Dispersion correction for finite difference approximations of the Helmholtz equation

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Continuous Helmholtz problem

- $\Omega \subset \mathbb{R}^d$ and $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$

$$\begin{cases} \mathcal{H}_k := -\Delta u(x) - k^2 u(x) & = f(x), \quad x \in \Omega, \\ u|_{\partial\Omega} & = g_D, \quad x \in \Gamma_D, \\ \partial_{\vec{n}} u & = g_N, \quad x \in \Gamma_N, \\ \partial_{\vec{n}} u - \mathrm{i}ku & = g_R, \quad x \in \Gamma_R. \end{cases}$$

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- k is the wavenumber.
- Model problem for frequency domain wave propagation.

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- If $\Gamma_R = \emptyset$ the Helmholtz equation is well-posed for $k \notin \mathcal{S}$.
- If $\Gamma_R \neq \emptyset$ the Helmholtz equation is well-posed for any $k > 0$.

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Main difficulties :

- $\mathcal{H}_k$ is not coercive.
- $\mathcal{H}_k$ is complex symmetric but not hermitian.
- Highly oscillatory solution e.g. $u(x) = \exp(\mathrm{i}k\, x \cdot \vec{\theta})$ for any $|\vec{\theta}| = 1$.

- Finite difference discretization of the Helmholtz equation :

$$(\mathcal{H}(k,h)u)_{i,j} = (-\Delta_h u)_{i,j} - k^2 u_{i,j},\ (v)_{i,j} = v(x_i, y_j).$$

Numerical dispersion and pollution effect

- Finite difference discretization of the Helmholtz equation :

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Numerical dispersion :

- $u_h = \exp(\mathrm{i} k_h(\theta) x \cdot \vec{\theta})$ satisfies $(\mathcal{H}(k,h)u_h)_{i,j} = 0$.
- $k_h(\theta)$ is the discrete wavenumber.
- $k_h(\theta) \neq k$.

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- $k_h(\theta) \neq k$.

Pollution effect :

- $\mathrm{e}_{\mathrm{poll}} = \|u_h - u_{\mathrm{int}}\|$ increases with k :

$$\|u - u_h\| \leq \mathrm{e}_{\mathrm{poll}} + \|u - u_{\mathrm{int}}\|.$$

- For example for $\mathbb{P}_1$-FEM :

$$\|u - u_h\|_{H^1} \leq \mathrm{e}_{\mathrm{poll}} + \|u - u_{\mathrm{int}}\|_{H^1} \lesssim k(kh)^2 + kh.$$

- Continuous Helmholtz operator :
$$\mathcal{H}_k = -\partial^2_{x^2} - k^2.$$
- Continuous plane waves :
$$u(x) = \exp(\pm \mathrm{i} k x)$$
- Discrete Helmholtz operator (3-pt stencil) :
$$(\mathcal{H}(k,h)u)_j = \frac{-u_{j-1} + 2u_j - u_{j+1}}{h^2} - k^2 u_j.$$
- Discrete plane wave solution $u_h(x) = \exp(\pm \mathrm{i} k_h(\theta) x)$
$$\cos(k_h(\theta)h) = 1 - \frac{k^2 h^2}{2}.$$

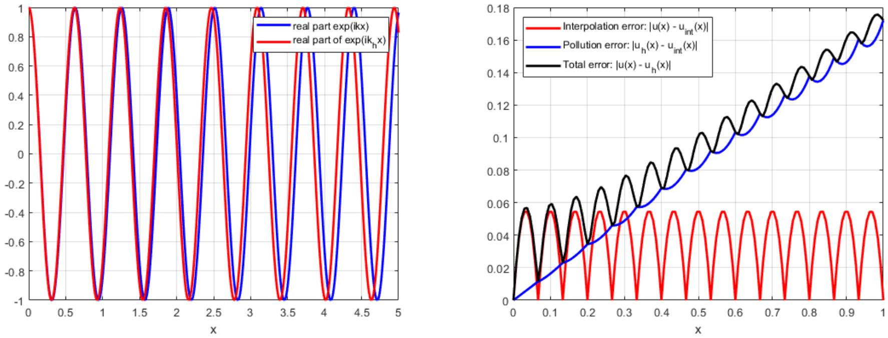

Figure – (Left) Dispersion error for $k = 10$ and $G = 2\pi/(kh) = 10$ for the 3-point stencil. (Right) Pollution effect for $k = 10$ and $G = 2\pi/(kh) = 10$.

Dispersion error $\Rightarrow$ Pollution effect.

- For $\mathbb{P}_n$-FEM, *CIP*−FEM and DG methods : No pollution if kh/n small enough and $n \geq C\log(k)$.
Babuska & Sauter, SINUM (1997) ; Melenk & Sauter, Math of comp. (2010), SINUM (2011), JSC (2013) ; Zu & Wu, SINUM (2013) ; Spence, CAMWA (2022) and ACM (2023).

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Goal of this talk : Do dispersion correction for standard schemes with explicit formula for the parameters.

General definitions

- Continuous symbol :

$$\sigma(k,\xi) = \mathrm{e}^{-\mathrm{i}\vec{x}\cdot\xi}\left((-\Delta - k^2)\mathrm{e}^{\mathrm{i}\vec{x}\cdot\xi}\right) = -k^2 + |\xi|^2.$$

- Discrete symbol :

$$\sigma(k,h,\xi) = \left(\mathrm{e}^{-\mathrm{i}\vec{x}\cdot\xi}\right)_{i,j}\left(\mathcal{H}(k,h)\mathrm{e}^{\mathrm{i}\vec{x}\cdot\xi}\right)_{i,j}.$$

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- Dispersion relations :

$$\mathcal{D} := \left\{\xi \in \mathbb{R}^N \mid \sigma(k,\xi) = 0\right\},$$

$$\mathcal{D}_h := \left\{\xi \in \mathbb{R}^N \mid \sigma(k,h,\xi) = 0\right\}.$$

- Discrete wavenumber $k_d = k_d(k,h,\vec{\theta})$:

$$\sigma(k,h,k_d\vec{\theta}) = 0,\ \vec{\theta} \in \mathcal{S}^{N-1}.$$

- Continuous symbol :

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Dispersion correction $\Leftrightarrow$ reducing $|k_d - k|$.

- 3-pt stencil :

$$(\mathcal{H}(k,h)u)_j = \frac{-u_{j-1} + 2u_j - u_{j+1}}{h^2} - k^2 u_j.$$

- Dispersion relations

$$\mathcal{D} := \{\pm k\},$$
$$\mathcal{D}_h := \left\{\xi \in \mathbb{R} \mid 2h^{-2}(1 - \cos(\xi h)) = k^2\right\}.$$

- Discrete wavenumber

$$k_d = \frac{1}{h}\arccos\left(1 - \frac{k^2 h^2}{2}\right).$$

- Gander's and Ernst's idea (2013) :

$$(\mathcal{H}(k,h)u)_j = \frac{-u_{j-1} + 2u_j - u_{j+1}}{h^2} - \widehat{k}(k,h)^2 u_j.$$

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- Discrete wavenumber

$$k_d = \frac{1}{h}\arccos\left(1 - \frac{\widehat{k}(k,h)^2 h^2}{2}\right).$$

- Choose $\widehat{k}(k,h)$ so that $k_d = k$:

$$\widehat{k}(k,h) = \sqrt{2h^{-2}(1-\cos(kh))}.$$

$\rightarrow$ No dispersion error !

Numerical example with Homogeneous Dirichlet boundary conditions

$$\begin{cases} -\partial^2_{x^2} u(x) - k^2 u(x) & = 1, \quad x \in [0,1], \\ u(0) & = 0, \\ u(1) & = 0. \end{cases}$$

$$u_{ex}(x) = -\frac{1}{k^2} + \frac{\cos(kx)}{k^2} + \frac{\sin(kx)}{k^2 \sin(k)} (1 - \cos(k))$$

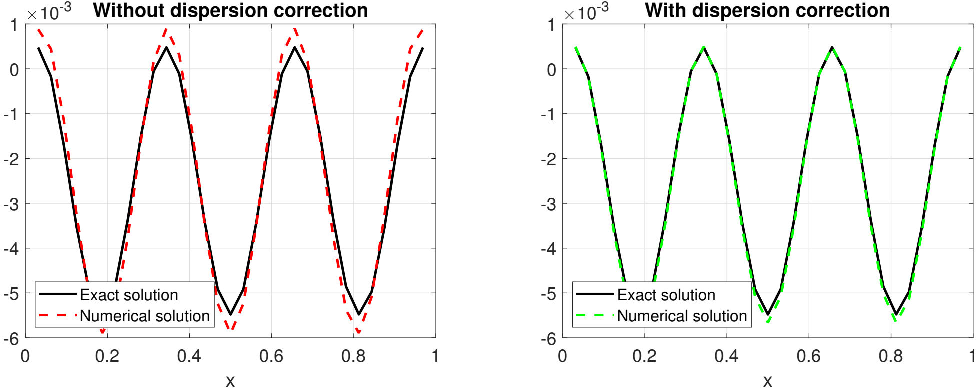
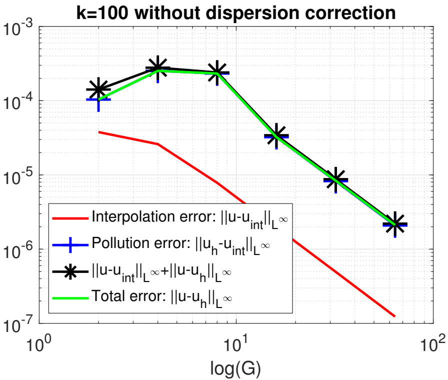


Figure – u_{ex} and u_h with $k = 20$ and $G = 10$ hence $n = 32$.



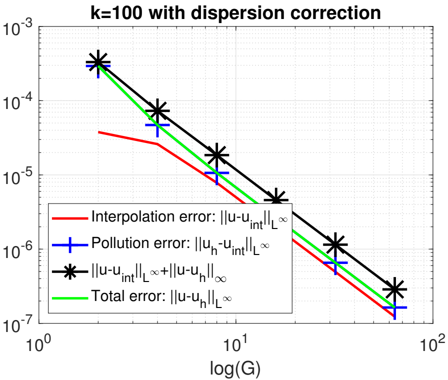


Figure – Errors without dispersion correction (Left) and with dispersion correction (Right) for $k = 100$ and $G = [2,\ 4,\ 8,\ 16,\ 32,\ 64]$.

Numerical example with Homogeneous Dirichlet boundary conditions

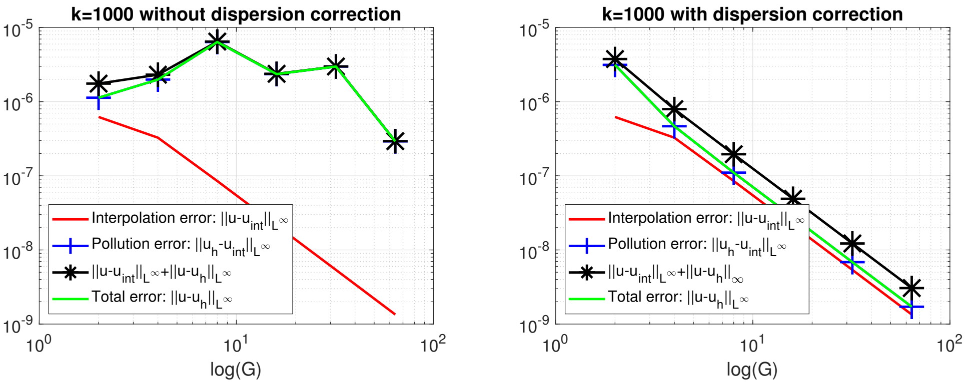


Figure – Errors without dispersion correction (Left) and with dispersion correction (Right) for $k = 1000$ and $G = [2,\ 4,\ 8,\ 16,\ 32,\ 64]$.

No dispersion $\Longrightarrow$ No pollution !

Assumptions : Let $k \notin \pi\mathbb{N}$ and f such that

$$\|f\|_{L^\infty(0,1)} \lesssim 1, \ \left\|f''\right\|_{L^\infty(0,1)} \lesssim k^2.$$

Let $\vec{e}_{\widetilde{k}} := (u_i - u(x_i))_{i=1}^n$ be the error for $\widetilde{k} \in \{k, \hat{k}\}$ and θ satisfying $\cos(\theta) = 1 - \frac{(kh)^2}{2}$.

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- $\left(\widetilde{k} = k\right)$ If $kh < 2$ and $\frac{4}{h^2}\sin\left(\frac{j\pi h}{2}\right)^2 - k^2 \neq 0$ for $j = 1, \cdots, n$ then

$$\|\vec{e}_k\|_\infty \lesssim \frac{k^2 h^3}{|\sin(\theta)||\sin(\theta/h)|}\left(1 + k\left(1 + \frac{1}{|\sin(k)|}\right)\right).$$

Assumptions : Let $k \notin \pi\mathbb{N}$ and f such that

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- $\left(\widetilde{k} = k\right)$ If $kh < 2$ and $\frac{4}{h^2} \sin\left(\frac{j\pi h}{2}\right)^2 - k^2 \neq 0$ for $j = 1, \cdots, n$ then

$$\begin{aligned} \|\vec{e}_k\|_\infty &\lesssim \frac{k^2 h^3}{|\sin(\theta)||\sin(\theta/h)|}\left(1 + k\left(1 + \frac{1}{|\sin(k)|}\right)\right). \\ &\lesssim \left((kh)^2 + k(kh)^4\right)\frac{1}{|\sin(k)|}\left(1 + \frac{1}{|\sin(k)|}\right). \end{aligned}$$

Assumptions : Let $k \notin \pi\mathbb{N}$ and f such that

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- $\left(\widetilde{k} = \widehat{k}\right)$ If $kh \notin \pi\mathbb{N}$ then $\theta = \pm kh$ and

$$\|\vec{e}_{\widehat{k}}\|_\infty \lesssim \frac{kh}{|\sin(kh)|}\frac{1}{|\sin(k)|}\left(\frac{(kh)^2}{k} + (kh)^2\left(1 + \frac{1}{|\sin(k)|}\right)\right).$$

$$\begin{cases} -\partial_{x^2}^2 u(x) - k(x)^2 u(x) &= 1, \quad x \in [-1,1], \\ u(-1) &= 0, \\ u(1) &= 0, \end{cases}$$

with

$$k(x) = \begin{cases} k_1 & \text{if } x < 0, \\ k_2 & \text{if } x > 0. \end{cases}$$

$$u_{ex}(x) = \begin{cases} A_1 \sin(k_1 x) + B_1 \cos(k_1 x) - \frac{1}{k_1^2} & \text{if } x < 0 \\ A_2 \sin(k_2 x) + B_2 \cos(k_2 x) - \frac{1}{k_2^2} & \text{if } x > 0. \end{cases}$$

- Uniform mesh with $2 \times n$ interior points including $x = 0$.
- Dispersion correction applied on each subinterval.
- Number of grid point per wavelength computed as $G = 2\pi / (\max\{k_1, k_2\} h)$.
- At $x = 0$, we set $k(0) = (k_1 + k_2)/2$.

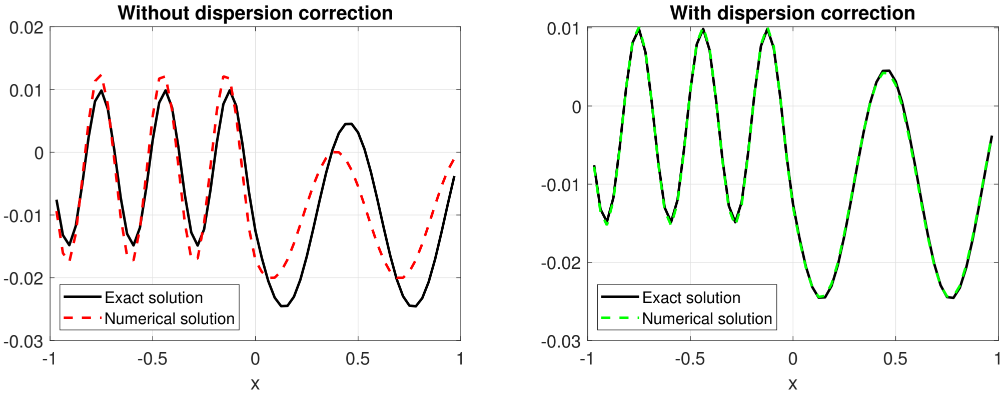

Figure – u_{ex} and u_h with $k_1 = 20$, $k_2 = 10$ and $G = 10$ hence $2 \times n = 64$.

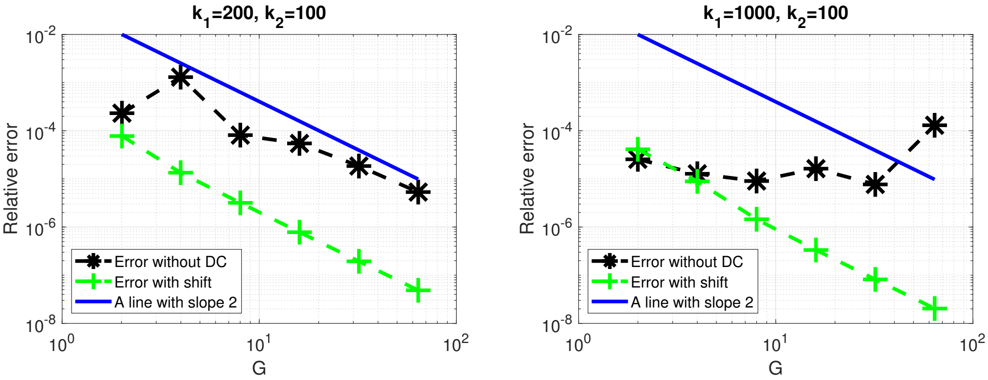

Figure – Errors with and without dispersion correction for (Right) $k_1 = 200,\ k_2 = 100$, (Left) $k_1 = 1000,\ k_2 = 100$ and $G = [2,\ 4,\ 8,\ 16,\ 32,\ 64]$.

- 5-point stencil :

$$(\mathcal{H}(k,h)u)_{i,j} = \frac{-u_{i,j-1} - u_{i,j+1} + 4u_{i,j} - u_{i-1,j} - u_{i+1,j}}{h^2} - k^2 u_{i,j}.$$

- Dispersion relation :

$$\mathcal{D} := \left\{ \xi \in \mathbb{R}^2 \mid \xi_1^2 + \xi_2^2 = k^2 \right\},$$

$$\mathcal{D}_h := \left\{ \xi \in \mathbb{R}^2 \mid (4 - 2\cos(\xi_1 h) - 2\cos(\xi_2 h)) = k^2 h^2 \right\}.$$

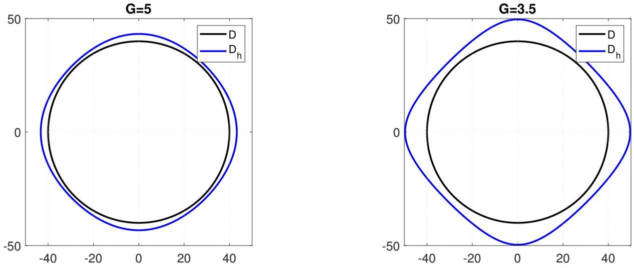

Figure – (Left) $k = 40$ and $G = 5$. (Right) $k = 40$ and $G = 3.5$.

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$$(\mathcal{H}(k,h)u)_{i,j} = \frac{-u_{i,j-1} - u_{i,j+1} + 4u_{i,j} - u_{i-1,j} - u_{i+1,j}}{h^2} - \widehat{k}(k,h)^2 u_{i,j}.$$

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Question : How to compute $\widehat{k}$ to minimize the dispersion error ?

Dispersion correction for a given angle : Directional shift

- Given $\theta_0 \in [0, 2\pi]$, compute $\widehat{k}^{\text{dir}}(k, h, \theta_0)$ so that $k(\cos(\theta_0), \sin(\theta_0)) \in \mathcal{D}_h$.

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- Given $\theta_0 \in [0, 2\pi]$, compute $\widehat{k}^{\text{dir}}(k, h, \theta_0)$ so that $k(\cos(\theta_0), \sin(\theta_0)) \in \mathcal{D}_h$.
- Any $\xi \in \mathcal{D}_h$ verifies

$$\frac{(4 - 2\cos(\xi_1 h) - 2\cos(\xi_2 h))}{h^2} = k^2,$$

Dispersion correction for a given angle : Directional shift

- Given $\theta_0 \in [0, 2\pi]$, compute $\widehat{k}^{\text{dir}}(k, h, \theta_0)$ so that $k(\cos(\theta_0), \sin(\theta_0)) \in \mathcal{D}_h$.
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$$\frac{(4 - 2\cos(\xi_1 h) - 2\cos(\xi_2 h))}{h^2} = k^2,$$

$$\widehat{k}^{\text{dir}}(k, h, \theta_0)^2 = \left(\frac{(4 - 2\cos(kh\cos(\theta_0)) - 2\cos(kh\sin(\theta_0)))}{h^2} \right).$$

Dispersion correction for a given angle : Directional shift

- Given $\theta_0 \in [0, 2\pi]$, compute $\widehat{k}^{\text{dir}}(k, h, \theta_0)$ so that $k(\cos(\theta_0), \sin(\theta_0)) \in \mathcal{D}_h$.
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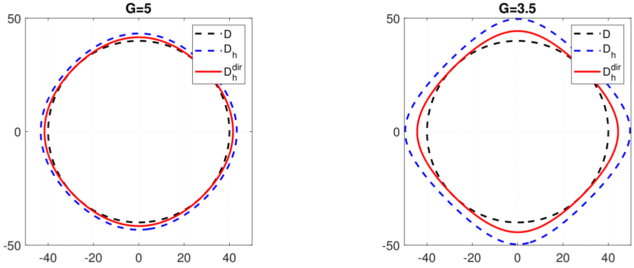

Figure – Dispersion relations using $\widehat{k}^{\text{dir}}$ for $\theta_0 = \frac{\pi}{4}$. (Left) $k = 40$ and $G = 5$. (Right) $k = 40$ and $G = 3.5$.

$$\begin{cases} -\Delta u - k^2 u &= 0, \quad \text{in } \Omega =]0,1[^2, \\ u &= f, \quad \text{on } \{0\} \times [0,1] \cup \{1\} \times [0,1], \\ \partial_n u + \mathrm{i} k u &= g, \quad \text{on } [0,1] \times \{0\} \cup [0,1] \times \{1\}, \end{cases}$$

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Relative error :

$$\mathrm{err}_\infty(\tilde{k}) = \frac{\left\| u - u_h(\tilde{k}) \right\|_\infty}{\|u\|_\infty}, \quad \tilde{k} \in \left\{ k, \ \widehat{k}^{\mathrm{dir}} \right\}$$

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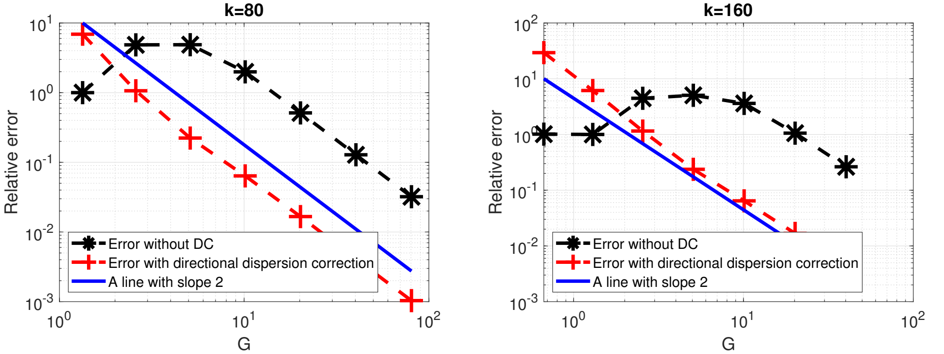

Figure – Relative error with and without shifted wavenumbers.

Solutions other than plane waves ?

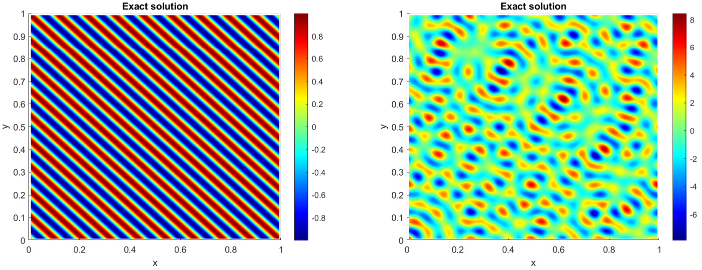

Figure – (Left) Plane wave with $\theta_0 = \pi/4$. (Right) Linear combinaison of 20 plane waves.

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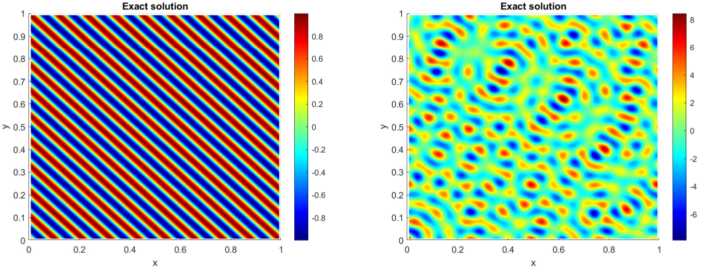

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<u>**Question :**</u> How to minimize dispersion error for several angles ?

Asymptotic optimal shift

- Discrete wavenumber $k_d(k, h, \theta)$ satisfies :

$$\frac{4 - 2(\cos(k_d h \cos(\theta)) + \cos(k_d h \sin(\theta)))}{h^2} - k^2 = 0$$

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- Setting $k_d = k_0 + k_1 h + k_2 h^2 + \cdots$ and identifying give

$$k_d(k, h, \theta) = k + \frac{k^3 h^2}{24}\left(2\cos(\theta)^4 - 2\cos(\theta)^2 + 1\right) + \cdots$$

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$$\widehat{k_d}(k, h, \theta) = k + \frac{k^3 h^2}{24} \left(2\cos(\theta)^4 - 2\cos(\theta)^2 + 1 + k_2 \frac{24}{k^3} \right) + \cdots$$

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- The asymptotic optimal shift is finally :

$$k_2^{\mathrm{asy}} = \underset{k_2}{\arg\min} \left(\max_{\theta} \left| 2\cos(\theta)^4 - 2\cos(\theta)^2 + 1 + k_2 \frac{24}{k^3} \right| \right).$$

Explicit formula for the asymptotic optimal shift

Proposition

The asymptotic optimal shift is

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- As a result

$$\max_\theta \left|2\cos(\theta)^4 - 2\cos(\theta)^2 + 1 + k_2 \frac{24}{k^3}\right| = \max\left(\left|1 + k_2 \frac{24}{k^3}\right|, \left|\frac{1}{2} + k_2 \frac{24}{k^3}\right|\right).$$

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- The solution to the min-max problem is finally reached at k_2 such that

$$1 + k_2 \frac{24}{k^3} = -\left(\frac{1}{2} + k_2 \frac{24}{k^3}\right).$$

Dispersion relation

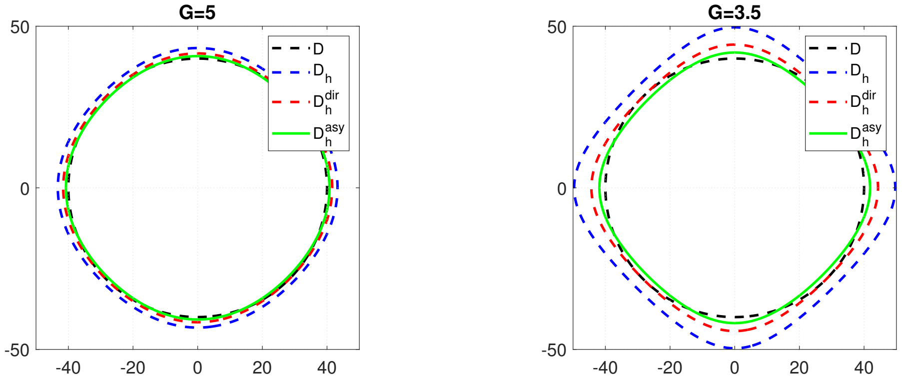
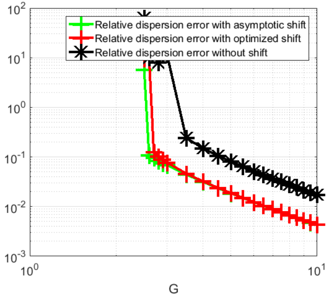


Figure – (Left) $k = 40$ and $G = 5$. (Right) $k = 40$ and $G = 3.5$.

Relative dispersion error :

$$\mathrm{Err}_{\mathrm{disp}}(\tilde{k}) = \max_{k\in\mathcal{K}} \max_{\theta} \frac{\left|k_d(\tilde{k}, h, \theta) - k\right|}{k},$$

$$\tilde{k} \in \left\{k,\ k^{\mathrm{asy}} = k + h^2 k_2^{\mathrm{asy}},\ \hat{k}^{\mathrm{opt}} = k + k_2^{\mathrm{opt}} h^2\right\}.$$



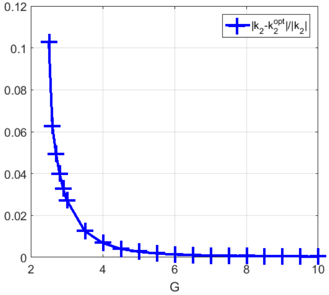


Figure – (Left) Log-log plot of $\mathrm{Err}_{\mathrm{disp}}(\tilde{k})$. (Right) $\frac{|k_2^{\mathrm{asy}} - k_2^{\mathrm{opt}}|}{|k_2^{\mathrm{asy}}|}$ as a function of G. We used $\mathcal{K} \subset [20, 600]$.

Helmholtz equation with Robin BC :

$$\begin{cases} -\Delta u - k^2 u & = 0, \quad \text{in } \Omega =]0,1[^2, \\ u & = f, \quad \text{on } \{0\} \times [0,1] \cup \{1\} \times [0,1], \\ \partial_n u + \mathrm{i} k u & = g, \quad \text{on } [0,1] \times \{0\} \cup [0,1] \times \{1\}, \end{cases}$$

with f, g so that the exact solution is $u(x,y) = \sum_{j=1}^{20} \alpha_j \mathrm{e}^{\mathrm{i}k\left\{x\cos(\theta_j)+y\sin(\theta_j)\right\}}$ with $\theta_j = \frac{2\pi j}{20}$.

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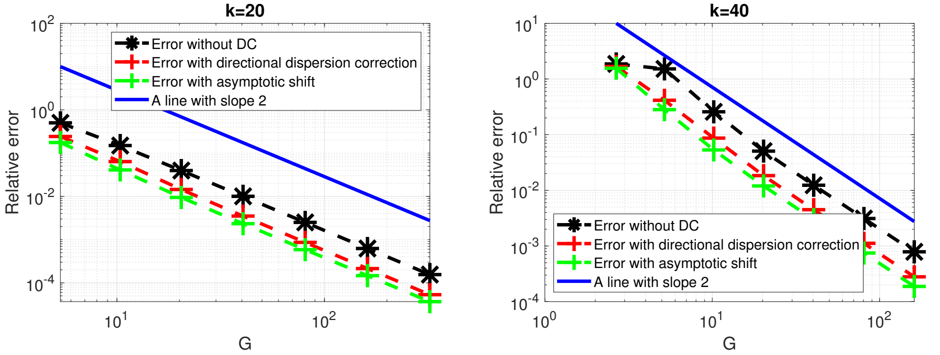

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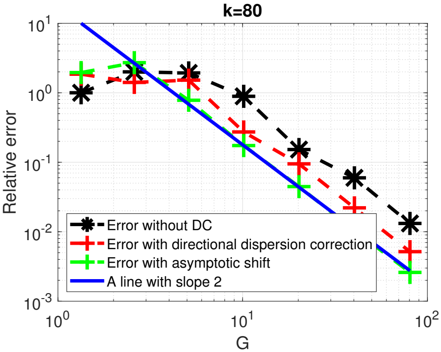

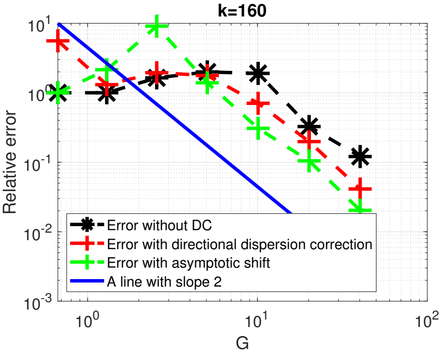

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n		2^4	2^5	2^6	2^7	2^8	2^9	2^{10}
$k = 20$	dir	2.0658	2.3522	2.7375	2.8637	2.9002	2.9111	2.9143
	asympt	2.8475	3.6653	4.1882	4.2924	4.2732	4.2440	4.2243
$k = 40$	dir	1.1114	3.6639	2.9673	2.7565	2.7488	2.7886	2.8125
	asympt	1.1960	5.3979	4.8432	4.2238	4.1404	4.1666	4.1886
$k = 80$	dir	0.5397	1.4187	1.2709	3.2589	1.6071	2.7043	2.5486
	asympt	0.5121	0.7373	2.4749	5.1185	3.4139	5.7096	5.0673
$k = 160$	dir	0.1789	0.7642	0.8434	1.1270	2.6926	1.6479	2.9300
	asympt	1.0000	0.4656	0.1801	1.4327	6.1770	3.1193	5.9436

Table – $\mathrm{err}_\infty(k)/\mathrm{err}_\infty(\widetilde{k})$ for varying meshsize $h = 1/(n+1)$ and wavenumber.

Formal definition

- Assume the discrete wavenumber can be expanded as follows

$$k_d(k, h, \theta) = k + h^p F_p(k, \theta) + \cdots$$

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Explicit formula for k_p^{asy}

Theorem

Assume there exists $\theta_{\min}, \theta_{\max}$ *such that*

$$\forall\theta : F_{\min} := F_p\left(k, \theta_{\min}\right) \leq F_p\left(k, \theta\right) \leq F_{\max} := F_p\left(k, \theta_{\max}\right).$$

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- If $F_{\min} = -F_{\max}$ then $k_p^{\mathrm{asy}} = 0$!

Application to some 6-th order 9-point stencil in 2d

$$
\begin{aligned}
(\mathcal{H}_h^{9-\mathrm{pt}} v)_{\vec{i}} := {} & \left(\frac{4a}{h^2} - k_g^2 b\right) v(x_i, y_j) + \left(\frac{1-2a}{h^2} - \frac{k_g^2 c}{4}\right) \left(v(x_{i-1}, y_j) + v(x_{i+1}, y_j) + v(x_i, y_{j-1}) + v(x_i, y_{j+1})\right) \\
& - \left(\frac{1-a}{h^2} + k_g^2 \frac{1-b-c}{4}\right) \left(v(x_{i-1}, y_{j-1}) + v(x_{i+1}, y_{j-1}) + v(x_{i-1}, y_{j+1}) + v(x_{i+1}, y_{j+1})\right),
\end{aligned}
$$

where a, b, c and k_g are

$$
a = \frac{5}{6}, \quad b = \frac{5}{6} - \frac{c}{2}, \quad c = \frac{8}{45} + c_2 G^{-2}, \; c_2 = -\frac{\pi^2}{54}, \quad k_g = k - \frac{\pi^4 k}{30} G^{-4}.
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- The discrete wavenumber is $k_d(k, h, \theta) = k + h^6 F_6(k, \theta) + \cdots$, with

$$
\begin{aligned}
F_6(k, \theta) \quad = \quad & \frac{k^7}{2 \times 6048 \pi^2} (2 \cos(\theta)^8 \pi^2 - 4 \cos(\theta)^6 \pi^2 + 6 \cos(\theta)^4 \pi^2 \\
& + 189 c_2 \cos(\theta)^4 - 4 \cos(\theta)^2 \pi^2 - 189 \cos(\theta)^2 c_2 + \pi^2).
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- Asymptotic optimal shift :

$$k_6^{\mathrm{asy}} = -\frac{k^7}{12288}.$$

Helmholtz equation with Dirichlet BC :

$$\begin{cases} -\Delta u - k^2 u &= 0, \quad \text{in } \Omega =]-1,1[^2, \\ u &= f, \quad \text{on } \partial\Omega, \end{cases}$$

with f so that $u(x,y) = \sum_{j=1}^{20} \alpha_j \mathrm{e}^{\mathrm{i}k\left\{x\cos(\theta_j) + y\sin(\theta_j)\right\}}$ with $\theta_j = \frac{2\pi j}{20}$ is the exact solution.

Relative error :

$$\mathrm{err}_\infty(\tilde{k}) = \frac{\left\| u - u_h(\tilde{k}) \right\|_\infty}{\|u\|_\infty}, \ \tilde{k} \in \left\{ k, k^{\mathrm{asy}} = k + k_6^{\mathrm{asy}} h^6 \right\}$$

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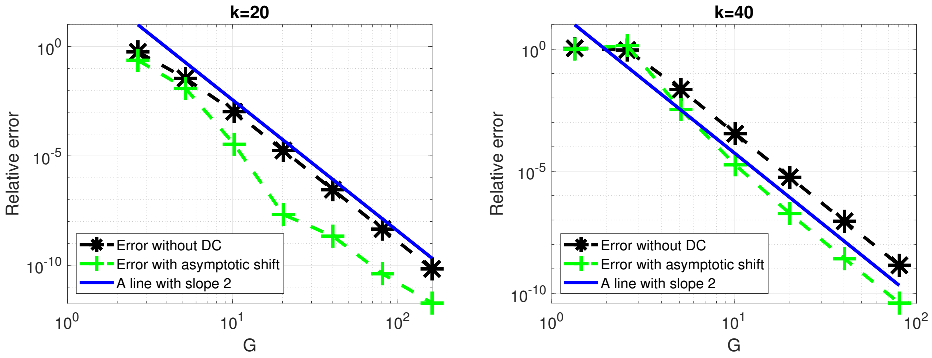

Figure – Relative error with and without shifted wavenumbers.

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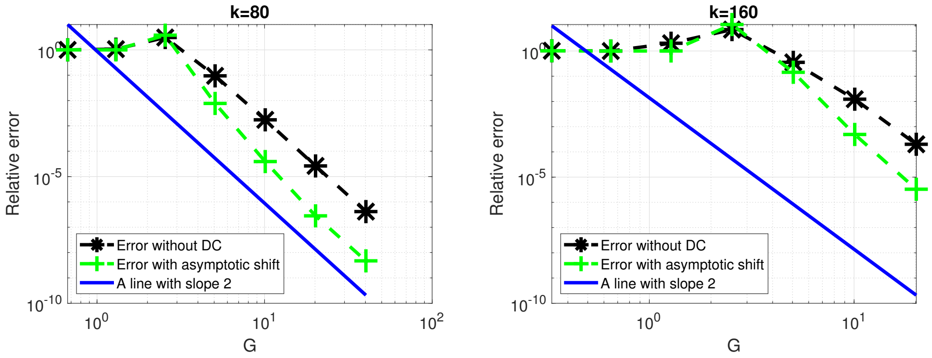

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n	2^4	2^5	2^6	2^7	2^8	2^9	2^{10}
$k=20$	2.4290	2.8762	31.0845	853.9139	132.8095	110.0423	36.5872
$k=40$	1.0733	0.6580	6.6486	18.8421	30.5103	34.3205	35.3280
$k=80$	1.0000	1.0700	0.8103	12.2690	44.4003	93.3499	87.8864
$k=160$	1.0000	1.0000	2.0232	0.6303	2.4774	25.0177	60.5840

Table – Ratio of the errors $\mathrm{err}_\infty(k)/\mathrm{err}_\infty(\widehat{k})$ for varying meshsize and wavenumber.

Conclusions :

- Dispersion correction for 1d Helmholtz equation $\Longrightarrow$ No pollution effect !
- Dispersion correction for 2d Helmholtz equation $\Longrightarrow$ Reduction of the relative error for large enough G.
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- Improvement of multigrid method, ...

Thank you for your attention