MueLu: Multigrid Framework for Advanced Architectures

SAND 2015-1808 C

FASTMath Team Members: Andrey Prokopenko (SNL), Jonathan Hu (SNL)

MueLu is a multigrid library in Sandia's Trilinos project and is designed to be flexible, easily extensible, and efficient on emerging architectures.

Design overview

MueLu is a multigrid solver library in the Sandia Trilinos project. MueLu is a part of the templated solver stack that is based upon Kokkos (intra-node parallelism) and Tpetra (inter-node parallelism).

- Aggregation-based algebraic multigrid algorithms (AMG) for Poisson, elasticity, convection-diffusion, Maxwell
- Design facilitates new algorithm development
- Scalar, local/global ordinals, and node template types. Permits architecture-specific algorithms & optimizations

https://trilinos.org

Reuse

Transient simulations may become prohibitively expensive due to a large number of time steps (10^4 or 10^5). In many cases, most of the time is spent in multigrid setup. Our research concentrates on reusing components of existing hierarchy for consecutive setups, particularly for the same mesh connectivity structure.

For instance, one can:

- Recompute only fine level smoother
- Reuse all prolongators and restrictors
- Reuse only tentative prolongator

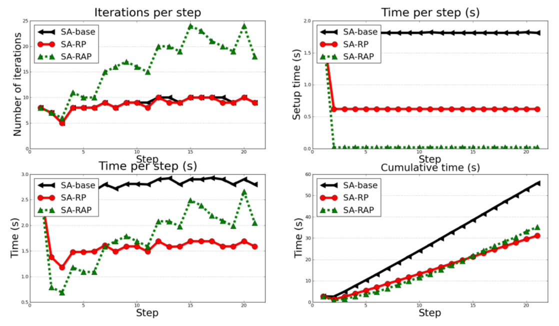


Fig 1: Impact of setup reuse on ice sheet simulation problem

AMG for Mixed Discretizations

A Q2-Q1 mixed FE discretization of the incompressible Navier-Stokes equations satisfies a discrete inf-sup condition. Standard AMG methods do not maintain this relationship. Energy minimizing multigrid methods (EMIN-AMG) provide flexibility in transfer sparsity patterns, which allows to maintain certain relationships between coarse pressures and velocities.

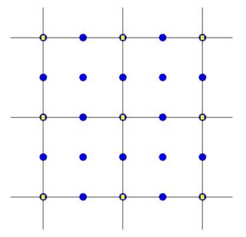


Fig 2: Q2-Q1 interpolation with collocated velocities

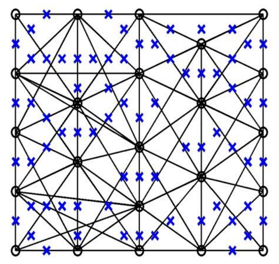


Fig 3: Automatically coarsened 17x17 mesh

Table 1: Convergence of EMIN-AMG with Vanka smoother on a model Stokes problem

DOF	Iterations	Complexity
659	20	2.01
2,467	25	1.81
37,607	27	1.85
592,387	28	1.91

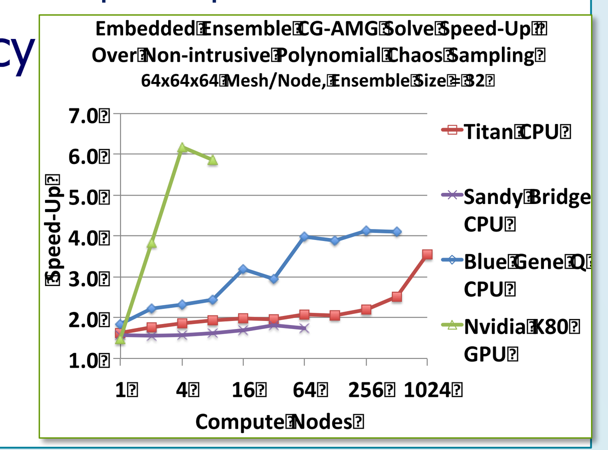
AMG in Uncertainty Quantification

Stokhos: embedded UQ methods

(E. Phipps, H.C. Edwards, J. Hu, M. D'Elia)

- Via *ensembles*, propagate *m* samples – block diagonal (nonlinear system)
- By commuting Kronecker products, each sample-dependent scalar can be replaced by length *m* array
  - ✓ Reuse non-sample dependent data
  - ✓ Amortize sparse communication latency
  - ✓ Amortize sparse access latency
  - ✓ Natural mapping to vector arithmetic
- Through templating, MueLu can be applied directly to ensemble system.

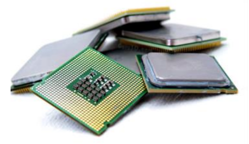
Fig 4: Embedded ensemble speed-up



A path to performance portability

MueLu heavily relies on two Trilinos libraries: **Kokkos**, and **Tpetra**.

- Kokkos provides a general node-level performance portable **programming model** across manycore devices (multicore CPU, NVidia GPU, Intel Xeon Phi). Kokkos introduces *Execution space* (where computational kernels are executed) and *Memory space* (where computational kernels' data is residing).
- Tpetra provides distributed sparse linear algebra kernels utilizing Kokkos for compute node performance.



Stokhos has demonstrated the benefit of the Tpetra/Kokkos SPMV for AMG solves. MueLu setup kernels are more varied and specialized (e.g., SPGEMM, MIS). Injecting Kokkos into these kernels will require porting and perhaps refactoring these algorithms.

1. Gaidamour et al, "Design considerations for a flexible multigrid preconditioning library", Scientific Programming, 20(3), 2012.
2. Lin et al, "Towards extreme-scale simulations for low Mach fluids with second-generation Trilinos", Parallel Process. Lett., 24(4), 2014.
3. Pawlowski et al, "Drekar:: cfd-a turbulent fluid-flow and conjugate heat transfer code: Theory manual version 1.0", SNL Techreport SAND2012-2697, 2012.
4. Phipps, "Embedded Uncertainty Quantification Methods via Stokhos", Handbook of Uncertainty, 2015 (to appear).

Application impact: MHD simulations

Drekar

(J. Shadid, R. Pawlowski, E. Cyr, T. Smith, T. Wildey)

Drekar is a scalable parallel implicit FE code for coupled physics (Navier-Stokes, MHD, LES, RANS). It relies on MueLu to provide the fully-coupled multigrid for solving monolithic systems.

By using the templated Trilinos solver stack, Drekar is now capable of performing significantly more detailed simulations.

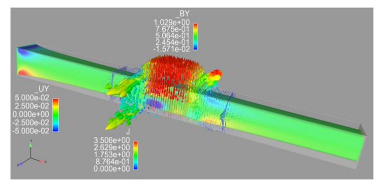


Fig 5: Steady-state 3D MHD generator (stabilized FE; fully-coupled multigrid preconditioned Newton-Krylov solve)

Table 2: Preliminary weak scaling for a steady MHD generator linear solve (P. Lin).

MPI tasks	unknowns	iter/Newt	Solve time/Newt(s)
128	845,000	17.4	4.11
1024	6,473,096	21.6	5.31
8192	50,658,056	31	7.89
65,536	400,799,240	53.3	14.2
524,288	3,188,616,200	104.8	29.8

Application impact: low Mach simulations

Nalu

(S. Domino)

Nalu is a generalized unstructured massively parallel low Mach flow code that uses MueLu and other Trilinos libraries for its solver needs. Nalu provides critical real-world performance tracking to identify/quantify performance bottlenecks. MueLu and new Trilinos stack provide the capability to run large simulations, such as 9 billion element fluid flow large eddy simulation (LES) problem on unstructured meshes with a 27 billion row matrix on 524,288 cores of an IBM Blue Gene/Q platform.

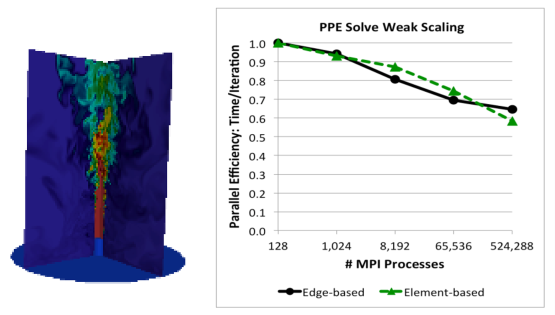


Fig 6: Pressure solve weak scaling for open-jet problem (P. Lin)

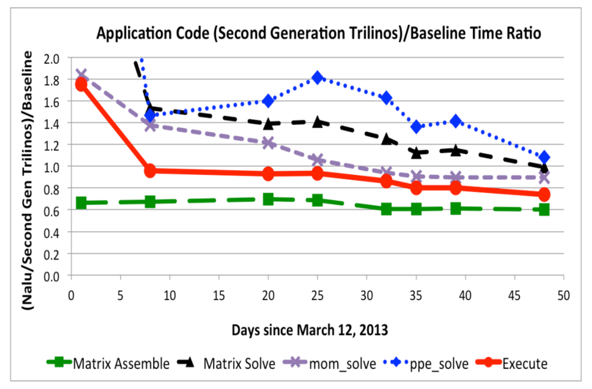


Fig 7: Tracking Nalu component performance over time (P. Lin)

Future Plans

- Continue research into multigrid algorithms exploiting mesh structure, *e.g.* coupling of unstructured and structured problems
- Investigate new multigrid algorithms for mixed discretizations
- Explore reducing setup cost through advanced reuse techniques
- Continue conversion of setup kernels to use Kokkos

More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

SciDAC Scientific Discovery through Advanced Computing