# A fast Fourier transform based direct solver for the Helmholtz problem

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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

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

$$\mathcal{B}u = 0$$
 on  $\Gamma$ , (2)

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

$$\mathcal{B}u = \nabla u \cdot \boldsymbol{n} = 0 \quad \text{on } \Gamma_N, \tag{3}$$
$$\mathcal{B}u = \nabla u \cdot \boldsymbol{n} - i\omega u = 0 \quad \text{on } \Gamma_B, \tag{4}$$

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

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

(7)

where

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

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

$$Au = f$$
,

where the matrix **A** has a separable tensor product form. The mesh will be equidistant in each direction  $x_i$ .

#### Discretization

For the two-dimensional (2d) case, the matrix A is given by

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

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

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

where  $K_j$  and  $M_j$  are one-dimensional (1d) stiffness and mass matrices, respectively, in the  $x_j$ -direction with possible modifications on or near the boundaries due to the ABC.



### Discretization

 $K_j$  and  $M_j$  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  $k_{1,1} = k_{n_j,n_j} = 1$ .

 $M_j$  is the same for both Neumann and (first-order) ABCs. Let the ABCs be given in direction of  $x_1$  for both (opposite) sides.

# **Fast solver**



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

The problem Au = f can be solved applying the following steps: 1. Solve Bv = f.

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



### Fast solver - the auxiliary problem

In case of periodic BCs in  $x_1$ -direction, the matrices  $K_1$  and  $M_1$  change to  $K_1^B$  and  $M_1^B$  and are given by

$$\boldsymbol{K}_{1}^{B} = \frac{1}{h_{1}} \begin{pmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ -1 & & & & -1 & 2 \end{pmatrix}, \qquad \boldsymbol{M}_{1}^{B} = \frac{h_{1}}{6} \begin{pmatrix} 4 & 1 & & & 1 \\ 1 & 4 & 1 & & & 1 \\ & \ddots & \ddots & & \\ & & & 1 & 4 & 1 \\ 1 & & & 1 & 4 \end{pmatrix},$$

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



### Fast solver

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

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

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

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

and only the matrix

$$\boldsymbol{C}_{bb} = \boldsymbol{B}_{bb} - \boldsymbol{A}_{bb} \tag{10}$$

has to be saved for the application of the fast solver.

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# Fast solver - some ideas behind applying the partial solution method

The eigenvectors given by the generalized eigenvalue problems

$$\boldsymbol{K}_1 \boldsymbol{V}_1 = \boldsymbol{M}_1 \boldsymbol{V}_1 \boldsymbol{\Lambda}_1^A$$
 and  $\boldsymbol{K}_1^B \boldsymbol{W}_1 = \boldsymbol{M}_1^B \boldsymbol{W}_1 \boldsymbol{\Lambda}_1^B$  (11)

diagonalize  $K_1$ ,  $K_1^B$  and  $M_1$ ,  $M_1^B$ .

The matrices  $\Lambda_1^A$  and  $\Lambda_1^B$  contain the eigenvalues as diagonal entries and the matrices  $V_1$  and  $W_1$  contain the corresponding eigenvectors as their columns. The eigenvectors have to be normalized in order to apply the partial solution method:

$$\boldsymbol{V}_{1}^{T}\boldsymbol{M}_{1}\boldsymbol{V}_{1} = \boldsymbol{I}_{1} \quad \text{and} \quad \boldsymbol{V}_{1}^{T}\boldsymbol{K}_{1}\boldsymbol{V}_{1} = \boldsymbol{\Lambda}_{1}^{A}, \quad (12)$$
$$\boldsymbol{W}_{1}^{T}\boldsymbol{M}_{1}^{B}\boldsymbol{W}_{1} = \boldsymbol{I}_{1} \quad \text{and} \quad \boldsymbol{W}_{1}^{T}\boldsymbol{K}_{1}^{B}\boldsymbol{W}_{1} = \boldsymbol{\Lambda}_{1}^{B}. \quad (13)$$

 $I_1$  denotes the identity matrix of length  $n_1$ , whereas  $I_j$  and  $I_{jk}$  denote the identity matrices of lengths  $n_j$  and  $n_j \times n_k$ . The eigenvalue problems (11) have to be solved only once during the solution process – in the initialization.

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# The 2d case



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## Fast solver (2d) - Reformulation of A and B

These conditions also lead to a convenient representation for the inverses of the system matrices A and B. Using (13) as follows

$$B = (W_1^{-T} \Lambda_1^B W_1^{-1} - \omega^2 W_1^{-T} I_1 W_1^{-1}) \otimes M_2 + (W_1^{-T} I_1 W_1^{-1}) \otimes K_2$$
  
=  $(W_1^{-T} (\Lambda_1^B - \omega^2 I_1) W_1^{-1}) \otimes M_2 + (W_1^{-T} I_1 W_1^{-1}) \otimes K_2$   
=  $(W_1^{-T} \otimes I_2)((\Lambda_1^B - \omega^2 I_1) \otimes M_2 + I_1 \otimes K_2)(W_1^{-1} \otimes I_2),$ 

the inverse of  $\boldsymbol{B}$  can be represented by

$$\boldsymbol{B}^{-1} = (\boldsymbol{W}_1 \otimes \boldsymbol{I}_2) \boldsymbol{H}_B^{-1} (\boldsymbol{W}_1^T \otimes \boldsymbol{I}_2),$$
  
$$\boldsymbol{H}_B = (\boldsymbol{\Lambda}_1^B - \omega^2 \boldsymbol{I}_1) \otimes \boldsymbol{M}_2 + \boldsymbol{I}_1 \otimes \boldsymbol{K}_2.$$
 (14)

Similarly using (12), we obtain

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Fast solver (2d) - LU decomposition

The LU decomposition of  $H_B$  and  $H_A$  are computed as follows

$$\boldsymbol{H}_B = \boldsymbol{L}_B \boldsymbol{U}_B$$
 and  $\boldsymbol{H}_A = \boldsymbol{L}_A \boldsymbol{U}_A$ . (16)

Then the linear system

$$\boldsymbol{H}_{B}\boldsymbol{y} = \boldsymbol{L}_{B}\boldsymbol{U}_{B}\boldsymbol{y} = \boldsymbol{r} \tag{17}$$

is solved by solving the respective two subproblems

$$\boldsymbol{L}_B \boldsymbol{z} = \boldsymbol{r}$$
 and  $\boldsymbol{U}_B \boldsymbol{y} = \boldsymbol{z}$  (18)

consecutively in the application of the fast solver (analogously for  $H_A$ ). The vector r denotes some right hand side which is in the different steps of the solver also different.

The structure of  $H_B$  and  $H_A$  is essential for the fast application of the solver: The diagonal blocks are tridiagonal which makes the LU decomposition fast. Computational complexity is optimal O(N).

Solve the auxiliary problem

$$\boldsymbol{B}\boldsymbol{v} = \boldsymbol{B}\begin{pmatrix} \boldsymbol{v}_b \\ \boldsymbol{v}_r \end{pmatrix} = \boldsymbol{f}, \tag{19}$$

but compute only  $\mathbf{v}_b$  and not  $\mathbf{v}_r$ .

(a) Compute the Fourier transformation  $\hat{f}$  of f using FFT (which corresponds to  $\hat{f} = (W_1^T \otimes I_2) f$ ), where its coefficients  $\hat{f}_k$  are given as follows

$$\hat{f}_k = \sum_{l=1}^{N} e^{-2\pi i \frac{(l-1)(k-1)}{N}} f_l \qquad \forall k = 1, \dots, N,$$
 (20)

and save it, since it will be needed in Step 3 as well. (b) Next, we apply the LU decomposition (17) with the right-hand side  $\hat{f}$ 

$$L_B z_1 = \hat{f}$$
 and  $U_B \tilde{z}_1 = z_1$ .

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(c) Performing the inverse FFT on the resulting vector  $\tilde{z}_1$  would provide both  $v_b$  and  $v_r$ , which would correspond to  $v = (W_1 \otimes I_2) \tilde{z}_1$ . Since we only need  $v_b$ , instead of that, we multiply the vector  $\tilde{z}_1$  by the matrix  $W_1^b$  (the eigenvectors of  $W_1$  which correspond only to the boundary  $\Gamma_B$ ): leading to

$$\boldsymbol{v}_b = (\boldsymbol{W}_1^b \otimes \boldsymbol{I}_2) \, \tilde{\boldsymbol{z}}_1, \tag{22}$$

which altogether resembles the representation (14) for  $B^{-1}$ . Computational complexity of step 1 is  $O(N \log N)$ .



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

$$\boldsymbol{A}\boldsymbol{w} = \boldsymbol{A}\begin{pmatrix} \boldsymbol{w}_b \\ \boldsymbol{w}_r \end{pmatrix} = (\boldsymbol{B} - \boldsymbol{A})\boldsymbol{v} = \begin{pmatrix} \boldsymbol{C}_{bb}\boldsymbol{v}_b \\ 0 \end{pmatrix}, \quad (23)$$

since

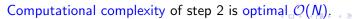
$$Aw = Au - Av = f - Av = Bv - Av, \qquad (24)$$

but compute only  $\boldsymbol{w}_b$  and not  $\boldsymbol{w}_r$  again:

(a) 
$$\boldsymbol{g}_b = (\boldsymbol{V}_1^{b^T} \otimes \boldsymbol{I}_2) \boldsymbol{C}_{bb} \boldsymbol{v}_b,$$
 (25)

(b)  $\boldsymbol{L}_{A}\boldsymbol{z}_{2} = \boldsymbol{g}_{b}$  and  $\boldsymbol{U}_{A}\tilde{\boldsymbol{z}}_{2} = \boldsymbol{z}_{2},$  (26)

(c) 
$$\boldsymbol{w}_b = (\boldsymbol{V}_1^b \otimes \boldsymbol{I}_2) \, \tilde{\boldsymbol{z}}_2.$$



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Solve now the problem

$$B\boldsymbol{u} = \boldsymbol{f} + (\boldsymbol{B} - \boldsymbol{A})(\boldsymbol{v} + \boldsymbol{w})$$
  
=  $\boldsymbol{f} + \begin{pmatrix} \boldsymbol{C}_{bb}(\boldsymbol{v}_b + \boldsymbol{w}_b) \\ 0 \end{pmatrix}$  (28)

due to Bu = Au + Bu - Au. (a) Use the Fourier transformation  $\hat{f}$  of f from step 1. Only need the Fourier transformation of the second term computed by

$$\boldsymbol{h}_{b} = (\boldsymbol{W}_{1}^{b^{T}} \otimes \boldsymbol{I}_{2}) \boldsymbol{C}_{bb}(\boldsymbol{v}_{b} + \boldsymbol{w}_{b})$$
(29)

leading to the Fourier transformation of the entire right-hand side of equation (28) denoted by  $\hat{f} + \hat{h}$ .

(b) 
$$\boldsymbol{L}_B \boldsymbol{z}_3 = \hat{\boldsymbol{f}} + \hat{\boldsymbol{h}}$$
 and  $\boldsymbol{U}_B \tilde{\boldsymbol{z}}_3 = \boldsymbol{z}_3$ . (30)

(c) In the last step all resulting components are needed (not only the ones corresponding to  $\Gamma_B$ ) to obtain the solution  $\boldsymbol{u}$  by applying the inverse Fourier transformation on  $\tilde{\boldsymbol{z}}_3$ , where its coefficients  $\hat{u}_k$  are given as follows

$$\hat{u}_k = \frac{1}{N} \sum_{l=1}^{N} e^{2\pi i \frac{(l-1)(k-1)}{N}} \tilde{z}_{3,l} \qquad \forall k = 1, \dots, N.$$
 (31)

The computation of the inverse Fourier transformation corresponds to the multiplication

$$\boldsymbol{u} = (\boldsymbol{W}_1 \otimes \boldsymbol{I}_2) \, \tilde{\boldsymbol{z}}_3.$$

Computational complexity of step 3 is  $\mathcal{O}(N \log N)$ .



# The 3d case



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## Fast solver (3d) - Reformulation of A and B

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

Analogously as in the 2d case

$$\boldsymbol{A}^{-1} = (\boldsymbol{V}_1 \otimes \boldsymbol{I}_{23}) \, \boldsymbol{H}_A^{-1} (\boldsymbol{V}_1^T \otimes \boldsymbol{I}_{23}) \tag{33}$$

and

$$\boldsymbol{B}^{-1} = (\boldsymbol{W}_1 \otimes \boldsymbol{I}_{23}) \boldsymbol{H}_B^{-1} (\boldsymbol{W}_1^T \otimes \boldsymbol{I}_{23}), \qquad (34)$$

where

$$\boldsymbol{H}_{A} = ((\boldsymbol{\Lambda}_{1}^{A} - \omega^{2}\boldsymbol{I}_{1}) \otimes \boldsymbol{M}_{2} + \boldsymbol{I}_{1} \otimes \boldsymbol{K}_{2}) \otimes \boldsymbol{M}_{3} + \boldsymbol{I}_{1} \otimes \boldsymbol{M}_{2} \otimes \boldsymbol{K}_{3}$$
(35)

and

$$\boldsymbol{H}_{B} = ((\boldsymbol{\Lambda}_{1}^{B} - \omega^{2}\boldsymbol{I}_{1}) \otimes \boldsymbol{M}_{2} + \boldsymbol{I}_{1} \otimes \boldsymbol{K}_{2}) \otimes \boldsymbol{M}_{3} + \boldsymbol{I}_{1} \otimes \boldsymbol{M}_{2} \overset{\text{(maximum constraints)}}{\overset{\text{(maximum constraints)}}{\overset{(maximum constraints$$

# Fast solver (3d) - Applying the 2d fast solver instead of LU decomposition

Since the LU decomposition is slow for very large problems in 3d, the linear systems with the block diagonal matrices  $H_B$  and  $H_A$  are efficiently implemented by applying the 2d fast solver  $n_1$  times for 2d subproblems of size  $n_2 \times n_3$  including the computation of the partial solution method in  $x_2$ -direction for

$$\mathbf{A}_{A,l} = (\mathbf{K}_2 - \underbrace{(\omega^2 - \mathbf{\Lambda}_{1,l}^A)}_{=:p_A} \mathbf{M}_2) \otimes \mathbf{M}_3 + \mathbf{M}_2 \otimes \mathbf{K}_3 \qquad (37)$$
$$\mathbf{A}_{B,l} = (\mathbf{K}_2 - \underbrace{(\omega^2 - \mathbf{\Lambda}_{1,l}^B)}_{=:p_B} \mathbf{M}_2) \otimes \mathbf{M}_3 + \mathbf{M}_2 \otimes \mathbf{K}_3, \qquad (38)$$

where  $l = 1, \ldots, n_1$ , solving the generalized eigenvalue problems

# **Numerical results**



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The numerical experiments have been computed in MATLAB 9.3, R2017b, on a laptop with Intel(R) Core(TM) i5-6267U CPU @ 2.90GHz processor and 16 GB 2133 MHz LPDDR3 memory.

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

Right-hand side is chosen as 0.01 for the first  $n_1$  entries and 1 for all the other entries

We compare the CPU times in seconds for computing the solution by applying Matlab's backslash and the fast solver presented. In our case, Matlab's backslash uses the sparse direct solver UMFPACK for computing the solution of the sparse linear systems. We present the times for the computations in the initialization process as well.

CPU times in seconds for different values of  $n = n_1 = n_2$ :

п	65	129	257	513	1025	2049
Initialization	0.07	0.09	0.31	1.74	13.38	118.99
Matlab's backslash	0.04	0.14	0.50	2.64	12.42	93.32
Fast solver	0.01	0.02	0.06	0.23	1.05	4.58

Largest numerical experiments in 2d have been computed for n = 2049 with 4 198 401 unknowns.



CPU times in seconds for different combinations of values for  $n_1$  and  $n_2$ :

<i>n</i> <sub>1</sub>	65	65	2049	2049
<i>n</i> <sub>2</sub>	65	2049	65	2049
Initialization	0.07	0.17	110.83	118.99
Matlab's backslash	0.04	0.98	1.07	93.32
Fast solver	0.01	0.10	0.12	4.58



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CPU times in seconds for different values of  $n = n_1 = n_2 = n_3$ :

п	9	17	33	65	129	257	513
Initialization	0.07	0.07	0.08	0.45	0.41	2.16	17.33
Matlab's backslash	0.02	0.28	6.39	572.91	-	_	-
Fast solver	0.09	0.12	0.21	1.03	8.43	69.55	672.27

Largest numerical experiments in 3d have been computed for n = 513 with 135 005 697 unknowns.



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## Numerical results (3d)

CPU times in seconds for different combinations of values for  $n_1$ ,  $n_2$  and  $n_3$ :

<i>n</i> <sub>1</sub>	9	9	9	513	9	513	513	513
<i>n</i> <sub>2</sub>	9	513	9	9	513	9	513	513
<i>n</i> <sub>3</sub>	9	9	513	9	513	513	9	513
Initialization	0.07	0.36	0.12	1.91	2.17	2.20	2.40	17.33
Matlab's backslash	0.02	1.06	0.96	0.90	_	_	_	_
Fast solver	0.09	0.22	0.25	0.62	10.95	8.00	7.01	672.27

The larger the size of the problem in 3d the more efficient the FFT based fast direct solver.

For large *n*, applying Matlab's lu on the subproblems as well as Matlab's kron are most time consuming.

 $\Rightarrow$  Can be expected that e.g. C++ implementation would the essentially faster.



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## Conclusions and outlook

#### Conclusions:

 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.

Outlook:

- Implementation in C++
- Application also to other problems

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# Thank you!

