9-jss and fd9-dc when $k = 10$. Algorithm 3.1 gives as optimized parameters for $G = 4$ the values $\alpha^* = [0.8027, 1.0532, 0.0002]$, $\hat{k}^* = 8.7725$, and for $G = 2.5$ the values $\alpha^* = [0.7662, 1.0553, 0.0003]$, $\hat{k}^* = 7.2186$. We see on the left that both schemes seem very good for $G = 4$, compared to the five point schemes in Figure 2, but on the

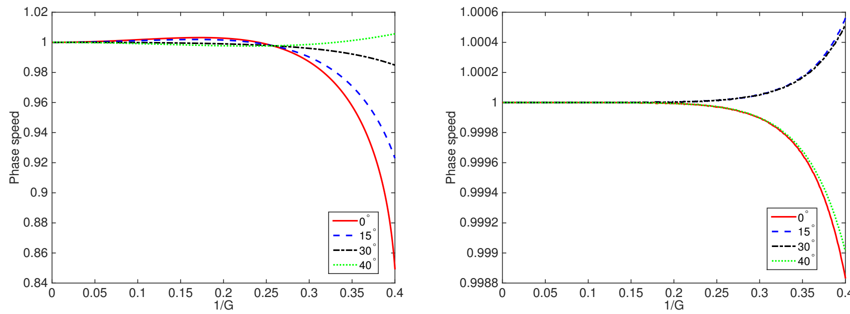

Fig. 4 Phase speed curves for fd9-jss (left) and fd9-dc (right) when $k = 10$.

h	fd5	fd9-jss	fd9-dc
0.05	1.30E5	5.41E3	5.35E3
0.1	5.57E2	1.70E3	1.36E3
0.2	1.28E16	4.37E2	3.77E2

Table 1 Condition number comparison for the linear systems obtained with the different schemes for varying mesh size when $k = 10$.

right for $G = 2.5$ the dispersion relation of fd9-dc is much better, still looking perfect for only 2.5 points per wavelength!

Figure 4 shows the phase speed curves $v_{\hat{k}^*}^{\alpha^*}$ for fd9-jss and fd9-dc for the angles $0°, 15°, 30°$ and $45°$ when $k = 10$ as a function of $1/G$. We can clearly see that the phase speed of fd9-dc is much closer to 1 than for fd9-jss (note the different scales).

We next investigate the accuracy in h. We consider the Helmholtz equation on $\Omega = (-1,1) \times (-1,1)$ with the exact plane wave solution $u_e^\theta(x) = e^{\mathbf{i}(k\cos(\theta)x_1 + k\sin(\theta)x_2)}$ and Dirichlet boundary conditions. The corresponding numerical solutions of fd9-jss and fd9-dc are $u_h^{\text{fd9-jss},\theta}$ and $u_h^{\text{fd9-dc},\theta}$, and the interpolated exact solution u_e^θ on the mesh with size h by $u_{i,h}^\theta$. We then measure the relative error of fd9-jss and fd9-dc by

$$err_{\text{fd9-jss}}(h,\theta) = \frac{\|u_h^{\text{fd9-jss},\theta} - u_{i,h}^\theta\|}{\|u_{i,h}^\theta\|},\; err_{\text{fd9-dc}}(h,\theta) = \frac{\|u_h^{\text{fd9-dc},\theta} - u_{i,h}^\theta\|}{\|u_{i,h}^\theta\|}.$$

In Figure 5, we show how the θ averaged errors

$$err_{\text{fd9-jss}}(h) = \frac{1}{2\pi}\int_0^{2\pi} err_{\text{fd9-jss}}(h,\theta)d\theta,\; err_{\text{fd9-dc}}(h) = \frac{1}{2\pi}\int_0^{2\pi} err_{\text{fd9-dc}}(h,\theta)d\theta,$$

behave when h becomes small, for $k = 5, 10$. We can clearly see that fd9-dc is 6-th order accurate, while fd9-jss is just second order accurate. We show in Table 1 the condition number of the corresponding linear systems for the different schemes for

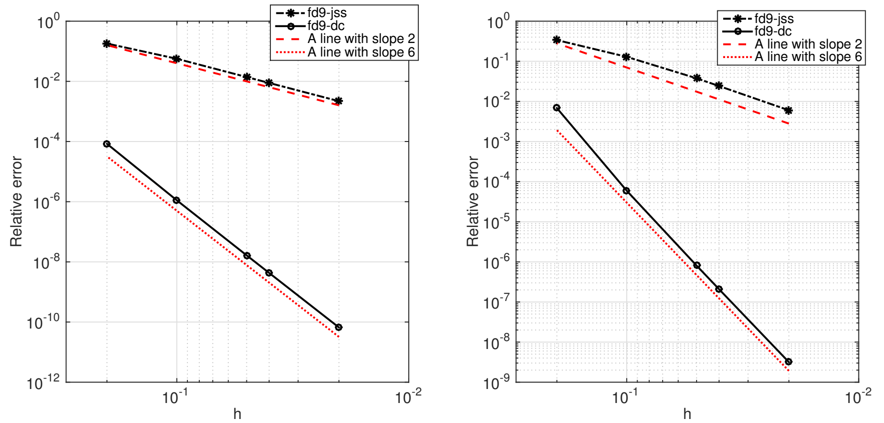

Fig. 5 Averaged relative errors of fd9-jss and fd9-dc for different mesh size h when $k=5$ (left) and $k=10$ (right).

different mesh sizes when $k=10$. We can clearly see that our new method (fd9-dc) also reduces the condition number compared to the original FDM (fd5) or the FDM proposed by Jo, Shin and Suh (fd9-jss).

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