Motivation

Among optimal hierarchical algorithms for the computational solution of elliptic problems, the Fast Multipole Method (FMM) stands out for its adaptability to emerging architectures, having high arithmetic intensity, tunable accuracy, and relaxed global synchronization requirements. We demonstrate that, beyond its traditional use as a solver in problems for which explicit free-space kernel representations are available, the FMM has applicability as a preconditioner in finite domain elliptic boundary value problems, by equipping it with boundary integral capability for finite boundaries and by wrapping it in a Krylov method for extensibility to more general operators. Compared with multilevel methods, it is capable of comparable algebraic convergence rates down to the truncation error of the discretized PDE, and it has superior multicore and distributed memory scalability properties on commodity architecture supercomputers.

Abstract

Among optimal hierarchical algorithms for the computational solution of elliptic problems, the Fast Multipole Method (FMM) stands out for its adaptability to emerging architectures, having high arithmetic intensity, tunable accuracy, and relaxed global synchronization requirements. We demonstrate that, beyond its traditional use as a solver in problems for which explicit free-space kernel representations are available, the FMM has applicability as a preconditioner in finite domain elliptic boundary value problems, by equipping it with boundary integral capability for finite boundaries and by wrapping it in a Krylov method for extensibility to more general operators. Compared with multilevel methods, it is capable of comparable algebraic convergence rates down to the truncation error of the discretized PDE, and it has superior multicore and distributed memory scalability properties on commodity architecture supercomputers.

Fast Multipole Method

- The FMM can be used as a numerical PDE solver for certain problems with Laplace, Stokes and Helmholtz operators, like multigrid.
- The FMM is a more promising approach for future architectures since it is compute-bound while multigrid methods are bandwidth-bound.
- The FMM may be of greatest value as a preconditioner for iterative methods:
  - High arithmetic intensity.
  - High degree of parallelism.
  - Potentially much less synchronous.
- The FMM does not naturally incorporate boundary conditions, as these do not appear in its original application of solving N-body problems; to overcome this obstacle we have coupled FMM to the boundary element method.

The FMM-BEM preconditioner

The FMM in its original form solves problems with free-field boundary conditions, since the formulation relies on free-space Green’s functions. FMM preconditioner can be extended to Dirichlet, Neumann or Robin boundary conditions for arbitrary geometries by coupling it with a boundary element method (BEM).

Boundary Element Method

- For Dirichlet boundary conditions, \( u \) is known and the boundary equation can be written in the following matrix form
  \[
  \mathbf{A} \mathbf{u} = \mathbf{f}
  \]
  Where \( N_b \) and \( N_i \) are the number of boundary nodes and internal nodes, respectively.
- The values of \( u \) and \( \partial u / \partial n \) will be known everywhere on the boundary after solving the linear system. Then it becomes possible to solve for the values inside the domain by solving the following
  \[
  \mathbf{u}(x) = \int_{\Gamma} G(x,y) f(y) dy
  \]
  In discrete form
  \[
  u_i = \sum_j G_{ij} f_j
  \]
  where \( G \) is a dense matrix, \( u \) and \( f \) are vectors.

- The third term on the right hand side involves an \( N_b \times N_i \) matrix, and is the dominant part of the computational load. This matrix-vector multiplication can be approached in \( O(N) \) time by using the FMM. We also use the FMM to accelerate all other matrix-vector multiplications.

Results

Convergence rate of the FMM preconditioner with different precision.

Time-to-solution for different problem sizes of the FMM and AMG preconditioners on a single core.

Strong scaling of the FMM and AMG preconditioners.

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