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24th of July 2018 – DD25, St. John's, Canada

Numerical Implementation of the Method of Reflections

as a Preconditioner for the Multiple Scattering Helmholtz Problem using BEM

1 The Multiple Scattering Helmholtz Problem

- 1 Multiple Scatt. Helmholtz Pb
- 2 Basics of DIE
- 3 Algorithm of the MOR
 - 4 Preconditioner for It. Solvers
- 5 Numerical Results
 6 Averaged MOR
 7 Multipreconditioned GCR
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Scattering Problem



Scattering problem: find $u \in H^1_{loc}(\mathbb{R}^d)$ such that: $\begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega^+ \\ u = -u^{\text{inc}} & \text{on } \Gamma \\ u \text{ outgoing} \end{cases}$

Outgoing→the Sommerfeld radiation condition:

$$\lim_{\|\mathbf{x}\|\to\infty} \|\mathbf{x}\|^{(d-1)/2} \left(\nabla u \cdot \frac{\mathbf{x}}{\|\mathbf{x}\|} - \mathrm{i}ku \right) = 0$$

and

$$\forall \boldsymbol{x} \in \mathbb{R}^d, \quad u^{\text{inc}}(\boldsymbol{x}) = e^{ik\boldsymbol{\beta}\cdot\boldsymbol{x}}$$

- Ω^- bounded open set of \mathbb{R}^d , d = 2, 3
- propagation domain $\Omega^+ = \mathbb{R}^d \setminus \overline{\Omega^-}$ connected
- the boundary of Ω^- : Γ

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Multiple Scattering Problem

- ► The domain Ω^- is a collection of N disjoint bounded open sets $\{\Omega_i^-\}_{i \in [\![1,N]\!]}$ of \mathbb{R}^d
- every domain $\mathbb{R}^d \setminus \overline{\Omega_i^-}$ is connected.



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2 Basics of Direct Integral Equations

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Well known properties that can be found in [Chandler-Wilde et al. 2012; McLean 2000] and references therein.

SINGLE-LAYER VOLUME OPERATOR

where G is the usual Green function for the Helmholtz problem

DOUBLE-LAYER VOLUME OPERATOR

$$\mathcal{M} : \begin{array}{c} H^{1/2}(\Gamma) \to H^1_{\text{loc}}(\mathbb{R}^d \backslash \Gamma) \\ \mathcal{M} : \\ \lambda \mapsto \mathcal{M}\lambda, \end{array} \qquad \qquad \mathcal{M}\lambda(\boldsymbol{x}) = -\int_{\Gamma} \partial_{\boldsymbol{n}_y} G(\boldsymbol{x}, \boldsymbol{y})\lambda(\boldsymbol{y}) d\Gamma(\boldsymbol{y}) \end{array}$$

Proposition

For every densities $\rho \in H^{-1/2}(\Gamma)$ and $\lambda \in H^{1/2}(\Gamma)$, the single-layer potential $\mathscr{L}\rho$ and the double-layer potential $\mathscr{M}\lambda$ are outgoing solutions of the Helmholtz equation in $\mathbb{R}^d \setminus \Gamma$. Moreover, the scattered field *u* can be written as

$$\forall \boldsymbol{x} \in \Omega^+, \quad u(\boldsymbol{x}) = -\mathscr{L}(\partial_{\boldsymbol{n}} u_{|\Gamma})(\boldsymbol{x}) - \mathscr{M}(u_{|\Gamma})(\boldsymbol{x}).$$

Proposition

The trace (γ_0) and the normal trace (γ_1) of the operators \mathscr{L} and \mathscr{M} are given by the following relations:

$$\begin{split} \gamma_0^{\pm} \mathcal{L} \rho &= L \rho, \qquad \gamma_0^{\pm} \mathcal{M} \lambda = \left(\mp \frac{1}{2} I + M \right) \lambda, \\ \gamma_1^{\pm} \mathcal{L} \rho &= \left(\mp \frac{1}{2} I + N \right) \rho, \quad \gamma_1^{\pm} \mathcal{M} \lambda = D \lambda, \end{split}$$

where *I* is the identity operator and,...

Proposition

...for $\mathbf{x} \in \Gamma$, $\rho \in H^{-1/2}(\Gamma)$ and $\lambda \in H^{1/2}(\Gamma)$, the four boundary integral operator are defined by

$$\begin{split} L &: H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma), \qquad L\rho(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y})\rho(\mathbf{y}) \mathrm{d}\Gamma(\mathbf{y}), \\ M &: H^{1/2}(\Gamma) \to H^{1/2}(\Gamma), \qquad M\lambda(\mathbf{x}) = -\int_{\Gamma} \partial_{\mathbf{n}_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y})\lambda(\mathbf{y}) \mathrm{d}\Gamma(\mathbf{y}), \\ N &: H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma), \qquad N\rho(\mathbf{x}) = \int_{\Gamma} \partial_{\mathbf{n}_{\mathbf{x}}} G(\mathbf{x}, \mathbf{y})\rho(\mathbf{y}) \mathrm{d}\Gamma(\mathbf{y}), \\ D &: H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma), \qquad D\lambda(\mathbf{x}) = -\partial_{\mathbf{n}_{\mathbf{x}}} \int_{\Gamma} \partial_{\mathbf{n}_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y})\lambda(\mathbf{y}) \mathrm{d}\Gamma(\mathbf{y}). \end{split}$$

Direct Integral Equations (DIE)

► Choosing an operator A (a trace operator)

Scattering problem:	DIE Problem
find $u \in H^1_{loc}(\mathbb{R}^d)$ s. t. $\begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega^+ \\ u = -u^{\text{inc}} & \text{on } \Gamma \\ u \text{ outgoing} \end{cases}$	find $\rho \in H^{-1/2}(\Gamma)$ s. t. $A \mathscr{L} \rho = -Au^{\text{inc}}, \text{ on } \Gamma$ $L_A \rho = -Au^{\text{inc}}, \text{ with } L_A \rho = A \mathscr{L} \rho$

Remark: Possible choices for A

► $A = \gamma_0^-: L_A \rho = -Au^{inc} \rightarrow L\rho = -u_{|\Gamma}^{inc}$ (EFIE formulation) ► $A = \gamma_1^-: L_A \rho = -Au^{inc} \rightarrow (\frac{1}{2}I + N)\rho = -\partial_n u_{|\Gamma}^{inc}$ (MFIE formulation) ► $A = (1 - \alpha)\gamma_0^- + \alpha\eta\gamma_1^-: \rightarrow linear combination$ (CFIE formulation) see [Thierry 2014] The single-layer volume integral operator \mathscr{L} can be written as the sum of N operators $\{\mathscr{L}_i\}_{i\in [\![1,N]\!]}$ defined by

$$\mathcal{L}_{i}: \begin{array}{c} H^{-1/2}(\Gamma_{i}) \to H^{1}_{\text{loc}}(\mathbb{R}^{d}) \\ \rho_{i} \mapsto \mathcal{L}_{i}\rho_{i}, \end{array}, \quad \mathcal{L}_{i}\rho_{i}(\boldsymbol{x}) = \int_{\Gamma_{i}} G(\boldsymbol{x}, \boldsymbol{y})\rho_{i}(\boldsymbol{y}) d\Gamma_{i}(\boldsymbol{y}) d$$

and

$$\forall \rho \in H^{-1/2}(\Gamma), \quad \mathscr{L}\rho = \sum_{i=1}^{N} \mathscr{L}_i \rho_i, \quad \text{with } \rho_i = \rho_{|\Gamma_i|}$$

Defining

$$\forall g \in H^1(\Omega^-), \quad A_i g = (Ag)_{|\Gamma_i|}$$

it holds that

$$\forall i \in [[1, N]], \quad \sum_{j=1}^{N} A_i \mathscr{L}_j \rho_j = -A_i u^{\text{inc}}$$

Complex linear system, non symmetric and dense (BEM)

$$\begin{split} L_{A}\rho &= -Au^{\text{inc}}: \\ \begin{pmatrix} L_{A}^{1,1} & L_{A}^{1,2} & \cdots & L_{A}^{1,N} \\ L_{A}^{2,1} & L_{A}^{2,2} & \cdots & L_{A}^{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ L_{A}^{N,1} & L_{A}^{N,2} & \cdots & L_{A}^{N,N} \end{pmatrix} \begin{pmatrix} \rho_{1} \\ \rho_{2} \\ \vdots \\ \rho_{N} \end{pmatrix} = - \begin{pmatrix} A_{1}u^{\text{inc}} \\ A_{2}u^{\text{inc}} \\ \vdots \\ A_{N}u^{\text{inc}} \end{pmatrix} \end{split}$$

- A: a trace operator
- ρ : unknown $(-\partial_{\mathbf{n}} u_{|\Gamma})$
- L_A: boundary operator

$$\forall \rho_j \in H^{-1/2}(\Gamma_j), L_A^{i,j}\rho_j = A_i(\mathscr{L}_j\rho_j)$$

- $L_A^{i,j}$ for $i \neq j$ interactions between domains
- Natural domain decomposition (decomposition of the boundary)

3 Algorithm of the Method of Reflections

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Parallel Method of Reflections (MOR)

- Parallel Method of Reflections ([G. M. Golusin 1934; Laurent, Legendre, and Salomon 2017]): domain decomposition method with natural partition (objects)
- ► Well suited for the **BEM** with a boundary decomposition
- Numerical application: is it useful?
- Example: Multiple Scattering Problem

Remark: Two versions of the Method of Reflections, one sequential [Smoluchowski 1911] and one parallel, we only consider here the second one.





4 Preconditioner for Iterative Solvers

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Preconditioner of Iterative Solvers

► Is the MOR useful as a solver? → No, compared to a GMRES solver applied to the global problem with hierarchical matrix structures

Preconditioned Block Jacobi Method

The method of reflections for the multiple scattering Helmholtz problem using direct integral equation is equivalent the the block Jacobi method, that is to say, the following iterative solver:

$$\forall \ell \in \mathbb{N}, \quad D_A \rho^{(\ell+1)} = D_A \rho^{(\ell)} + (F - L_A \rho^{(\ell)})$$

where
$$D_A = \text{diag}((L_A^{i,i})_{i \in \llbracket 1,N \rrbracket})$$
 and $F = -Au^{\text{inc}}$

Proved by induction

Preconditioner

- ▶ Preconditioner: D_A^{-1} for an iterative solver, *i.e.*, Generalized Conjugate Residual (GCR), GMRES, etc. (see [Saad 2003])
- The convergence of the MOR (Jacobi) is not guaranteed, but convergence occurs for Krylov subspace methods
- Structure of

$$D_A^{-1} = \begin{pmatrix} L_A^{1,1} & 0 & \cdots & 0 \\ 0 & L_A^{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & L_A^{N,N^{-1}} \end{pmatrix}$$

 \rightarrow Parallel preconditioner

5 Numerical Results

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Numerical Results with GCR algorithm

• Set of spheres with different radius in 3D



Numerical Results with GCR algorithm

- Set of spheres with different radius in 3D
- Operator matrices computed by BEMPP (python)¹ ([Scroggs et al. 2017]), linear problem solved with a homemade preconditioned GCR solver (python+numpy)
- Useful when the spheres are close to each other
- Well known preconditioner: see [Thierry 2014]
- Numerical study depending on the number of spheres using the (small) cluster of the laboratory CEREMADE, Université Paris-Dauphine: one node with 40CPUs and 128Go of RAM

8 Spheres



27 Spheres



64 Spheres



- Distance between centers of spheres is 3.3, and random radius are between 1 and 1.6
- 3D positioning

Number of Spheres	D.o.F.	GCR it.	Precond. GCR it.
8	3464	412	30
27	12246	>500	52
64	34024	>500	240



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Weighted Preconditioner of Iterative Solvers

Weighted Preconditioned Block Jacobi Method

The method of reflections for the multiple scattering Helmholtz problem using direct integral equation is equivalent to the weighted block Jacobi method, that is to say, the following iterative solver:

$$\forall \ell \in \mathbb{N}, \forall i \in [[1, N]] \quad \rho_i^{(\ell+1)} = \rho_i^{(\ell)} + \omega_i L_A^{i, i^{-1}} \left(F_i - \sum_{j=1}^N L_A^{i, j} \rho_j^{(\ell)} \right)$$

- Once again proved by induction
- Preconditioner: $\mathbf{H} = \sum_{i=1}^{N} \omega_i R_i^T L_A^{i,i^{-1}} R_i$ where R_i is the restriction operator
- How to choose the weights ω_i ?

Connection with Multipreconditioning

Averaged MOR preconditioner:

$$\mathbf{H} = \sum_{k=1}^{N} \omega_k R_k^T L_A^{k,k^{-1}} R_k$$

 Additive Schwarz with Variable Weights [Greif, Rees, and Szyld 2012]: sequence of preconditioners

$$M^{(i)} = \sum_{k=1}^{N} \alpha_k^{(i)} R_k^T A_k^{-1} R_k$$

- Multipreconditioning with the MOR preconditioner gives sequence (ω_k⁽ⁱ⁾)_{k∈[[1,N]}
- Implementation of a multipreconditioned CGR

7 Multipreconditioned GCR

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(Multi)Preconditioned GCR I

• MOR Preconditioner:
$$\mathbf{H} = D_A^{-1} = \sum_{k=1}^N R_k^T L_A^{k,k^{-1}} R_k = \sum_{k=1}^N \mathbf{H}^k$$

Preconditioned GCR Multipreconditioned GCR $\mathbf{r}_{0} = \mathbf{b} - \mathbf{A}\mathbf{x}_{0}; \mathbf{Z}_{0} = [\mathbf{H}^{1}\mathbf{r}_{0} | \dots | \mathbf{H}^{N}\mathbf{r}_{0}]; \mathbf{P}_{0} = \mathbf{Z}_{0}$ 1 $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$; $\mathbf{z}_0 = \mathbf{H}\mathbf{r}_0$; $\mathbf{p}_0 = \mathbf{z}_0$ $q_0 = Ap_0$ $\mathbf{Q}_0 = \mathbf{A}\mathbf{P}_0$ **3** for *i* = 0, 1, ..., conv. do **for** *i* = 0, 1, ..., *conv.* **do** 4 $\Delta_i = \mathbf{q}_i^{\mathsf{T}} \mathbf{q}_i; \quad \gamma_i = \mathbf{q}_i^{\mathsf{T}} \mathbf{r}_i; \quad \alpha_i = \Delta_i^{-1} \gamma_i$ 5 $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{p}_i \alpha_i \quad \leftarrow \alpha_i \in \mathbb{R}, \, \mathbf{p}_i \in \mathbb{R}^n$ $\Delta_i = \mathbf{Q}_i^{\top} \mathbf{Q}_i; \quad \gamma_i = \mathbf{Q}_i^{\top} \mathbf{r}_i; \quad \alpha_i = \Delta_i^{-1} \gamma_i$ $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i \alpha_i \qquad \leftarrow \alpha_i \in \mathbb{R}^N, \, \mathbf{P}_i \in \mathbb{R}^{n \times N}$ $\begin{cases} \mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1} \\ \mathbf{z}_{i+1} = \mathbf{H}\mathbf{r}_{i+1} \\ \forall j \in [[0, i]], \Phi_{i,j} = \mathbf{q}_j^{\mathsf{T}}(\mathbf{A}\mathbf{z}_{i+1}) \\ \rho \end{cases}$ $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{q}_i \alpha_i$ $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{O}_i \alpha_i$ $\mathbf{Z}_{i+1} = \begin{bmatrix} \mathbf{H}^1 \mathbf{r}_{i+1} \end{bmatrix} \dots \begin{bmatrix} \mathbf{H}^N \mathbf{r}_{i+1} \end{bmatrix} \qquad \leftarrow Multi.$ $\forall j \in \llbracket 0, i \rrbracket, \Phi_{i,i} = \mathbf{Q}_i^\top (\mathbf{A} \mathbf{Z}_{i+1});$ $\beta_{i,i} = \Delta_j^{-1} \Phi_{i,j}$ $\beta_{i,i} = \Delta_j^{-1} \Phi_{i,j}$ 9 $\mathbf{p}_{i+1} = \mathbf{z}_{i+1} - \sum_{j=0}^{1} \mathbf{p}_j \beta_{i,j} \quad \leftarrow Ortho.$ $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{i=0} \mathbf{P}_j \beta_{i,j}$ $\leftarrow Ortho.$ $\mathbf{q}_{i+1} = (\mathbf{A}\mathbf{z}_{i+1}) - \sum_{i=0}^{i} \mathbf{q}_{i}\beta_{i,j}$ $\mathbf{Q}_{i+1} = (\mathbf{A}\mathbf{Z}_{i+1}) - \sum_{i=0}^{i} \mathbf{Q}_{i}\beta_{i,i}$ 10 11 end end 12 Return \mathbf{x}_{i+1} Return \mathbf{x}_{i+1}

_ Recall of Properties of (Multi)Preconditioned GCR _

$$\|\mathbf{r}_i\|_{\ell_2} = \|\mathbf{x}_* - \mathbf{x}_i\|_{\mathbf{A}^\top \mathbf{A}} = \min\left\{\|\mathbf{x}_* - \mathbf{x}\|_{\mathbf{A}^\top \mathbf{A}}; \mathbf{x} \in \mathbf{x}_0 + \bigoplus_{j=0}^{i-1} \operatorname{range}(\mathbf{P}_j)\right\},\$$

- $\mathbf{P}_i^{\top}(\mathbf{A}^{\top}\mathbf{A})\mathbf{P}_j = \mathbf{0}$ for every j = 0, ..., i 1.
- ▶ See [Bovet, Gosselet, and Spillane 2017; Bridson and Greif 2006]
- MOR multipreconditioner:

$$\mathbf{H}^{(i)} = \sum_{k=1}^{N} \omega_{k}^{(i)} R_{k}^{T} L_{A}^{k,k^{-1}} R_{k}$$

8 Spheres Test



27 Spheres Test



Perspectives

- CPU time \rightarrow be sure about what to compare
- Numerical study of the influence of the distance between the spheres and the consequence for the weights
- More irregular objects
- Adaptive Multipreconditioning
- Improve preconditioning with a coarse space coming from a simpler problem (smaller objects with a rough discretization?)

Thank you!





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