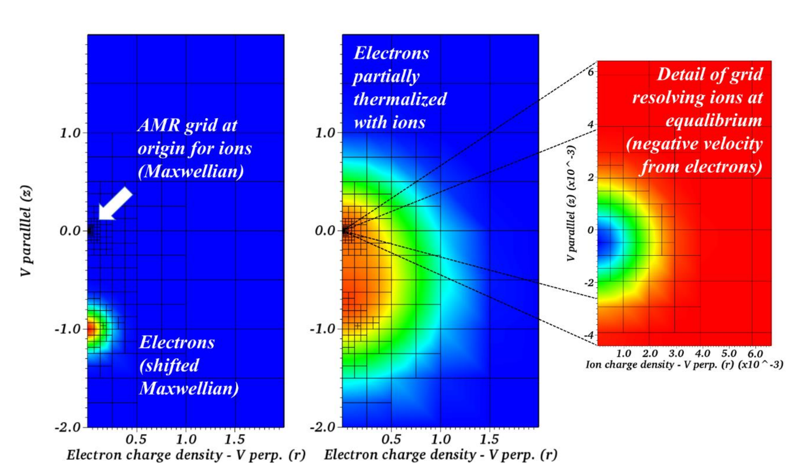
Linear Solver Technologies: Recent Developments

Emerging architectures are forcing the reevaluation of both iterative and direct solvers to ensure continued high performance. At the same time new algorithms need to be developed to solve increasingly complex problems. FASTMath linear solvers include various multilevel methods, with excellent numerical scalability, as well as direct factorization methods capable of solving highly indefinite and ill-conditioned linear systems.

Solver Integrated Tree-based Adaptive Refinement (SITAR) in PETSc

Scientific Achievement

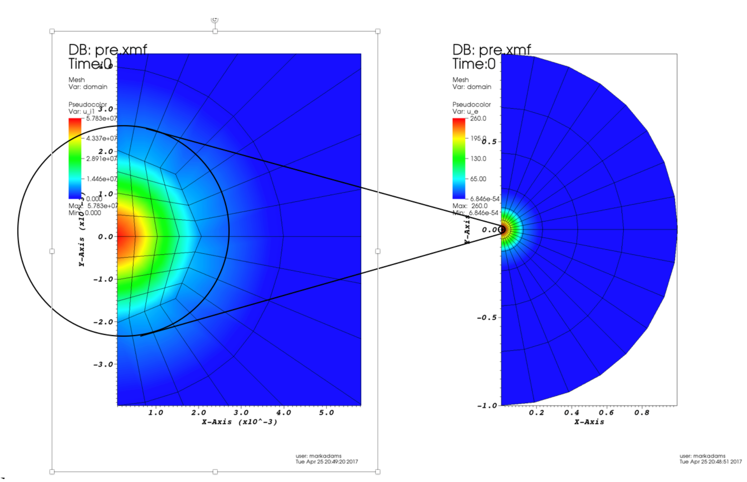
Integrate algebraic solvers with discretizations and mesh management for high value applications.



Research Details

Build on existing algebraic multigrid (AMG) solvers in PETSc. Hybridize with geometric multigrid for speed and matrix-free. Uses *h* and *p* multigrid.

Meta-multigrid, used in 2015 Gordon Bell Prize:
- **matrix-free geometric multigrid (GMG) on finest grids**
- **Nonlinear FAS multigrid**
- **P refinement**
- **H refinement**
- **GMG with algebraic, Galerkin, coarse grids,**
- **Full AMG on coarsest grids**



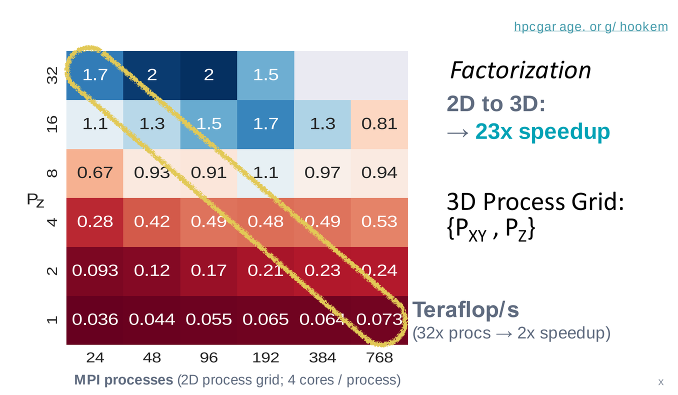
Integrate solver with PETSc's new FE, FV and DG support, and with new adaptivity support for semi-structured (top) and unstructured (bottom) mesh adaptivity.

Contact: Mark Adams

SuperLU: Direct Solver for Sparse Linear Systems

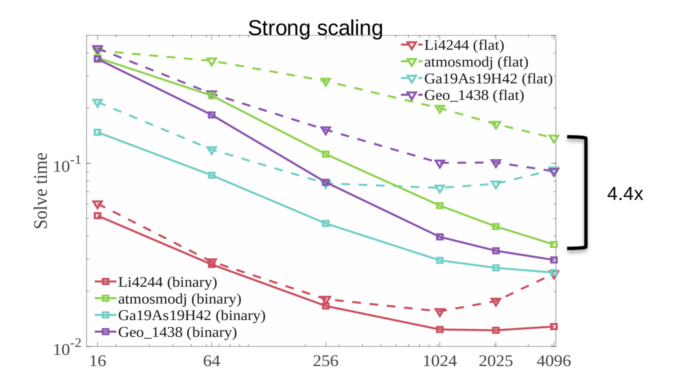
Scientific Achievement

Developed new parallelization strategies that reduce communication. Exposed task parallelism and vectorization for irregular loops involving sparse indirect addressing to better use on-node resources.



Significance and Impact

Sparse factorization is a critical solution technology for highly indefinite and ill-conditioned sparse linear systems and widely used in accelerator engineering, chemical science, earth science, fusion and materials science



Triangular solution, 4 sparse matrices, compared to baseline algorithm

Research Details

Developed a novel communication-avoiding factorization algorithm using 3D process grid, trading off memory for reduced communication and increased parallelism. Demonstrated 27x improvement and strong scaling to 24,000+ cores. Developed asynchronous tree-based algorithms for collective communication, reducing synchronization cost and communication hotspot in triangular solution. Demonstrated 6x improvement and unprecedented strong scaling to 4000+ cores.

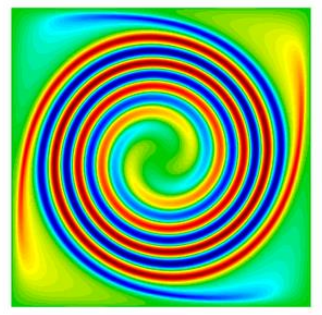
Contact: Sherry Li

This research was funded by ECP

A New AMG Method for Nonsymmetric Systems in *hypre*

Scientific Achievement

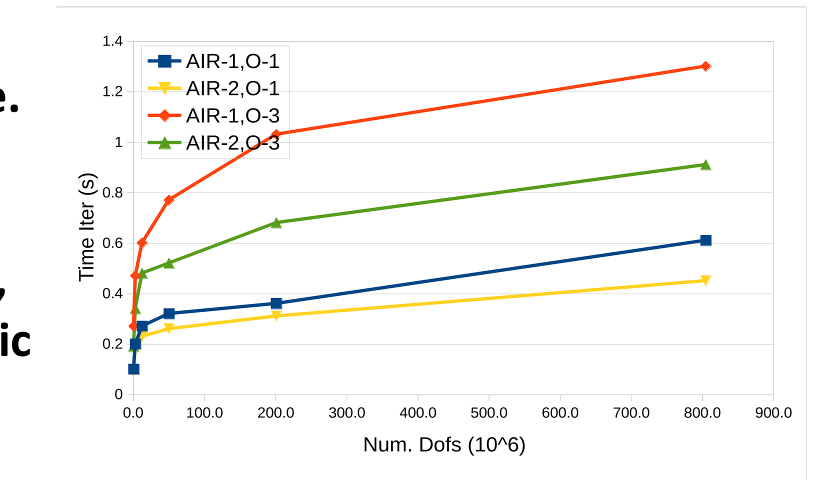
Developed new algebraic multigrid method, pAIR (parallel Approximate Ideal Restrictions), capable of solving highly non-symmetric problems that conventional AMG methods are unable to solve or only solve poorly; integrated the new methods in hypre.



Using pAIR to solve nonsymmetric linear systems from a time-dependent advection equation (solution pictured), discretized by DG (order 1 and 3) using MFEM.

Significance and Impact

Nonsymmetric advection dominated problems, occurring e.g. in transport, often present a challenge for algebraic multigrid methods. The new AMG method enables significantly faster solution.



Weak scalability (up to 16384 cores) of pAIR (with AMG restriction distance 1 and 2) for DG advection problem. Standard AMG, if combined with GMRES, can only solve the two smallest problems, but is much (~4x,~8x) slower.

Research Details

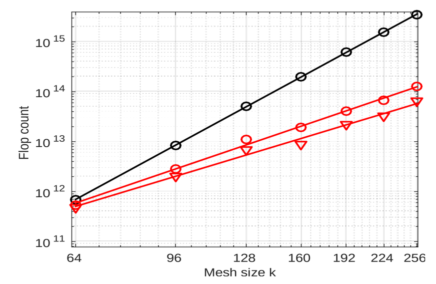
pAIR is a localized multigrid reduction method that approximates the ideal restriction from a local neighborhood and uses a low-complexity interpolation. It has been implemented in hypre and tested on various nonsymmetric problems, leading to significant speedups and solving some problems that could not be solved with AMG before.

Contact: Ruipeng Li

STRUMPACK Solver and Preconditioner for Sparse Linear Systems

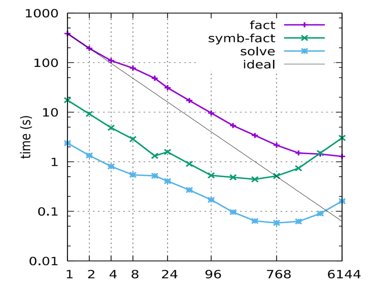
Scientific Achievement

Developed low-rank approximate factorization algorithms that have quasi-linear arithmetic and communication complexity in problem size. Developed new parallelization for irregular computations involving sparse data structures.



Scaling with mesh size for Helmholtz.

black: direct solve)O(N^(3/2).
red: HSS



Strong scale to 6000+ cores for unstructured mesh (Flan1565) on NERSC Cori Haswell.

Significance and Impact

Factorization based preconditioning is critical for many extreme-scale multiphysics and multiscale simulation codes involving highly indefinite and ill-conditioned sparse linear systems.

Research Details

Developed a new randomized sampling method for low-rank HSS matrix construction, which is used in a new matrix-free dense factorization and a fully structured HSS-embedded sparse multifrontal factorization. Developed new stopping criteria to stabilize the adaptive randomized sampling for low-rank detection. This ensures sufficient samples to achieve accuracy, but not too many samples to degrade performance.

Contact: Pieter Ghysels

This research was funded by ECP

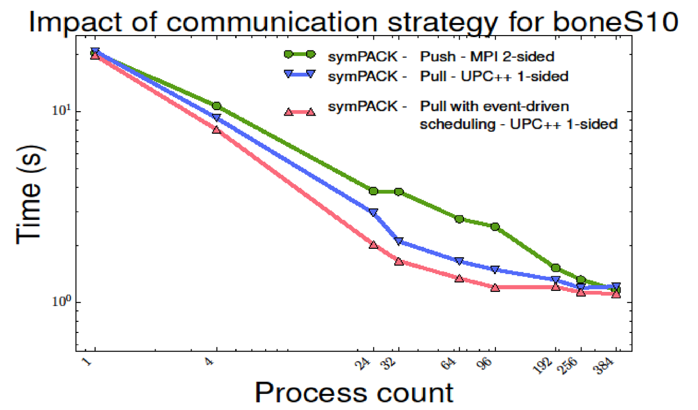
Improved Performance and Scalability of symPACK

Scientific Achievement

Improved performance of symPACK, a software package for sparse symmetric linear systems through new communication strategies.

Significance and Impact

Sparse symmetric systems occur in many applications. Integration of symPACK into the electronic structure calculation code PEXSI led to reduced compute and storage cost and improved overall computation time.



Strong scalability of symPACK using various Communication strategies on NERSC Edison

Research Details

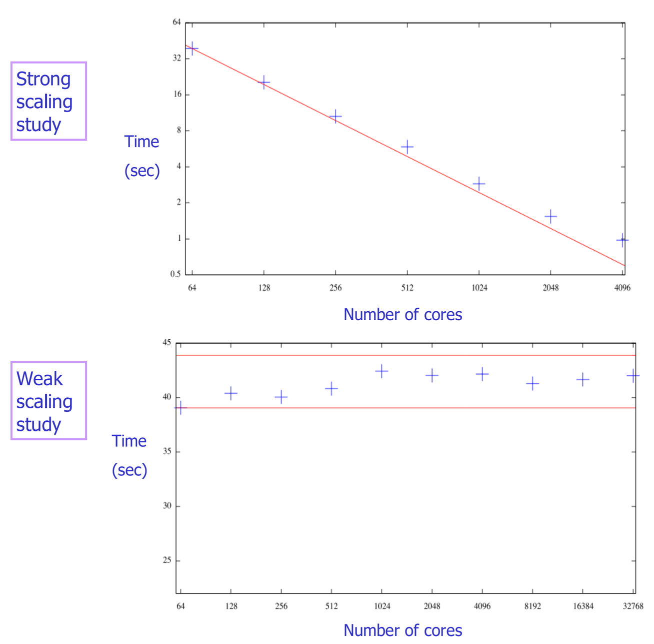
The original MPI two-sided communication in symPACK was replaced with UPC++ for asynchronous remote function calls, one-sided communication and event-driven scheduling, leading to more efficient communication and overall better scalability

Contact: Mathias Jacqelin

A Low Communication Method to Solve Poisson's Equation

Scientific Achievement

A new algorithm and high-performance implementation for solving Poisson's equation with free-space boundary conditions has 1/10 the communication cost of previous methods.



Significance and Impact:

The method will enable multiscale simulations in fluid dynamics, astrophysics, and plasma physics on exascale computers.

Research Details:

The present method is based on a new representation of the nonlocal coupling that leads to communication costs corresponding to a single iterations of multigrid. The computational kernels are multidimensional Fast Fourier Transforms on small domains, which can be implemented efficiently on current and emerging HPC node architectures.

Contact: Peter McCorquodale

Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-POST-755480

More Information: http://www.fastmath-scidac.org or contact Ulrike Yang, LLNL, yang11@llnl.gov, 925-422-2850

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