Parallel Optimizations for the Hierarchical Poincaré-Steklov Scheme (HPS)

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Abstract Parallel optimizations for the 2D Hierarchical Poincaré-Steklov (HPS) discretization scheme are described. HPS is a multi-domain spectral collocation scheme that allows for combining very high order discretizations with direct solvers, making the discretization powerful in resolving highly oscillatory solutions to high accuracy. HPS can be viewed as a domain decomposition scheme where the domains are connected directly through the use of a sparse direct solver. This manuscript describes optimizations of HPS that are simple to implement, and that leverage batched linear algebra on modern hybrid architectures to improve the practical speed of the solver. In particular, the manuscript demonstrates that the traditionally high cost of performing local static condensation for discretizations involving very high local order $p$ can be reduced dramatically.

1 Introduction

We describe methods for solving boundary value problems of the form

\[
\begin{align*}
\mathcal{A}u(x) &= f(x), & x &\in \Omega, \\
u(x) &= g(x), & x &\in \Gamma,
\end{align*}
\]

(1)

where $\mathcal{A}$ is a second order elliptic differential operator, and $\Omega$ is a rectangular domain in two dimensions with boundary $\Gamma$. For the sake of concreteness, we will focus on the case where $\mathcal{A}$ is a variable coefficient Helmholtz operator

\[
\mathcal{A}u(x) = -\Delta u(x) - \kappa^2 b(x) u(x),
\]

(2)

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where \( \kappa \) is a reference wavenumber, and where \( b(x) \) is a smooth non-negative function that typically satisfies \( 0 \leq b(x) \leq 1 \). Upon discretizing (1), one obtains a linear system

\[
Au = f
\]

involving a sparse coefficient matrix \( A \in \mathbb{R}^{N \times N} \). The focus of this work is on efficiently solving the sparse system (3) for the Hierarchical Poincaré-Steklov (HPS) discretization. HPS is a multi-domain spectral collocation scheme that allows for relatively high choices of \( p \), while interfacing well with sparse direct solvers. For (1) discretized with HPS with local polynomial order \( p \), the cost of factorizing \( A \) directly is

\[
T_{\text{build}} = O \left( p^4 N + N^{3/2} \right). \tag{4}
\]

After the leaf operations are complete, the cost to factorize the system directly has no pre-factor dependence on \( p \). The pre-factor cost of the leaf operations, however, has long been viewed as prohibitively expensive. This manuscript describes simple parallel optimizations using batched linear algebra that substantially accelerate the leaf operations and shows compelling results for \( p \) up to 42. We also demonstrate that the choice of \( p \) does not have substantial effects on the build time for the direct factorization stage, allowing \( p \) to be chosen based on physical considerations instead of practical concerns.

High order discretization is crucial in resolving variable-coefficient scattering phenomena due to the well known "pollution effect" that generally requires the number of points per wavelength to increase, the larger the computational domain is. The pollution effect is very strong for low order discretizations, but quickly gets less problematic as the discretization order increases \([1, 2]\). HPS is less sensitive to pollution because the scheme allows for high choices of local polynomial order \( p \) \([3, 4]\). Combining HPS discretization with efficient sparse direct solvers provides a powerful tool for resolving challenging scattering phenomena to high accuracy, especially for situations where no efficient preconditioners are known to exist (e.g. trapped rays, multiple reflections, backscattering) \([5]\).

## 2 HPS Discretization and Interfacing with Sparse Direct Solvers

We next discuss the HPS discretization and efficient methods to interface the resulting sparse linear system with direct solvers. We introduce the HPS briefly for the simple model problem (1), and refer the reader to \([6, 7, 8]\) for details and extensions. An important limitation of the discretization is that we assume the solution is smooth and that the coefficients in the operator \( \mathcal{A} \) of (1) are smooth as well.

The domain \( \Omega \) is partitioned into non-overlapping subdomains. The discretization is described by two parameters, \( a \) and \( p \), which are the element size and local polynomial order, respectively. On each subdomain, we place a \( p \times p \) tensor product mesh of Chebyshev points. Internal to each subdomain, the PDE is enforced locally
via spectral differentiation and direct collocation. On element boundaries, we enforce that the flux between adjacent boundaries is continuous. On each subdomain of \( p^2 \) nodes, the spectral differentiation operators lead to a dense matrix of interactions of size \( p^2 \times p^2 \). To improve efficiency of sparse direct solvers for HPS discretizations, we “eliminate” the dense interactions of nodes interior to each subdomain. This process is referred to as “static condensation” \([9, 10]\). The remaining active nodes are on the boundaries between subdomains. As a result of the leaf elimination, we produce a smaller system \( \tilde{A} \) of size \( \frac{N}{p} \) with equivalent body load \( \tilde{f} \) on the active nodes

\[
\tilde{A} \tilde{u} = \tilde{f}.
\]

See Figure 2 for the full grid of points and the remaining active nodes after static condensation.

The leaf elimination requires independent dense linear algebraic operations on \( \frac{N}{p^2} \) systems each of size \( p^2 \times p^2 \), resulting in overall cost \( O(p^3 \log p) \) to produce the equivalent system \( (5) \). For \( p \) up to 42, these operations can be efficiently parallelized with batched linear algebra (BLAS). For larger \( p \), methods that produce an sparser equivalent system are more fitting \([11, 12]\). Traditionally, it may be challenging to achieve high arithmetic intensity for many small parallel tasks due to overhead costs. Batched BLAS is a highly optimized software for parallel operations on matrices that are small enough to fit in the top levels of the memory hierarchy (i.e. smaller than the L2 cache size) \([13]\). The framework operates by grouping small inputs into larger “batches” and can achieve particularly good performance on high-throughput architectures, such as GPUs.

We combined the fast leaf factorization procedure with two methods for solving the reduced system \( (5) \). The first option for solving \( (5) \) uses a black-box sparse direct solver with the nested dissection (ND) ordering. ND is a based on a multi-level graph partitioning of nodes and produces a sparse factorization with minimal fill-in \([14, 15]\). In 2D, sparse factorization using the ND ordering requires \( O(N^{3/2}) \) time to build and \( O(N \log N) \) time to apply.

As a second option for solving \( (5) \), we used a scheme we refer to as SlabLU, which is a simplified two-level scheme (as opposed to standard hierarchical schemes) that is designed for ease of parallelization \([16]\). To be precise, SlabLU uses a decomposition of the domain into elongated “slab” subdomains. The nodes internal to each slab are eliminated in parallel, and the resulting block-tridiagonal system on
slab interfaces is solved directly. The resulting two-level scheme has complexity $O(N^{5/3})$ to factorize $\tilde{A}$ directly and $O(N^{7/6})$ complexity to apply the computed factors to solve (5). SlabLU is simple scheme that leverages high concurrency and batched BLAS to achieve high performance on modern hybrid architectures. Despite the asymptotically higher costs, SlabLU performs favorably compared to multi-level nested dissection schemes in its build time and memory footprint, as we demonstrate in Section 3.

Remark 1 Since the leaf computations are very efficient, we saved memory and reduced communication by not explicitly storing the factorizations of the local spectral differentiation matrices. Instead, these are reformed and refactored after each solve involving the reduced system (5).

3 Numerical Experiments

We next demonstrate the effectiveness of HPS, combined with efficient sparse direct solvers, in solving high frequency Helmholtz equations. The experiments are run on a desktop with a 16-core Intel i9-12900k CPU with 128GB of memory and a NVIDIA RTX 3090 GPU with 24GB of memory.

![Time for HPS leaf operations for various p](image)

Fig. 2 Leaf Operations for HPS require $O(p^4 N)$ operations, though the practical scaling for parallel operations has a small constant prefactor for $p$ up to 42. Parallel HPS leaf operations are further accelerated on GPUs, with a speed-up of at least 4x.

We demonstrate that simple parallel optimizations allow us to efficiently do leaf operations for various local polynomial order $p$; see Figure 2. After the leaf operations, we directly factorize the reduced system (5) using efficient sparse direct solvers and demonstrate that the choice of $p$ does not have much effect on the time to factorize $\tilde{A}$. Having freedom over the choice of $p$ allows the user to resolve highly oscillatory PDEs to high order accuracy, without concern for how the choice may affect the cost of solving (5) directly.

To demonstrate the effectiveness of the HPS discretization resolving oscillatory solutions to high accuracy, we report results for a PDE with a known analytic solution.
\[
\begin{aligned}
-\Delta u(x) - \kappa^2 u(x) &= 0, \quad x \in \Omega, \\
\quad u(x) = u_{\text{true}}(x), \quad x \in \Gamma,
\end{aligned}
\]

(6)

where the true solution \( u_{\text{true}} \) is given by \( u_{\text{true}} = J_0(\kappa|x|) \), where \( x \mapsto J_0(\kappa|x|) \) is the free-space fundamental solution to the Helmholtz equation.

In the experiments, we discretize (6) using HPS for various choices of \( p \) and set the wavenumber \( \kappa \) to increase with \( \mathcal{N} \) to maintain 10 points per wavelength with increasing problem size.

After applying a direct solver to solve (5) on the reduced HPS grid, we re-factorize the linear systems on interior leaf nodes to calculate the solution \( u_{\text{calc}} \) on the full HPS grid. The leaf solver requires time \( O(p^4 \mathcal{N}) \), but is particularly efficient using the parallel optimizations described. The reported build times and solve times include the leaf operations, which are done with batched BLAS on a GPU. We report relative error with respect to the residual of the discretized system (3). When a true solution is known, we also report relative error with respect to the true solution \( u_{\text{true}} \) evaluated on the collocation points of the full HPS grid

\[
\text{relerr}_{\text{res}} = \frac{\|A u_{\text{calc}} - f\|_2}{\|f\|_2}, \quad \text{relerr}_{\text{true}} = \frac{\|u_{\text{calc}} - u_{\text{true}}\|_2}{\|u_{\text{true}}\|_2}.
\]

(7)

3.1 Comparison of Sparse Direct Solvers

The system (5) is solved using two different sparse direct solvers, SuperLU and SlabLU. SuperLU is a black-box solver that finds an appropriate ordering of the system that minimizes fill-in while increasing concurrency by grouping nodes into “super-nodes” [17]. SuperLU is accessed through the Scipy interface (version 1.8.1) and called with the COLAMD ordering. This version of Scipy uses the CPU only.

Not many GPU-aware sparse direct solvers are widely available, though this is an active area of research. SuperLU also uses a pivoting scheme that can exchange rows between supernodes to attain almost machine precision accuracy in the residual of the computed solutions. SlabLU uses an ordering based on a decomposition of the domain into “slabs” that has a limited pivoting scheme. Despite this limitation, SlabLU can achieve 10 digits of accuracy in the residual, which gives also gives high order true relative accuracy, depending on the choice of \( p \).

SlabLU is a simple two-level framework that achieves large speedups over SuperLU by leveraging batched BLAS and GPU optimizations. See Figure 3.1 for a comparison between SuperLU and SlabLU in factorizing \( \tilde{A} \) to solve (5). See Figure 4 for a comparison of accuracies in the computed solutions for various \( p \). For PDEs on rectangular domains, SlabLU, compared to SuperLU, is able to solve larger sparse systems (5) with a smaller memory footprint. We demonstrate the ability of HPS for various \( p \), combined with SlabLU, to solve Helmholtz problems of size up to 900.\( l \times 900.\l (\text{for which } \mathcal{N}=81M) \) to high order accuracy. See Figure 5 which reports
build and solve times for various choices of \( p \). See Figure 6 which reports how the choice of \( p \) affects the accuracy of the computed solutions.

![Build Time and Memory Comparison](image)

**Fig. 3** Build time and memory footprint comparison between SuperLU and SlabLU for (6) discretized with HPS \((p=22)\), where \( \kappa \) is increased to maintain 10 points per wavelength. For \( N=5.06M\), the SlabLU build time is faster by a factor of 16x and the memory footprint is less by a factor of 14x.

![Accuracy Comparison](image)

**Fig. 4** Accuracy comparison between SuperLU and SlabLU for (6) discretized with HPS \((p=22,42)\), where \( \kappa \) is increased to maintain 10 points per wavelength. SuperLU uses a more sophisticated pivoting scheme to achieve high accuracy in the residual error. For \( p=22 \), SlabLU and SuperLU both resolve the solution to 6 digits in the true relative accuracy. For \( p=42 \), SuperLU is able to achieve 10 digits in the true relative accuracy, while SlabLU achieves 8 digits.

### 3.2 Variable-Coefficient Scattering Problems

We next demonstrate the ability of HPS, combined with SlabLU as a sparse direct solver, to solve complicated scattering phenomena. To be precise, we solve BVP (1) with the variable-coefficient Helmholtz operator (2) and discretize using HPS with \( p=32 \). The problems physically correspond to an antenna releasing an electromagnetic signal in a closed room. Due to the boundary conditions, multiple reflections occur because the wave cannot escape the closed domain. The Dirichlet data \( u_{\text{dir}} \) for the experiments in this section is given by a Gaussian pulse on the left boundary of the domain.
Fig. 5 Build time and solve time for HPS with various $p$ for (6) where $\kappa$ is increased with $N$ to maintain 10 points per wavelength. The choice of $p$ does not substantially affect the time needed to factorize the sparse linear system with SlabLU. As $p$ increases, the memory footprint required to store the factorization decreases and the solve time increases.

Fig. 6 Solution accuracy for HPS with various $p$ for (6) where $\kappa$ is increased with $N$ to maintain 10 digits of relative accuracy in the residual. With increasing $p$, one can calculate solutions with higher relative accuracy, compared to the true solution of the PDE.

$$u_{\text{dir}}(x) = \begin{cases} \exp\left(-2000(x_1 - 0.5)^2\right), & \text{when } x_0 = 0 \\ 0, & \text{otherwise.} \end{cases} \quad (8)$$

See Figure 3.2 for the computed solution with smooth variable coefficient media $b$, which mimics the presence of a crystal that blocks the propagating pulse.
4 Conclusions

HPS is a high-order convergent discretization scheme that interfaces well with sparse direct solvers. This manuscript describes parallel optimizations of the scheme that allow for the rapid and memory efficient direct solution of (4) of the resulting linear systems. First, we perform the leaf operations in parallel using batched BLAS, then we factorize a smaller system (5) of size $N/p$ using sparse direct solvers, where $p$ denotes the local order of convergence (which we show can be chosen as high as 40). The numerical results feature comparisons between sparse direct solvers and demonstrate that SlabLU can factorize systems corresponding to domains of size up to $900 \times 900 \lambda$ (for which $N=81M$) in less than 20 minutes. The approach is effective in resolving challenging scattering problems to high accuracy.

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