

Scalable Linear Solvers

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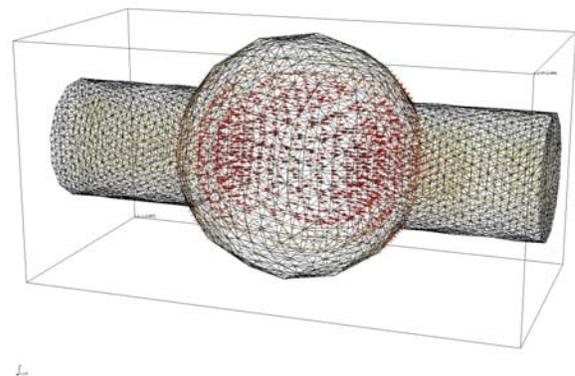
Summary

The goal of this project is to develop parallel multigrid methods for solving the large linear systems of equations that arise in many DOE scientific simulation codes. These methods have the potential to reduce simulation times dramatically (by as much as a factor of 10 or more), enabling new advancements in science.

At the core of many DOE simulation codes is the need to solve huge linear systems on thousands of processors. Multigrid methods are so-called *scalable* or *optimal* methods because they can solve a linear system with N unknowns with only $O(N)$ work. This property makes it possible to solve ever larger problems on proportionally larger parallel machines in constant time.

Multigrid methods achieve this optimality by employing two complementary processes *smoothing* and *coarse-grid correction*. In the classical setting, the smoother is a simple iterative method like Gauss-Seidel that is effective at reducing high-frequency error. The remaining low-frequency error is then accurately represented and efficiently eliminated on coarser grids via the coarse-grid correction step. Applying this simple multigrid idea to get a scalable method often involves considerable algorithmic research, however. One has to decide which method to use as a smoother, how to coarsen the problem, and how to transfer information between the grids. When designed properly, a multigrid solver will be scalable.

In general, multigrid methods must exploit the character of the near null space of the operator. A near null space vector x is nearly invisible under the action of the operator A , that is $Ax \approx 0$. In the classical setting, these vectors are geometrically smooth (low-frequency), but for applications such as electromagnetics, the near null space is huge ($O(N)$) and geometrically oscillatory. In addition, these problems are often posed on unstructured grids (see figure below). The *algebraic multigrid* (AMG) approach is well suited for addressing these challenges, and is the focus of our research.



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The majority of the AMG algorithms we develop are implemented in *hypre*, a library of parallel preconditioners. Through *hypre*, we have moved much of our earlier multigrid methods research into parallel application codes, impacting such diverse areas as heterogeneous porous-media flow, radiation hydrodynamics, laser plasma interaction, and structural mechanics.

Our main accomplishment this past year concerns the scalable solution of the definite Maxwell's equations. The major difficulty with developing scalable solvers for these equations is the oscillatory, huge near null space. Previous attempts to construct AMG methods have had only partial success.

Our new auxiliary-space Maxwell solver (AMS) is based on our work developing so-called auxiliary mesh preconditioners. The latter is a technique to solve problems on unstructured meshes that exploits available geometric multigrid methods for structured meshes (see Figure 1). One disadvantage of the auxiliary mesh approach is that it requires a re-discretization of the problem on a related uniform mesh.

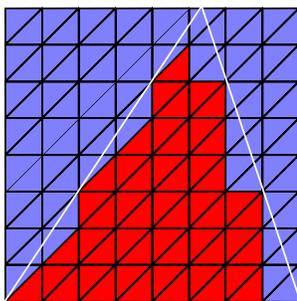


Figure 1. A uniform auxiliary mesh (red) for a triangular domain (white). The unstructured original mesh for the domain is not shown.

A computationally more attractive approach was recently announced by Ralph Hiptmair and Jinchao Xu. Their method borrows the main tool from the auxiliary mesh method,

namely, an interpolation operator that maps functions from a standard conforming finite element space into the respective Nédélec finite element space. The approach does not require re-meshing the domain, but does require explicit knowledge of the curl-free components of the Nédélec space (these are just gradients of an H^1 -conforming scalar finite element space).

Based on our experience with the auxiliary mesh method, our new AMS solver is an improved version of the Hiptmair/Xu solver. AMS is the first provably scalable solver for the definite Maxwell's equations on quasi-uniform unstructured meshes that requires minimal additional information from the user. An illustration of its performance is shown in Figure 2.

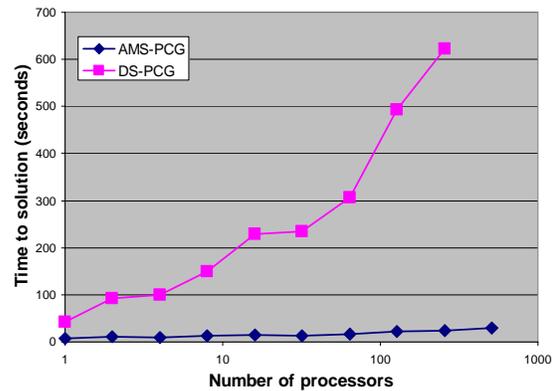


Figure 2. Weak scaling results (105K unknowns per processor) for the AMS preconditioner and diagonally-scaled conjugate gradient (DS-PCG).

Our research was in close collaboration with Tzanio Kolev at LLNL and researchers at Texas A&M and Penn State Universities. See our publications at http://www.llnl.gov/CASC/linear_solvers/.

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