Multipole-Based Preconditioners for Large Sparse Linear Systems

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Overview

- Summary of Contributions
- Generalized Stokes Problem
- Solenoidal Basis Methods and Preconditioning
- Multipole Methods as Preconditioners
- Performance of Multipole-Based Preconditioners
- Parallelization of Solver/Preconditioner
- Parallel Performance
- Concluding Remarks

Summary of Contributions

- Problem Formulation
- Excellent Convergence Properties of Multipole-Based Preconditioners
- Parallelism in Multipole Methods
- Highly Scalable and Efficient Parallel Formulations

Generalized Stokes Problem

- Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u} = -\nabla p + \frac{1}{R} \Delta \mathbf{u} \quad \text{in } \Omega$$

$$\nabla \bullet \mathbf{u} = \mathbf{0} \quad \text{in } \Omega$$

$$\mathbf{u} = \mathbf{g} \quad \text{on } \partial\Omega$$

- Incompressibility Condition $\nabla \bullet \mathbf{u} = 0$

Generalized Stokes Problem

- Linear system

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathrm{u} \\ \mathrm{p} \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

- B^T is the discrete divergence operator and A collects all the velocity terms.

- Navier-Stokes:

$$A = \frac{1}{\Delta t} M + C + \frac{1}{R} L$$

- Generalized Stokes Problem:

$$A = \frac{1}{\Delta t} M + \frac{1}{R} L$$

Solenoidal Basis Methods [Sarin 2001]

- Class of projection based methods
- Basis for divergence-free velocity
- Solenoidal basis matrix *P*: $B^T P = 0$
- Divergence free velocity: $\mathrm{u} = P\mathrm{x}$

$$B^T \mathrm{u} = B^T P\mathrm{x} = 0$$

- Modified system

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathrm{u} \\ \mathrm{p} \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} \quad \Rightarrow \quad AP\mathrm{x} + B\mathrm{p} = f$$

Solenoidal Basis Method

- Reduced system:

$$B^T P = P^T B = 0$$

$$AP\mathrm{x} + B\mathrm{p} = f \quad \Rightarrow \quad P^T AP\mathrm{x} = P^T f$$

- Reduced system solved by suitable iterative methods such as CG or GMRES.

- Velocity obtained by : $\mathrm{u} = P\mathrm{x}$

- Pressure obtained by: $Bp = f - APx$

Preconditioning

- Observations

$$y = P^T u \quad \Rightarrow \quad \boldsymbol{\xi} = \nabla \times \mathbf{u}$$

$$u = Pw \quad \Rightarrow \quad \mathbf{u} = \nabla \times \boldsymbol{\psi}$$

$$y = P^T P w \quad \Rightarrow \quad \boldsymbol{\xi} = \nabla \times \nabla \times \boldsymbol{\psi}$$

- Vorticity-Velocity function formulation:

$$\frac{\partial \boldsymbol{\xi}}{\partial t} = -\frac{1}{R} \nabla \times \nabla \times \boldsymbol{\xi}, \qquad \boldsymbol{\xi} = -\Delta \boldsymbol{\psi}$$

Preconditioning

- Reduced system approximation:

$$P^T A P \approx \left[\frac{1}{\Delta t} M + \frac{1}{R} P^T P \right] P^T P$$

- Preconditioner:

$$G \approx \left[\frac{1}{\Delta t} M + \frac{1}{R} L_s \right] L_s$$

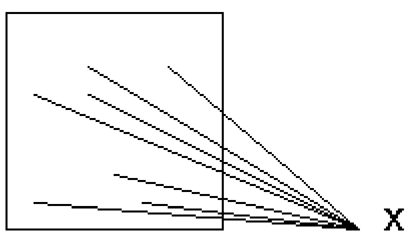
- Low accuracy preconditioning is sufficient

Preconditioning

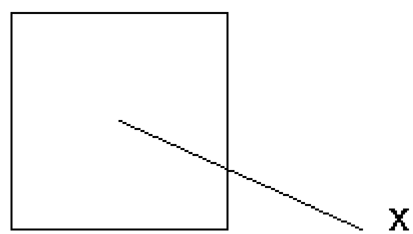
- Preconditioning can be affected by an approximate Laplace solve followed by a Helmholtz solve.
- The Laplace solve can be performed effectively using a Multipole method.

Overview of Multipole Methods

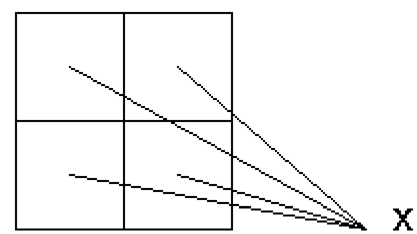
- Consider the problem of computing the trajectory of particles in space.
- Multipole methods use hierarchical approximations to reduce computational cost.



set of particles impacting x.



Can they be approximated by their center of mass?



If not, divide domain and recursively apply the same criteria to sub-domains.

Overview of Multipole Methods

- Accurate formulation requires $O(n^2)$ force computations (mat-vec with a coefficient matrix of Green's functions)
- Hierarchical methods reduce this complexity to $O(n)$ or $O(n \log n)$
- Since particle distributions can be very irregular, the tree can be highly unbalanced
- Commonly used hierarchical methods include FMM and the Barnes-Hut methods.

Overview of Multipole Methods

- Interactions (direct force computations) are replaced by Gaussian quadratures.
- Far-field interactions are replaced by multipole series representing remote Gauss points.
- Each matrix-vector product now becomes a single tree traversal taking O(n) or O(n log n) time.
- This mat-vec can be encapsulated in iterative solvers for dense systems.

Overview of Multipole Methods

- A number of results relating to the complexity of hierarchical methods [Rokhlin, Greengard], error analysis and control [Grama, Sarin, Sameh], and their use in dense solvers [Grama, Kumar, Sameh] have been shown. Their applications in applications such as inductance extraction [White, Sarin] have also been demonstrated.

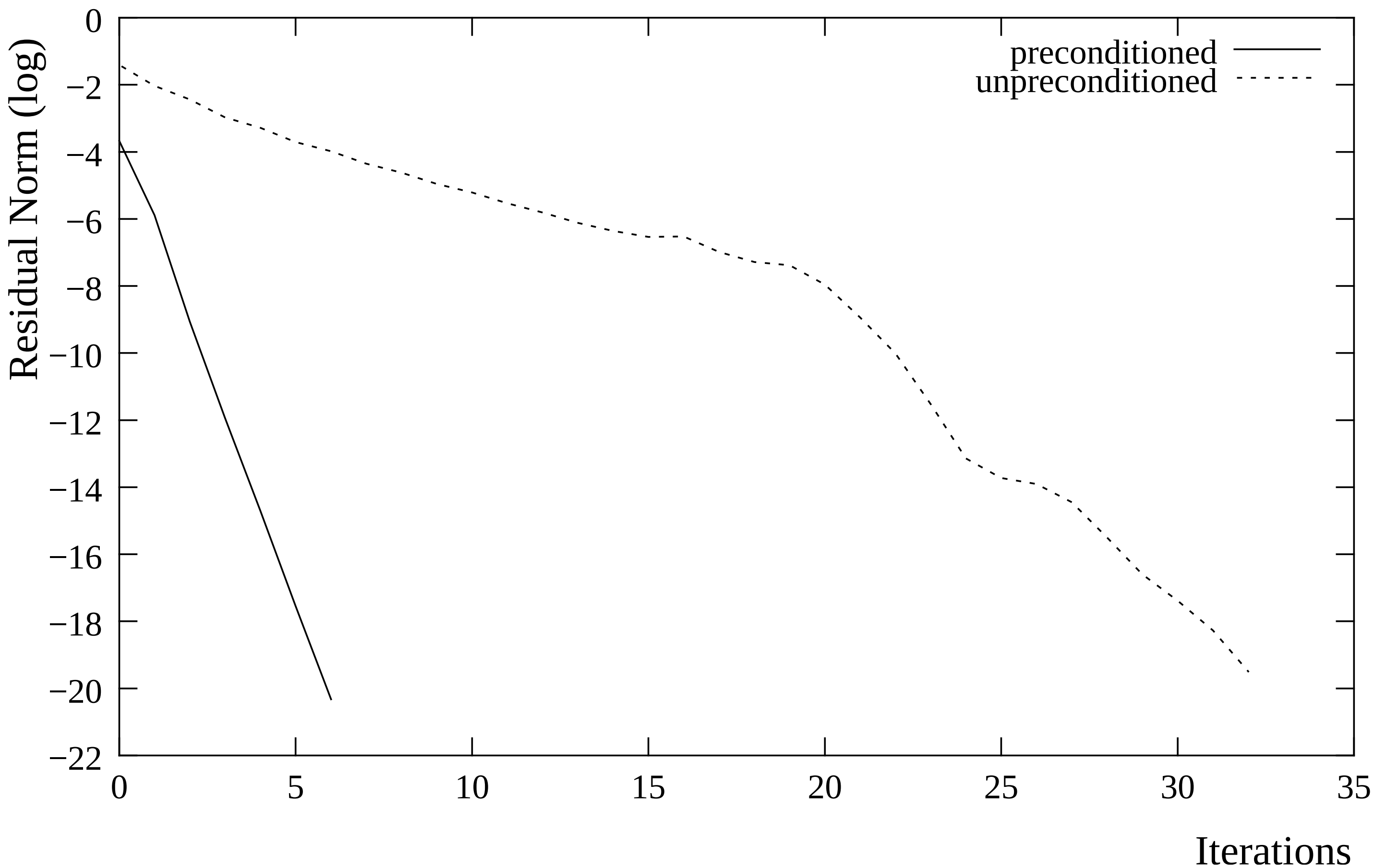
Numerical Experiments

- 3D driven cavity problem in a cubic domain.
- Marker-and-cell scheme in which domain is discretized uniformly.
- Pressure unknowns are defined at node points and velocities at mid points of edges.
- x, y, and z components of velocities are defined on edges along respective directions.

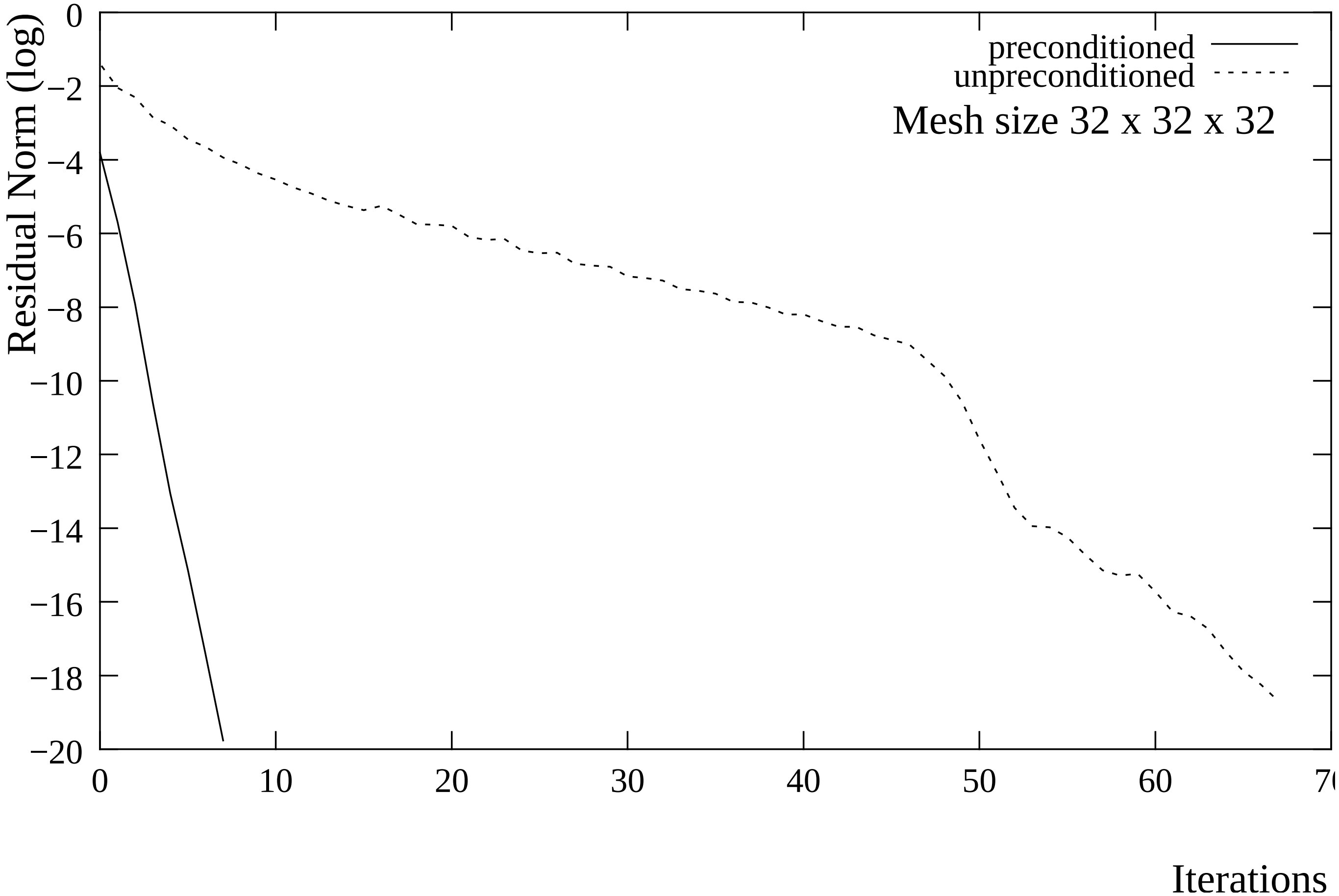
Sample Problem Sizes

Mesh	Pressure	Velocity	Solenoidal Functions
8x8x8	512	1,344	1,176
16x16x16	4,096	11,520	10,800
32x32x32	32,768	95,232	92,256

Preconditioning Performance



Preconditioning Performance



Parallel Formulation - Outer Solve

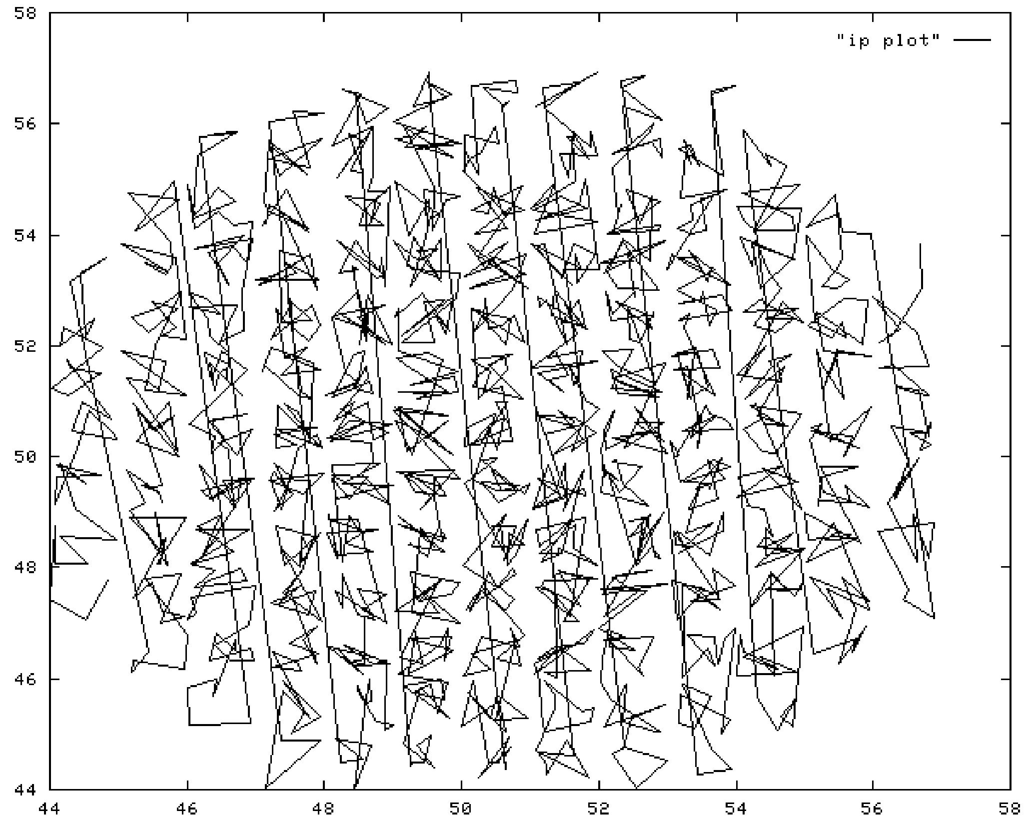
- Partition domain across processors
- Computation and storage of solenoidal basis matrix P
- Matrix-vector products: $y = P^T APx$
  - Local operations on the grid
- Vector operations
- Preconditioning
- Scalable parallel implementations have been developed for all these operations
- Matrix free approach
- SGI Origin 2000 with OpenMP and MPI

Parallel Formulation (Multipole Solve)

- Each node evaluation can potentially be executed as a thread.
- Since there may be a large number of nodes, this may lead to too many threads. In general, we build some granularity into the thread by gathering k nodes into a single thread.
- The Barnes-Hut tree is a read-only data structure. Therefore, good performance can be achieved if we can build spatial and temporal locality (and the working set size does not exceed local memory).

Parallel Formulation(Multipole Solve)

- Spatially proximate particles are likely to interact with nearly identical parts of the tree. Therefore particles must be traversed in a spatial-proximity preserving order.

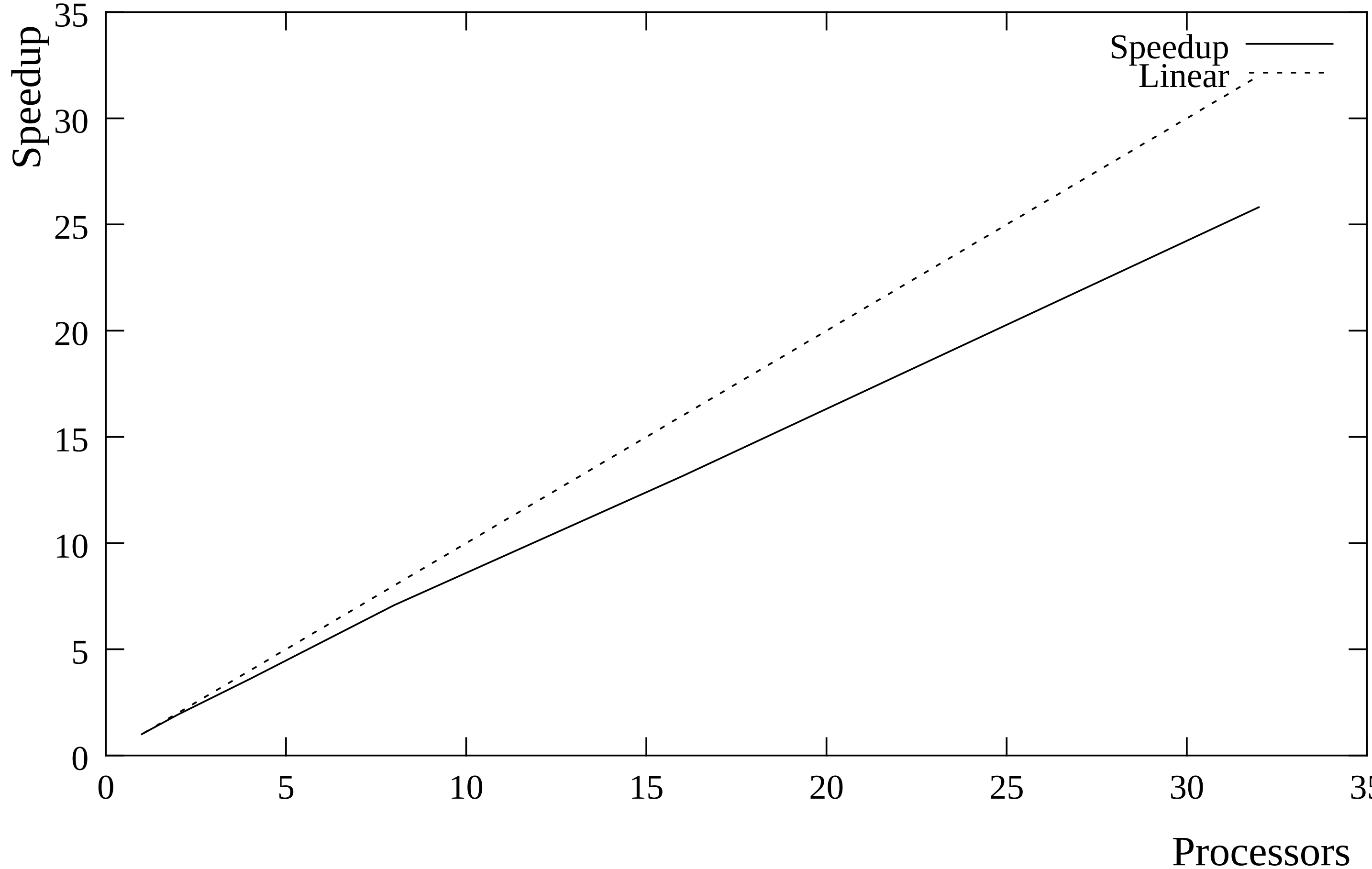


Parallel Performance

- Mesh size 32 x 32 x 32

Number of processors	Processor grid	Time (sec)	Speed-up	Efficiency
1	1 x 1 x 1	929	-	1.0
2	2 x 1 x 1	483	1.92	0.96
4	2 x 2 x 1	257	3.61	0.90
8	2 x 2 x 2	131	7.08	0.88
16	4 x 2 x 2	70	13.15	0.82
32	4 x 4 x 2	36	25.81	0.80

Parallel Performance



Concluding Remarks

- Multipole methods provide highly effective preconditioning techniques that yield excellent parallel speedups.
- The accuracy parameters of the multipole solve (degree, multipole acceptance criteria) significantly impact time (but less so convergence rate).
- Rely on closed form Green's function, but can be adapted to other scenarios.