A Fast Fourier transform based direct solver for the Helmholtz problem

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Content

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Model problem

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a d-dimensional rectangular domain. The pressure field satisfies the **Helmholtz** partial differential equation

$$-\triangle u - \omega^2 u = f \qquad \text{in } \Omega, \tag{1}$$

$$\mathcal{B}u = 0 \qquad \text{on } \Gamma, \tag{2}$$

where ω denotes the wave number. The boundary $\Gamma = \partial\Omega = \Gamma_N \cup \Gamma_B$ is decomposed into Neumann boundary condition (BC) Γ_N and (first-order) absorbing BC (ABC) Γ_B:

$$\mathcal{B}u = \nabla u \cdot \boldsymbol{n} = 0 \qquad \text{on } \Gamma_N, \tag{3}$$

$$\mathcal{B}u = \nabla u \cdot \boldsymbol{n} - i\omega u = 0 \qquad \text{on } \Gamma_B, \tag{4}$$

where $\boldsymbol{n}$ denotes the outward normal to the boundary. Equation (2) is an approximation for the Sommerfeld radiation condition.

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Discretization

Weak formulation for the Helmholtz problem (1)–(2): Find $u \in V = H^1(\Omega)$ such that

$$a(u,v) = \int_\Omega fv \, d\boldsymbol{x} \qquad \forall v \in V, \tag{5}$$

where

$$a(u,v) = \int_\Omega \left(\nabla u \cdot \nabla v - \omega^2 uv\right) d\boldsymbol{x} - i\omega \int_{\partial\Omega} uv \, ds. \tag{6}$$

Discretizing (5) by bilinear or trilinear finite elements on an orthogonal mesh leads to a system of linear equations given by

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}, \tag{7}$$

where the matrix $\boldsymbol{A}$ has a separable tensor product form. The mesh will be equidistant in each direction x_j.

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Discretization

For the two-dimensional (2d) case, the matrix $\boldsymbol{A}$ is given by

$$\boldsymbol{A} = (\boldsymbol{K}_1 - \omega^2 \boldsymbol{M}_1) \otimes \boldsymbol{M}_2 + \boldsymbol{M}_1 \otimes \boldsymbol{K}_2,$$

whereas in three dimensions (3d) it is given by

$$\boldsymbol{A} = (\boldsymbol{K}_1 - \omega^2 \boldsymbol{M}_1) \otimes \boldsymbol{M}_2 \otimes \boldsymbol{M}_3 + \boldsymbol{M}_1 \otimes (\boldsymbol{K}_2 \otimes \boldsymbol{M}_3 + \boldsymbol{M}_2 \otimes \boldsymbol{K}_3),$$

where $\boldsymbol{K}_j$ and $\boldsymbol{M}_j$ are one-dimensional stiffness and mass matrices, respectively, in the x_j-direction with possible modifications on or near the boundaries due to the ABC.

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Discretization

$\boldsymbol{K}_j$ and $\boldsymbol{M}_j$ are computed by 1d numerical quadrature on $[0,1]$:

$$\boldsymbol{K}_j = \frac{1}{h_j}\begin{pmatrix} k_{1,1} & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & k_{n_j,n_j} \end{pmatrix}, \qquad \boldsymbol{M}_j = \frac{h_j}{6}\begin{pmatrix} 2 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 2 \end{pmatrix}$$

where the first and last entries are including the corresponding BCs. ABCs (4) yield the entries $k_{1,1} = k_{n_j,n_j} = 1 - i\omega h_j$, whereas Neumann BCs lead to $k_{1,1} = k_{n_j,n_j} = 1$.

$\boldsymbol{M}_j$ is the same for both Neumann and (first-order) ABCs.

Let the ABCs be given in direction of x_1 for both (opposite) sides.

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Fast solver - idea

The main idea for solving the problem $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}$ is to consider an auxiliary problem $\boldsymbol{B}\boldsymbol{v} = \boldsymbol{f}$, where the system matrix $\boldsymbol{B}$ is derived by changing the ABCs to periodic ones.
The key is that we can solve the modified (periodic) problem $\boldsymbol{B}\boldsymbol{v} = \boldsymbol{f}$ now by using the FFT method, which is not possible for the original problem $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}$.

The problem $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}$ can be solved applying the following steps:

1. Solve $\boldsymbol{B}\boldsymbol{v} = \boldsymbol{f}$.
2. Solve $\boldsymbol{A}\boldsymbol{w} = \boldsymbol{f} - \boldsymbol{A}\boldsymbol{v} = \boldsymbol{B}\boldsymbol{v} - \boldsymbol{A}\boldsymbol{v} = (\boldsymbol{B} - \boldsymbol{A})\boldsymbol{v}$, $\boldsymbol{u} = \boldsymbol{v} + \boldsymbol{w}$.
3. Solve $\boldsymbol{B}\boldsymbol{u} = \boldsymbol{f} + (\boldsymbol{B} - \boldsymbol{A})(\boldsymbol{v} + \boldsymbol{w})$.

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Fast solver - the auxiliary problem

In case of periodic BCs in x_1-direction, the matrices $\boldsymbol{K}_1$ and $\boldsymbol{M}_1$ change to $\boldsymbol{K}_1^B$ and $\boldsymbol{M}_1^B$ and are given by

$$\boldsymbol{K}_1^B = \frac{1}{h_1}\begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}, \quad \boldsymbol{M}_1^B = \frac{h_1}{6}\begin{pmatrix} 4 & 1 & & & 1 \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ 1 & & & 1 & 4 \end{pmatrix},$$

which means that the BCs on the two opposite x_1-boundaries have been changed to be of periodic type. The matrix $\boldsymbol{B}$ is given by

$$\boldsymbol{B} = (\boldsymbol{K}_1^B - \omega^2 \boldsymbol{M}_1^B) \otimes \boldsymbol{M}_2 + \boldsymbol{M}_1^B \otimes \boldsymbol{K}_2 \quad \text{(2d)},$$

$$\boldsymbol{B} = (\boldsymbol{K}_1^B - \omega^2 \boldsymbol{M}_1^B) \otimes \boldsymbol{M}_2 \otimes \boldsymbol{M}_3 + \boldsymbol{M}_1^B \otimes (\boldsymbol{K}_2 \otimes \boldsymbol{M}_3 + \boldsymbol{M}_2 \otimes \boldsymbol{K}_3) \text{ (3d)}.$$

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Fast solver

After a suitable permutation $\boldsymbol{A}$ and $\boldsymbol{B}$ have the block forms

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_{bb} & \boldsymbol{A}_{br} \\ \boldsymbol{A}_{rb} & \boldsymbol{A}_{rr} \end{pmatrix} \quad \text{and} \quad \boldsymbol{B} = \begin{pmatrix} \boldsymbol{B}_{bb} & \boldsymbol{A}_{br} \\ \boldsymbol{A}_{rb} & \boldsymbol{A}_{rr} \end{pmatrix}, \tag{8}$$

the subscripts b and r correspond to the nodes on the Γ_B boundary and to the rest of the nodes, respectively. Note that the matrix $\boldsymbol{B} - \boldsymbol{A}$ has the structure

$$\boldsymbol{B} - \boldsymbol{A} = \begin{pmatrix} \boldsymbol{B}_{bb} - \boldsymbol{A}_{bb} & 0 \\ 0 & 0 \end{pmatrix}. \tag{9}$$

Fast solver - some ideas behind applying partial solution method

The eigenvectors given by the generalized eigenvalue problems

$$\boldsymbol{K}_1 \boldsymbol{V} = \boldsymbol{M}_1 \boldsymbol{V} \boldsymbol{\Lambda}_A \qquad \text{and} \qquad \boldsymbol{K}_1^B \boldsymbol{W} = \boldsymbol{M}_1^B \boldsymbol{W} \boldsymbol{\Lambda}_B \tag{10}$$

diagonalize $\boldsymbol{K}_1$, $\boldsymbol{K}_1^B$ and $\boldsymbol{M}_1$, $\boldsymbol{M}_1^B$.
The matrices $\boldsymbol{\Lambda}_A$ and $\boldsymbol{\Lambda}_B$ contain the eigenvalues as diagonal entries and the matrices $\boldsymbol{V}$ and $\boldsymbol{W}$ contain the corresponding eigenvectors as their columns. The eigenvectors have to form a basis in $\mathbb{C}^{n_1}$ in order to apply the partial solution method:

$$\boldsymbol{V}^T \boldsymbol{M}_1 \boldsymbol{V} = \boldsymbol{I}_1 \qquad \text{and} \qquad \boldsymbol{V}^T \boldsymbol{K}_1 \boldsymbol{V} = \boldsymbol{\Lambda}_A, \tag{11}$$

$$\boldsymbol{W}^T \boldsymbol{M}_1^B \boldsymbol{W} = \boldsymbol{I}_1 \qquad \text{and} \qquad \boldsymbol{W}^T \boldsymbol{K}_1^B \boldsymbol{W} = \boldsymbol{\Lambda}_B. \tag{12}$$

$\boldsymbol{I}_1$ denotes the identity matrix of length n_1, whereas $\boldsymbol{I}_j$ and $\boldsymbol{I}_{jk}$ denote the identity matrices of lengths n_j and $n_j \times n_k$.
The eigenvalue problems (10) have to be solved only once during the solution process – in the initialization.

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Fast solver

These conditions also lead to a convenient representation for the inverses of the system matrices $\boldsymbol{A}$ and $\boldsymbol{B}$.
We obtain for the system matrix $\boldsymbol{B}$ the following representation:

$$\boldsymbol{B}^{-1} = (\boldsymbol{W} \otimes \boldsymbol{I}_2)\, \boldsymbol{H}_B^{-1} (\boldsymbol{W}^T \otimes \boldsymbol{I}_2),$$
$$\boldsymbol{H}_B = (\boldsymbol{\Lambda}_B - \omega^2 \boldsymbol{I}_1) \otimes \boldsymbol{M}_2 + \boldsymbol{I}_1 \otimes \boldsymbol{K}_2$$

for 2d as well as

$$\boldsymbol{B}^{-1} = (\boldsymbol{W} \otimes \boldsymbol{I}_{23})\, \boldsymbol{H}_B^{-1} (\boldsymbol{W}^T \otimes \boldsymbol{I}_{23}),$$
$$\boldsymbol{H}_B = ((\boldsymbol{\Lambda}_B - \omega^2 \boldsymbol{I}_1) \otimes \boldsymbol{M}_2 + \boldsymbol{I}_1 \otimes \boldsymbol{K}_2) \otimes \boldsymbol{M}_3 + \boldsymbol{I}_1 \otimes \boldsymbol{M}_2 \otimes \boldsymbol{K}_3$$

for 3d.
The representation for $\boldsymbol{A}$ goes completely analogously.

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Fast solver - efficient computation for the inverses of $\boldsymbol{H}_B$ and $\boldsymbol{H}_A$

2d: Compute the LU decomposition of $\boldsymbol{LU} = \boldsymbol{H}_B$. Instead of directly computing the inverse of $\boldsymbol{H}_B$, solve the linear system

$$\boldsymbol{H}_B\boldsymbol{y} = \boldsymbol{LUy} = \boldsymbol{r}$$

by solving the problems

$$\boldsymbol{Lz} = \boldsymbol{r} \qquad \text{and} \qquad \boldsymbol{Uy} = \boldsymbol{z} \tag{13}$$

iteratively (with $\boldsymbol{r}$ being some right-hand side).
3d: Instead of solving the problems (13) with the block diagonal matrices $\boldsymbol{L}$ and $\boldsymbol{U}$, split them into n_1 subproblems of size $n_2 \times n_3$ corresponding to the respective diagonal blocks.
Then solve the independent n_1 subproblems in the same iterative scheme (13) leading to a faster implementation for the 3d problem.

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Fast solver - Step 1

Compute the Fourier transformation $\hat{\boldsymbol{f}}$ of $\boldsymbol{f}$ using FFT and save it, since it will be needed in Step 3 as well. Solve the auxiliary problem

$$\boldsymbol{B}\boldsymbol{v} = \boldsymbol{B}\begin{pmatrix}\boldsymbol{v}_b \\ \boldsymbol{v}_r\end{pmatrix} = \boldsymbol{f}, \qquad (14)$$

but compute only $\boldsymbol{v}_b$ and not $\boldsymbol{v}_r$. Performing the inverse Fourier transformation would provide both $\boldsymbol{v}_b$ and $\boldsymbol{v}_r$. Instead of that, it is efficient to solve problem $\boldsymbol{H}_B\boldsymbol{y} = \boldsymbol{L}\boldsymbol{U}\boldsymbol{y} = \hat{\boldsymbol{f}}$ and then multiply the resulting vector by the eigenvectors of $\boldsymbol{W}$ which correspond to the boundary Γ_B.

Recall, e.g., in 2d, $\boldsymbol{B}^{-1} = (\boldsymbol{W} \otimes \boldsymbol{I}_2)\,\boldsymbol{H}_B^{-1}(\boldsymbol{W}^T \otimes \boldsymbol{I}_2)$.

Fast solver - Step 2

Introduce an additional vector $\boldsymbol{w}$ given by $\boldsymbol{w} = \boldsymbol{u} - \boldsymbol{v}$, and solve the problem

$$\boldsymbol{A}\boldsymbol{w} = \boldsymbol{A}\begin{pmatrix} \boldsymbol{w}_b \\ \boldsymbol{w}_r \end{pmatrix} = (\boldsymbol{B} - \boldsymbol{A})\boldsymbol{v} = \begin{pmatrix} (\boldsymbol{B}_{bb} - \boldsymbol{A}_{bb})\boldsymbol{v}_b \\ 0 \end{pmatrix}, \tag{15}$$

since

$$\boldsymbol{A}\boldsymbol{w} = \boldsymbol{A}\boldsymbol{u} - \boldsymbol{A}\boldsymbol{v} = \boldsymbol{f} - \boldsymbol{A}\boldsymbol{v} = \boldsymbol{B}\boldsymbol{v} - \boldsymbol{A}\boldsymbol{v}, \tag{16}$$

but compute only $\boldsymbol{w}_b$ and not $\boldsymbol{w}_r$. Problem (15) can be solved efficiently using the diagonalization with multiplications by the eigenvector matrices $\boldsymbol{V}^T$ and $\boldsymbol{V}$ of $\boldsymbol{A}$ corresponding to the boundary Γ_B.

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Fast solver - Step 3

Solve now the problem

$$\begin{aligned} \boldsymbol{B}\boldsymbol{u} &= \boldsymbol{f} + (\boldsymbol{B} - \boldsymbol{A})(\boldsymbol{v} + \boldsymbol{w}) \\ &= \boldsymbol{f} + \begin{pmatrix} (\boldsymbol{B}_{bb} - \boldsymbol{A}_{bb})(\boldsymbol{v}_b + \boldsymbol{w}_b) \\ 0 \end{pmatrix} \end{aligned} \tag{17}$$

due to $\boldsymbol{B}\boldsymbol{u} = \boldsymbol{A}\boldsymbol{u} + \boldsymbol{B}\boldsymbol{u} - \boldsymbol{A}\boldsymbol{u}$. Use the Fourier transformation $\hat{\boldsymbol{f}}$ of $\boldsymbol{f}$ from Step 1. The Fourier transformation of the second term

$$\boldsymbol{g} = (\boldsymbol{B} - \boldsymbol{A})(\boldsymbol{v} + \boldsymbol{w}) = \begin{pmatrix} (\boldsymbol{B}_{bb} - \boldsymbol{A}_{bb})(\boldsymbol{v}_b + \boldsymbol{w}_b) \\ 0 \end{pmatrix} \tag{18}$$

can be performed efficiently by multiplying it by $\boldsymbol{W}^T$ as the term (18) is sparse again.

Finally, solve $\boldsymbol{H}_B\boldsymbol{y} = \boldsymbol{L}\boldsymbol{U}\boldsymbol{y} = \hat{\boldsymbol{f}} + \hat{\boldsymbol{g}}$ and then perform the inverse FFT on the resulting vector leading to the solution $\boldsymbol{u}$ of the original problem $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}$.

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Numerical results

The numerical experiments have been computed in Matlab.

$\Omega = [0, 1]^d$, $\omega = 2\pi$, uniform meshes wrt each x_j, step size $h = 1/n$

Right-hand side is chosen as 0.01 for the first n entries and 1 for all the other entries

We compare the CPU times in seconds for computing the solution by applying Matlab's backslash, the fast solver presented as well as second version of it, where in step 1 and 3 we use the FFT instead of the multiplications by $\boldsymbol{W}$. We present the times for the computations in the initialization process as well.

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Numerical results (2d)

CPU times in seconds:

n_j	65	129	257	513	1025
Initialization	0.11	0.26	0.82	3.93	22.92
Matlab's backslash	0.04	0.16	0.52	3.17	13.11
Fast Solver	0.02	0.05	0.13	0.47	2.09
Fast Solver version 2	0.01	0.03	0.07	0.37	1.74

Numerical results (3d)

CPU times in seconds:

n_j	9	17	33	65	129	257
Initialization	0.09	0.13	0.32	1.95	15.32	152.28
Matlab's backslash	0.06	0.31	7.33	671.77	–	–
Fast Solver	0.06	0.13	0.53	4.64	63.94	631.39
Fast Solver version 2	0.08	0.12	0.51	4.45	61.41	647.46

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Conclusions and outlook

Efficient numerical method employing FFT combined with a fast direct solver for the Helmholtz problem with ABCs. Solving the Helmholtz equation is in general difficult or impossible to solve efficiently with most numerical methods.

E. Heikkola, T. Rossi, and J. Toivanen, *Fast direct solution of the Helmholtz equation with a perfectly matched layer or an absorbing boundary condition* , International journal for numerical methods in engineering, 57(14), 2007–2025, 2003.

J. Toivanen and M. Wolfmayr, *A Fast Fourier Transform based direct solver for the Helmholtz problem*, in preparation, 2017.

Outlook:

- More complicated domains and data
- Combine this solver with domain decomposition methods for layered media
- Parallel implementation

Ευχαριστώ !

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