Fast Calderón preconditioning of the PCMHWT formulation for scattering by multiple dielectric particles

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Abstract

The discrete PMCHWT formulation for the single and multi-particle transmission problem suffers from ill-conditioning. Calderón preconditioning is a well-known technique to remedy this, reducing the number of iterations required by the linear solver, albeit at the expense of an increased number of matvecs per iteration. For single-particle problems, we find that the Calderón method is often outperformed by a simple mass-matrix preconditioner. For multi-particle problems a block-diagonal Calderón preconditioner provides a significant reduction in computational cost. We explore the capabilities of a bi-parametric Calderón preconditioner, which uses high quadrature orders and small $\mathcal{H}$-matrix tolerances for the assembly of the operator, but low quadrature orders and larger $\mathcal{H}$-matrix tolerances for the preconditioner. Finally, we investigate the effect of using only near-field interactions in the preconditioner. The performance of the different approaches is compared using the Bempp software package.

Keywords: Boundary element method, electromagnetic scattering, multiple bodies, Bempp

1 Introduction

We consider 3D electromagnetic scattering by M disjoint isotropic homogeneous dielectric scatterers in a homogeneous exterior medium. The electric and magnetic fields in the interior domains $(\mathbf{E}^i_m, \mathbf{H}^i_m)$, and the exterior domain $(\mathbf{E}^e, \mathbf{H}^e)$ are assumed to satisfy the time-harmonic Maxwell equations, which, written in second-order form for the electric fields $\mathbf{E}^i_m$, $\mathbf{E}^e$, are

$$\nabla \times (\nabla \times \mathbf{E}) - k^2 \mathbf{E} = 0,$$

where $k = k_m = \omega\sqrt{\mu_m \epsilon_m}$ and $k = k_e = \omega\sqrt{\mu_e \epsilon_e}$ are the wavenumbers for the respective domains. The exterior field is assumed to satisfy the Silver-Müller radiation condition.

2 Boundary Integral Operators

We define electric and magnetic potentials

$$\mathcal{E}\mathbf{v}(\mathbf{x}) := \mathrm{i}k \int_\Gamma \mathbf{v}(\mathbf{y}) G(\mathbf{x},\mathbf{y}) d\Gamma(\mathbf{y}) - \frac{1}{\mathrm{i}k} \nabla_\mathbf{x} \int_\Gamma \nabla_\mathbf{y} \cdot \mathbf{v}(\mathbf{y}) G(\mathbf{x},\mathbf{y}) d\Gamma(\mathbf{y}),$$

$$\mathcal{H}\mathbf{v}(\mathbf{x}) := \nabla_\mathbf{x} \times \int_\Gamma \mathbf{v}(\mathbf{y}) G(\mathbf{x},\mathbf{y}) d\Gamma(\mathbf{y}),$$

with $G(x,y) = \frac{\exp(\mathrm{i}k|\mathbf{x}-\mathbf{y}|)}{4\pi|\mathbf{x}-\mathbf{y}|}$, and interior $(-)$ and exterior $(+)$ Dirichlet and Neumann traces

$$\gamma_D^\pm \mathbf{u}^\pm(\mathbf{x}) = \mathbf{u}^\pm(\mathbf{x}) \times \mathbf{n}(\mathbf{x}), \qquad \mathbf{x} \in \Gamma,$$

$$\gamma_N^\pm \mathbf{u}^\pm(\mathbf{x}) = \frac{1}{ik} \gamma_D^\pm \left(\nabla \times \mathbf{u}^\pm(\mathbf{x})\right), \quad \mathbf{x} \in \Gamma.$$

We define the electric and magnetic boundary integral operators (with $\{\gamma_\cdot\} := (\gamma_\cdot^+ + \gamma_\cdot^-)/2$)

$$\mathcal{S} := \{\gamma_D\}\mathcal{E} = -\{\gamma_N\}\mathcal{H}, \quad \mathcal{C} := \{\gamma_D\}\mathcal{H} = \{\gamma_N\}\mathcal{E},$$

and the block operators and vectors

$$\mathcal{A}^i_m = \begin{bmatrix} \mathcal{C}^i_m & \frac{\mu_m}{k_m}\mathcal{S}^i_m \\ -\frac{k_m}{\mu_m}\mathcal{S}^i_m & \mathcal{C}^i_m \end{bmatrix}, \quad \mathbf{u}^i_m = \begin{bmatrix} \gamma^-_{D,m}\mathbf{E}^i_m \\ \frac{k_m}{\mu_m}\gamma^-_{N,m}\mathbf{E}^i_m \end{bmatrix},$$

$$\mathcal{A}^e_m = \begin{bmatrix} \mathcal{C}^e_m & \frac{\mu_e}{k_e}\mathcal{S}^e_m \\ -\frac{k_e}{\mu_e}\mathcal{S}^e_m & \mathcal{C}^e_m \end{bmatrix}, \quad \mathbf{u}^s_m = \begin{bmatrix} \gamma^+_{D,m}\mathbf{E}^s \\ \frac{k_e}{\mu_e}\gamma^+_{N,m}\mathbf{E}^s \end{bmatrix},$$

$$\mathcal{A}_{m\ell} = \begin{bmatrix} \mathcal{C}^e_{m\ell} & \frac{\mu_e}{k_e}\mathcal{S}^e_{m\ell} \\ -\frac{k_e}{\mu_e}\mathcal{S}^e_{m\ell} & \mathcal{C}^e_{m\ell} \end{bmatrix}, \quad \mathbf{u}^{inc}_m = \begin{bmatrix} \gamma^+_{D,m}\mathbf{E}^{inc} \\ \frac{k_e}{\mu_e}\gamma^+_{N,m}\mathbf{E}^{inc} \end{bmatrix},$$

where e.g. $\mathcal{S}^e_{m\ell}$ is $\mathcal{S}$ acting on scatterer ℓ, evaluated on scatterer m, with wavenumber $k = k_e$.

3 The PMCHWT formulation

The multi-particle PMCHWT formulation is

$$\mathcal{A}\mathbf{u}^s = \left(\frac{1}{2}\mathcal{I} - \mathcal{A}^i\right)\mathbf{u}^{inc}, \tag{1}$$

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where

$$\mathcal{A} = \begin{bmatrix} \mathcal{A}_1^e + \mathcal{A}_1^i & \mathcal{A}_{12} & \cdots & \mathcal{A}_{1M} \\ \mathcal{A}_{21} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathcal{A}_{(M-1)M} \\ \mathcal{A}_{M1} & \cdots & \mathcal{A}_{M(M-1)} & \mathcal{A}_M^e + \mathcal{A}_M^i \end{bmatrix},$$

$$\mathcal{A}^i = \begin{bmatrix} \mathcal{A}_1^i & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mathcal{A}_M^i \end{bmatrix}, \quad \mathbf{u}^s = \begin{bmatrix} \mathbf{u}_1^s \\ \mathbf{u}_2^s \\ \vdots \\ \mathbf{u}_M^s \end{bmatrix},$$

$$\mathcal{I} = \begin{bmatrix} \mathcal{I}_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mathcal{I}_M \end{bmatrix}, \quad \mathbf{u}^{inc} = \begin{bmatrix} \mathbf{u}_1^{inc} \\ \mathbf{u}_2^{inc} \\ \vdots \\ \mathbf{u}_M^{inc} \end{bmatrix}.$$

4 Calderón Preconditioning

Galerkin discretisation of (1) produces an ill-conditioned linear system, leading to slow convergence of iterative solvers. This occurs because $\mathcal{C}_m^i$ and $\mathcal{C}_m^e$ are compact, with eigenvalues accumulating at zero, while $\mathcal{S}_m^i$ and $\mathcal{S}_m^e$ are the sum of a compact operator, with eigenvalues accumulating at zero, and a hypersingular operator, with eigenvalues accumulating at infinity. As was shown in [1], one can remedy this at the continuous level by applying $\mathcal{A}$ to (1), obtaining the preconditioned system

$$\mathcal{A}^2 \mathbf{u}^s = \mathcal{A}\left(\frac{1}{2}\mathcal{I} - \mathcal{A}^i\right)\mathbf{u}^{inc}, \qquad (2)$$

which has better spectral properties than (1) due to the Calderón identities

$$\mathcal{S}^2 = -\frac{1}{4}\mathcal{I} + \mathcal{C}^2, \quad \mathcal{CS} + \mathcal{SC} = 0.$$

In a recent study of Calderón preconditioners for single- and multi-particle dielectric scattering [2], we found that the standard Calderón preconditioner (2) is actually no more efficient than a simple mass-matrix preconditioner in terms of the total matvecs required to reach GMRES convergence. But for the multi-particle case we found that a significant saving in computational cost can be obtained by performing block-diagonal Calderón preconditioning in which (1) is multiplied by only the block-diagonal part $\mathcal{D}$ of $\mathcal{A}$. Numerical experiments were performed for scatterers representing complex ice crystals, an example of which is shown in Fig. 1.

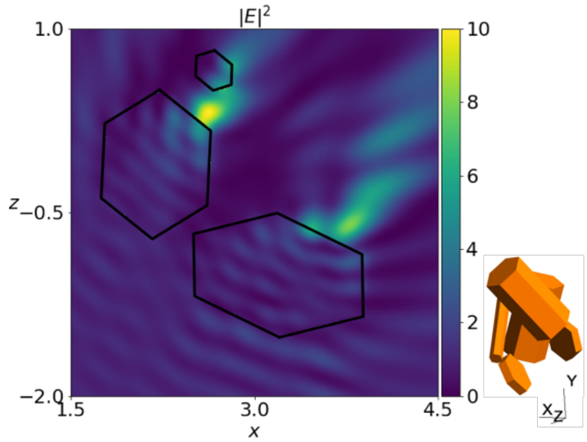

Figure 1: Squared magnitude of the electric field created by a plane incident wave travelling across an aggregate of ice crystals.

In [3], a bi-parametric Calderón preconditioner was introduced for the EFIE problem. We apply this bi-parametric approach to the PMCHWT multi-particle problem, with the operator $\mathcal{A}$ discretised by RWG basis functions and assembled with a high order quadrature and small $\mathcal{H}-$matrix tolerance, and the preconditioner $\mathcal{D}$ discretised by BC functions and assembled with a minimum number of quadrature points and a larger $\mathcal{H}-$matrix tolerance. In addition, we explore the possibility of including only the near-field interactions in the preconditioner, which results in a sparse matrix.

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