A comparison between Hierarchical Poincaré-Steklov approaches for the 3D Helmholtz equation with variable coefficients.

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Abstract

We present two solvers for the Hierarchical Poincaré-Steklov (HPS) discretization of 3D variable coefficient Helmholtz problems. An iterative approach uses a `GMRES` solver coupled with a leaf-wise block-Jacobi preconditioner. The preconditioner is built using two nested local solvers accelerated by local homogenization. Both the operator and preconditioner are implemented in a matrix-free fashion and with distributed memory. The solver can tackle problems approximately 50 wavelengths in each direction requiring more than a billion unknowns to get approximately 7 digits of accuracy in less than an hour.

We compare with an extension to 3D of the direct solver shown in [1,2]. Iterative local solvers, matrix compression and a modified discretization accelerate the solution and reduce memory footprint. We test both approaches and their performance with application examples.

Keywords: Helmholtz, Domain-Decomposition, Poincaré-Steklov

1 Introduction

We consider the variable coefficient Helmholtz problem with impedance boundary conditions given below

$$\begin{aligned} -\Delta u(\boldsymbol{x}) - \kappa^2(1-b(\boldsymbol{x}))u(\boldsymbol{x}) &= s(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \\ \frac{\partial u}{\partial n} + \mathrm{i}\eta u(\boldsymbol{x}) &= t(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial\Omega. \end{aligned} \tag{1}$$

$\Omega = (0,1)^3$, $u(\boldsymbol{x})$ is the complex unknown solution, $\kappa \in \mathbb{R}$ is the wave number, $b(\boldsymbol{x})$ is a given smooth scattering potential and n is the outward normal unit vector to the boundary of the domain. The functions $s(\boldsymbol{x})$ and $t(\boldsymbol{x})$ are assumed to be smooth complex functions.

We discretize the geometry into a collection of disjoint patches or **leaves**. Leaves are sized so that a local boundary value problem can be solved to high accuracy via a high degree Chebyshev spectral collocation method. Impedance-to-impedance (ItI) constraints are required between neighboring leaves. By using this operator for the coupling of elements, the HPS discretization is able to avoid artificial resonances and does not appear to observe the so-called *pollution effect* [1].

Problem size in leaves	$64 \times 64 \times 64$
MPI distributed memory procs	4096
Degrees of Freedom	1027M
GMRES time (1114 iterations)	2206s

Table 1: Performance for 50 wavelengths across, 10^{-8} residual reduction, Chebyshev degree 16.

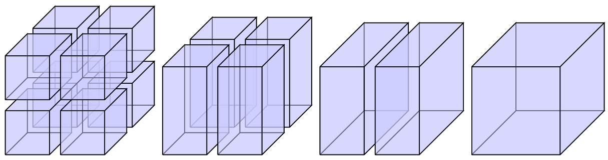

Figure 1: Merging subdomains in 3D

The iterative technique relies on the fact that the matrix that results from HPS is block sparse, where all non-zero blocks are also sparse and can be applied *matrix-free*. To solve the linear system we utilize a leaf-wise block-Jacobi preconditioned `GMRES` solver. The proposed block-Jacobi preconditioner and the system matrix are applied via matrix-free operations and exploit the tensor product nature of the element wise discretization matrices. The local nature of the blocks and the preconditioner make the solution technique naturally parallelizable in a distributed memory model. Numerical tests show that the solution technique is efficient and capable of tackling problems with a billion degrees of freedom (DoFs) in less than forty minutes in parallel (see Table 1).

The direct technique is an extension of [1,2] to 3D, it consists of two main steps after local spectral discretization:

- Approximate boundary (Poincaré–Steklov) and solution operators are constructed for each patch, starting with the leaves.
- In a hierarchical fashion, using Schur com-

plements obtain new patches by "glueing" patches together two at a time by enforcing ItI conditions via the Poincaré-Steklov operators on the boundaries of each patch. The procedure is illustrated in Figure 1. For each merged patch, corresponding boundary and solution operators are constructed.

2 Leaf discretization and solver

Let τ be a leaf, we seek to approximate the solution to (1) on Ω^τ using classical spectral collocation. Discretizing this way we obtain the matrix $\boldsymbol{A}_c^\tau := -\boldsymbol{D}_x^2 - \boldsymbol{D}_y^2 - \boldsymbol{D}_z^2 - \boldsymbol{C}^\tau$. $\boldsymbol{C}^\tau$ is a diagonal matrix with entries $\{\kappa^2\ (1 - b(\boldsymbol{x}_k))\}_{k=1}^n$, $\boldsymbol{D}_x^2$, $\boldsymbol{D}_y^2$ and $\boldsymbol{D}_z^2$ are Chebyshev differentiation matrices with corner and edge interaction entries removed.

The incoming and outgoing impedance operators in eq. (1) are approximated using the matrices $\boldsymbol{F}^\tau = \boldsymbol{N} + \mathrm{i}\eta\boldsymbol{I}$ and $\boldsymbol{G}^\tau = \boldsymbol{N} - \mathrm{i}\eta\boldsymbol{I}$. $\boldsymbol{I}$ is the identity matrix and $\boldsymbol{N}$ approximates the derivative at the boundary and is composed of submatrices of $\boldsymbol{D}_x$, $\boldsymbol{D}_y$ and $\boldsymbol{D}_z$.

Let $\boldsymbol{A}^\tau := \begin{pmatrix} \boldsymbol{A}_c^\tau(I_i^\tau, I^\tau) \\ \boldsymbol{F}^\tau \end{pmatrix}$, where I_i^τ are the interior node indices and I^τ are the indices for all nodes. Reordering we obtain a leaf system of the form

$$\boldsymbol{A}^\tau := \begin{pmatrix} \boldsymbol{A}_{ii}^\tau & \boldsymbol{A}_{ib}^\tau \\ \boldsymbol{F}_{bi}^\tau & \boldsymbol{F}_{bb}^\tau \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_i^\tau \\ \boldsymbol{u}_b^\tau \end{pmatrix} = \mathbf{RHS}^\tau, \quad (2)$$

where the subscript i stands for "interior" and b for "boundary" nodes of the leaf. The matrix $\boldsymbol{A}_{ii}^\tau$ is sparse can be applied rapidly thanks to its Kronecker product structure and $\boldsymbol{A}_{ib}^\tau$, $\boldsymbol{F}_{bi}^\tau$, $\boldsymbol{F}_{bb}^\tau$ are also sparse.

When $b(\boldsymbol{x})$ varies slowly, we solve this system by using the 2×2 block-matrix inversion formula. The formula needs the inverse of the Schur complement $\boldsymbol{S}^\tau$ and the inverse of $\boldsymbol{A}_{ii}^\tau$ which we apply iteratively using two nested `GMRES` solvers preconditioned with the inverses of homogenized versions of $\boldsymbol{A}_{ii}^\tau$ and $\boldsymbol{S}^\tau$. Given their structure, such homogenized inverses are relatively cheap to calculate.

3 Iterative method

The efficient leaf solver discussed in section 2 makes a leaf-wise block-Jacobi preconditioner a natural choice for the `GMRES` global solver. Thus we use a total of 3 nested `GMRES` solvers for leaves and global systems. Further details are given in [3] and some performance results are given in Table 1.

The solver can efficiently tackle very big problems to obtain a single solution. Inverse problems involving solving for several body loads and boundary conditions are better addressed with a direct method as we explain hereafter.

4 Direct method

The direct technique used in [1,2] demonstrated an excellent performance in 2D. We extend the technique to 3D overcoming many dimensionality challenges.

Increased dimensionality requires a large amount of DoFs in each leaf. We accelerate inversion using a modified spectral discretization. Leaf matrices being sparse, we apply a local iterative technique from section 3 when possible.

Operators for merging patches are significantly larger in 3D. However, large patch operators are rank-deficient up to the desired accuracy, especially for high frequency. Interpolative compression is used to reduce memory footprint. Linear algebra is parallelized with distributed memory akin to multifrontal solvers.

For inverse problems where the solution for many body loads and boundary conditions is needed, a direct technique outperforms an iterative solution. We study and compare both techniques with application examples including seismic inversion.

5 References

References

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