Algebraic Solvers in FASTMath

Argonne Training Program on Extreme-Scale Computing
August 2016



Algebraic Solvers in FASTMath

- HYPRE – see detailed presentation
- PARPACK
- PETSc – see detailed presentation
- SUNDIALS – see detailed presentation
- SuperLU, STRUMPACK – see detailed presesntation
- Trilinos-ML,NOX

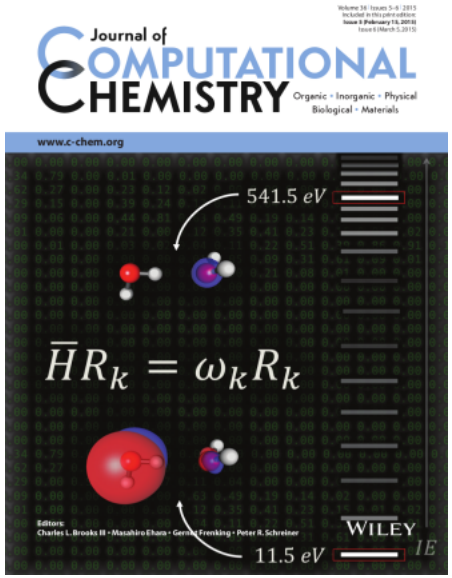
PARPACK

- **Capabilities:**
  - Compute a few eigenpairs of a Hermitian and non-Hermitian matrix
  - Both standard and generalized eigenvalues
  - Extremal and interior eigenvalues
  - Reverse communication allows easy integration with application
  - MPI/BLACS communication
- **Download:**

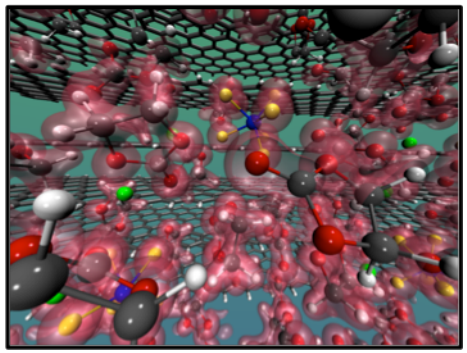
  http://www.caam.rice.edu/software/ARPACK/

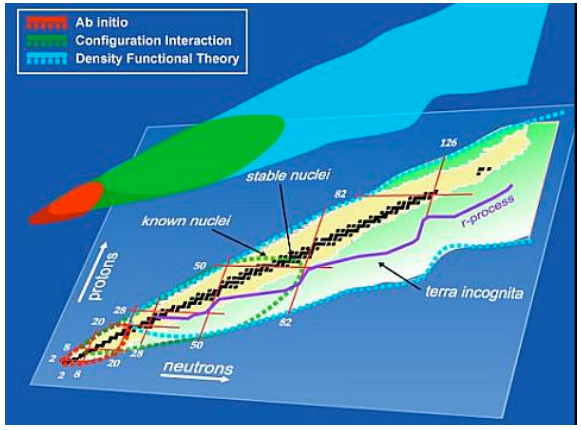
Applications

- Computational chemistry and materials science
  - Density functional theory based calculation
  - Excited states calculationed based on one and two-particle Green's function formalism
  - Many-body wavefunction methods (configuration interaction, coupled cluster equation-of-motion), MCSCF
- Nuclear physics
  - Nuclear CI calculation
- Accelerator cavity modeling



Li-ion battery simulation





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New Development

- **PPCG** (Projected Preconditioned Conjugate Gradient) method for symmetric eigenvalue problems with reduced Rayleigh-Ritz cost
- **RLOBPCG** (A robust implementation of the locally optimal block preconditioned conjugate gradient algorithm)
- **GPLHR** (Generalized Preconditioned Local Harmonic Ritz) method for interior eigenvalues of a non-Hermitian sparse matrix
- **pEVSL** (parallel eigenvalue slicing) spectrum slicing technique for computing a relatively large number of eigenpairs of a Hermitian matrix
- **BSEPACK** Structure preserving eigensolver for linear response eigenvalue problems of the form

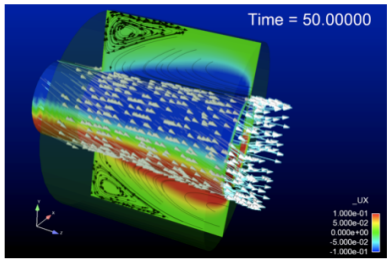
$$(■A\&B@-B\ \&-A\ )(■x@y\ )=\lambda(■x@y\ ),\ A=A\uparrow H\ ,\ B=B\uparrow T$$

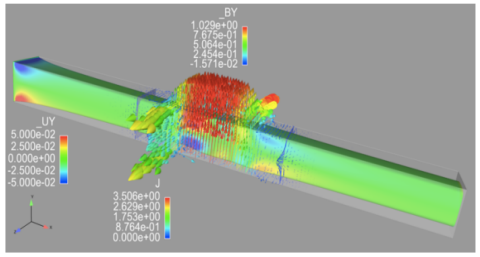
ML and MueLu: Multigrid Libraries in Trilinos

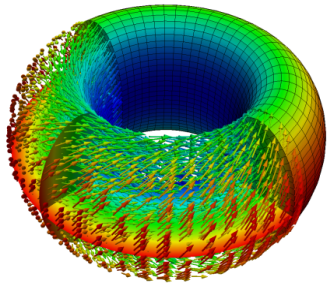
- **ML: aggregation-based algebraic multigrid algorithms**
  - Support for scalar problems (diffusion, convection-diffusion), PDE systems (elasticity), electromagnetic problems (eddy current)
  - Various coarsening and data rebalancing options
  - Smoothers (SOR, polynomial, ILU, block variants, line, user-provided)
  - Written in C
- **MueLu: templated multigrid framework**
  - Support for energy minimizing multigrid algorithms in addition to many algorithms from ML
  - Leverages Trilinos templated sparse linear algebra stack
    - Optimized kernels for multiple architectures (GPU, OpenMP, Xeon Phi)
    - Templated scalar type allowing mixed precision, UQ, …
  - Advanced data reuse possibilities, extensible by design
  - Written in C++
- **Download/further information:** www.trilinos.org

ML and MueLu: Application Highlights

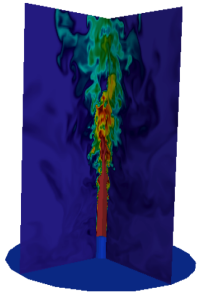
- **Magnetohydrodynamics (Drekar)**
  ML scales to 512K cores on BG/Q and to 128K cores on Titan

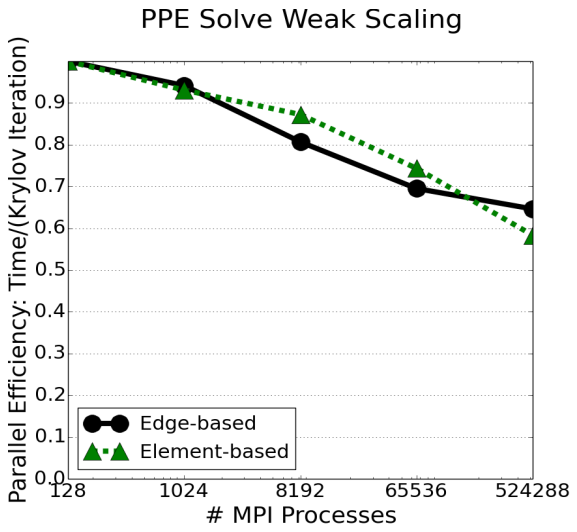






- **Fluid dynamics (Nalu)**
  MueLu scales to 524K cores of BG/Q



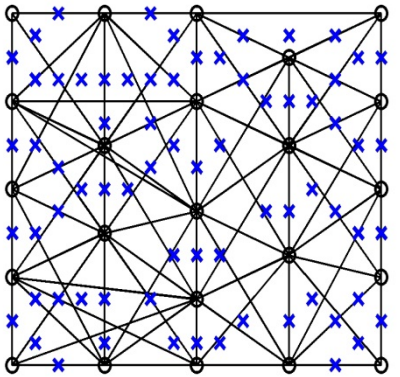


MueLu: Research Framework

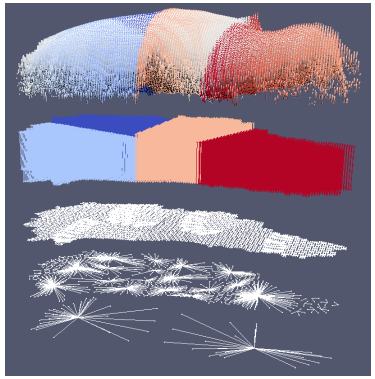
- **Component reuse** in multigrid can be effective in reducing setup costs while maintaining solver convergence. We have demonstrated that reuse can yield 2.5x speedup on 25K cores of Cray XE6.

- **Block systems** arise naturally in mixed discretizations. Our new multigrid algorithm preserves such block structure on coarse levels for Stokes and Navier-Stokes systems.

- MueLu/ML provide a specialized AMG for **PISCEES** project through **semi-coarsening** and **line smoothers** that exploit partial structure in meshes arising in ice sheet modeling.



Automatically generated coarse mesh for Q2-Q1 discretization of a Stokes system



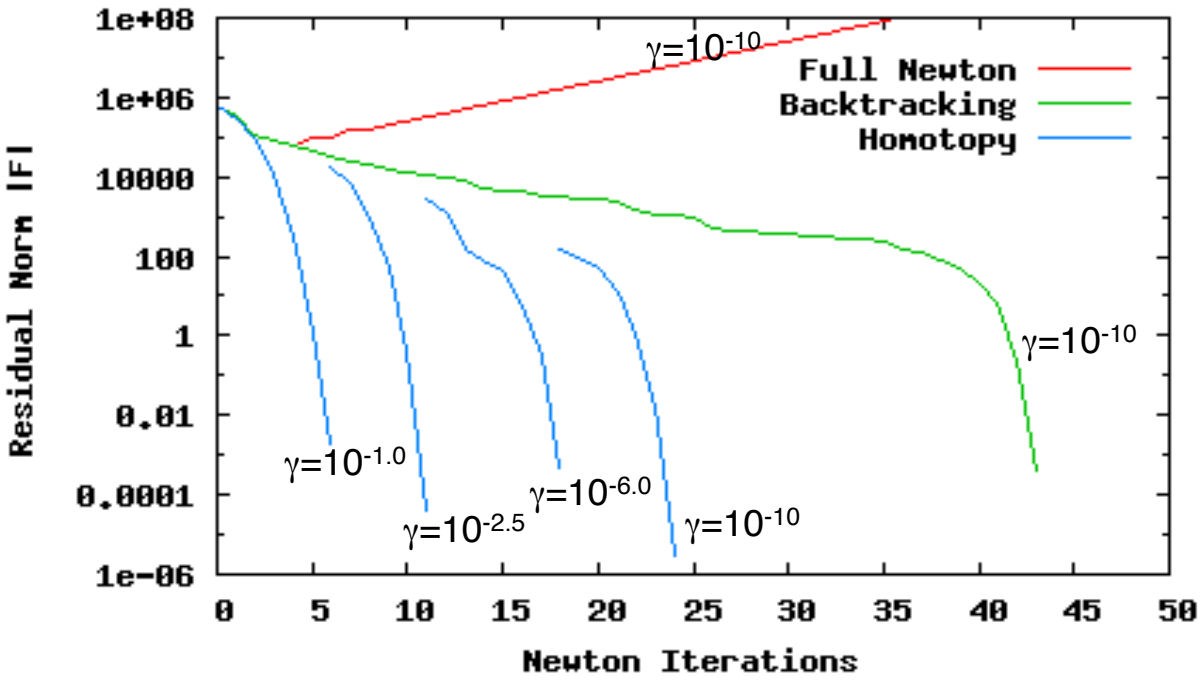
Semicoarsening followed by regular 2D coarsening for Greenland model.

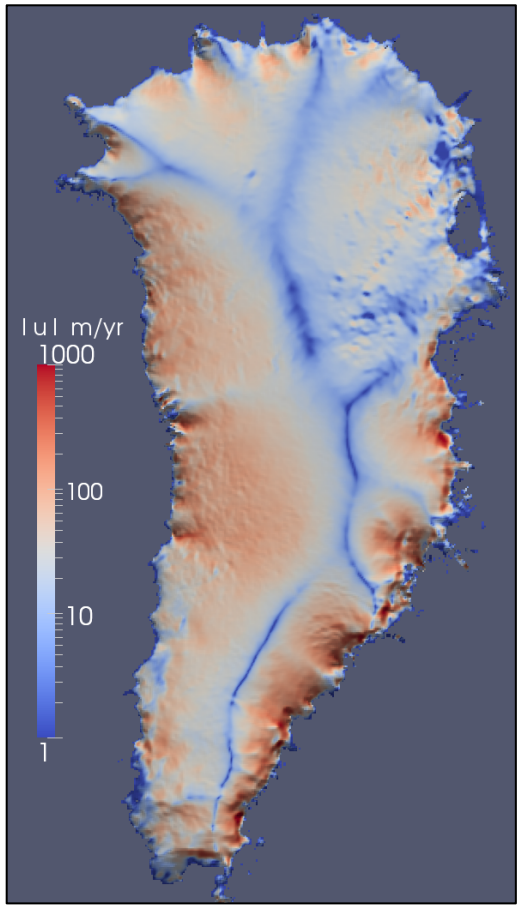
Trilinos/NOX Nonlinear Solver

- **Capabilities:**
  - Newton-Based Nonlinear Solver
    - Linked to Trilinos linear solvers for scalability
    - Matrix-Free option
  - Anderson Acceleration for Fixed-Point iterations
  - Globalizations for improved robustness
    - Line Searches, Trust Region, Homotopy methods
  - Customizable: C++ abstractions at every level
  - Extended by LOCA package
    - Parameter continuation, Stability analysis, Bifurcation tracking
- **Download: Part of Trilinos (trilinos.sandia.gov)**
- **Further information: Andy Salinger [agsalin@sandia.gov]**

Trilinos/NOX: Robustness for Ice Sheet Simulation:
PISCEES SciDAC Application project (BER-ASCR)

- Ice Sheets modeled by nonlinear Stokes's equation
  - Initial solve is fragile: Full Newton fails
  - Homotopy continuation on regularization parameter "γ" saves the day





Greenland Ice Sheet
Surface Velocities
(constant friction model)

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NOX and ML are part of larger Trilinos solver stack: Linear solvers, Equations solvers, Analysis tools