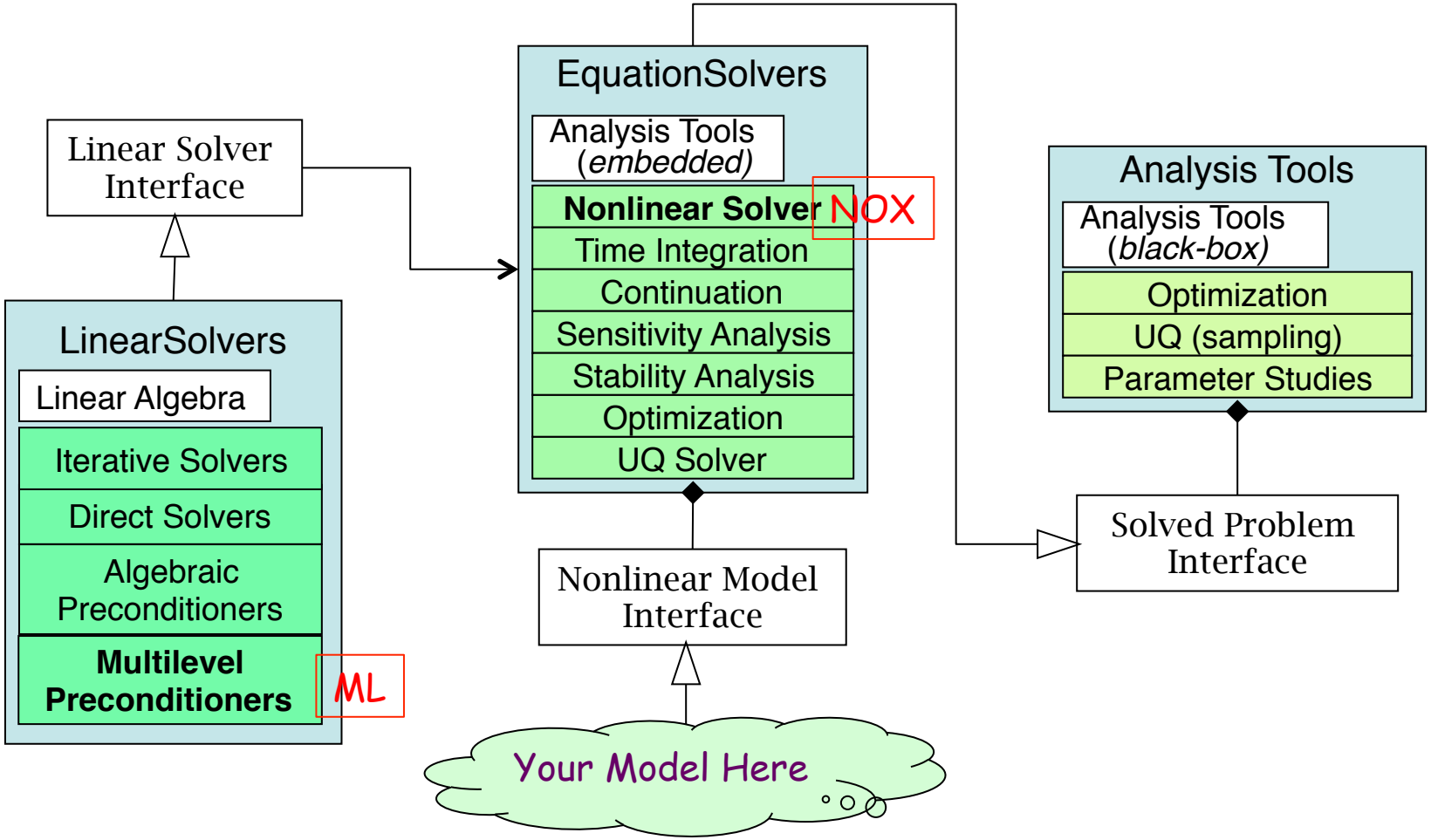
Trilinos/NOX Nonlinear Solver

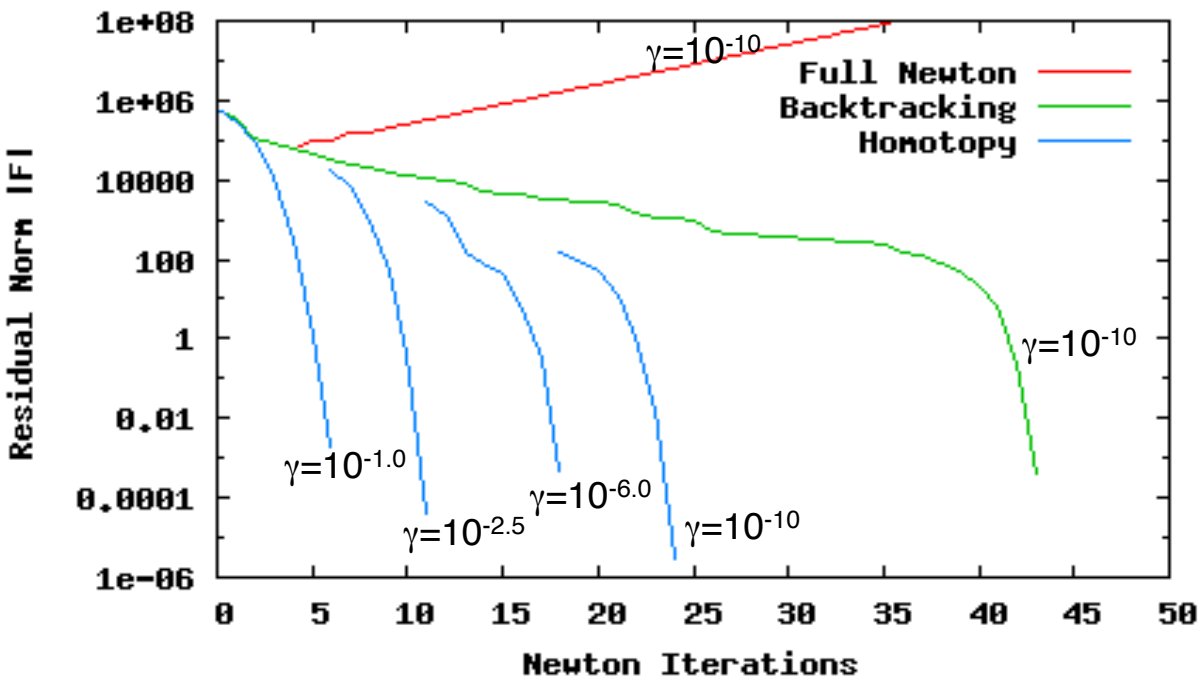
- **Capabilities:**
  - Newton-Based Nonlinear Solver
    - Linked to Trilinos linear solvers for scalability
    - Matrix-Free option
  - Anderson Acceleration for Fixed-Point iterations
  - Globalizations for improved robustness
    - Line Searches, Trust Region, Homotopy methods
  - Customizable: 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]**

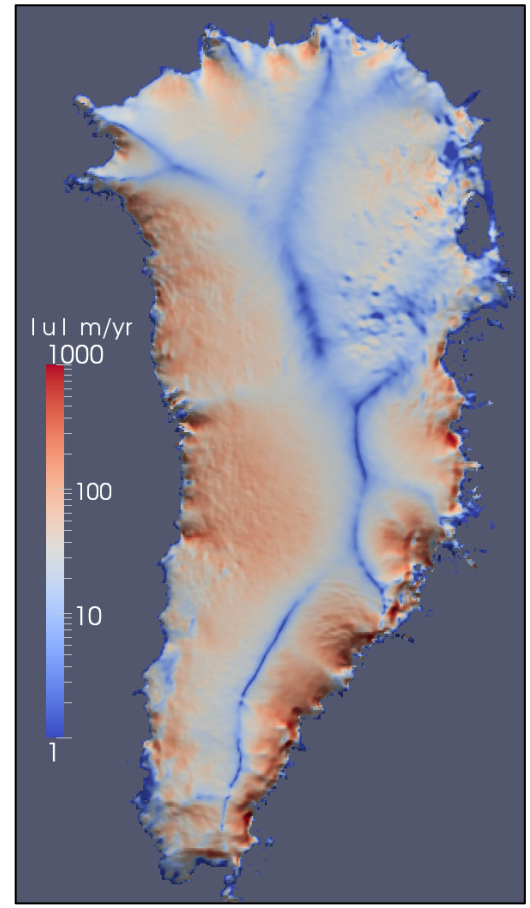
NOX and ML are part of larger Trilinos solver stack: Linear solvers, Equations solvers, Analysis tools



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)

Multigrid in Trilinos

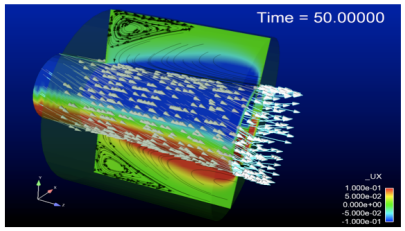
- **ML: algebraic multigrid (AMG)**
  - Aggregation-based AMG for
    - Poisson, elasticity, convection-diffusion, eddy current (E&M)
  - Various coarsening and data rebalancing options
  - Smoothers: SOR, polynomial, ILU, block variants, user-provided

- **MueLu: templated multigrid framework**
  - Same main algorithms as above, plus energy minimizing AMG
  - Leverages Trilinos templated sparse linear algebra stack
    - Can use kernels optimized for various compute node types
    - Templated scalar type allows for mixed precision, UQ, …
  - Advanced data reuse possibilities, extensible by design

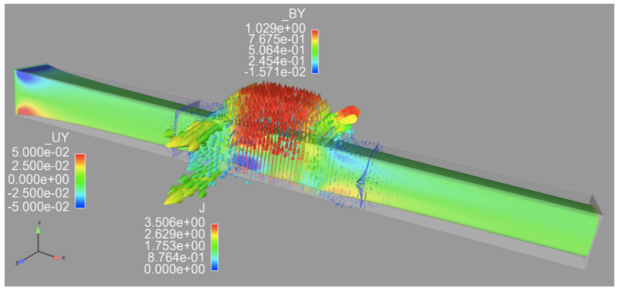
- **Download/further information:** www.trilinos.org

ML and MueLu: Application highlights

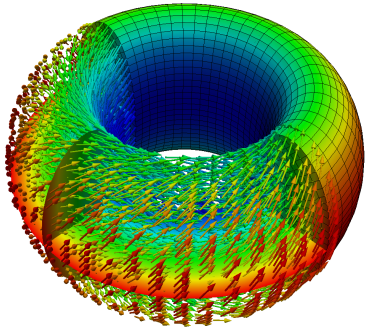
ML scales up to 512K BG/Q & 128K Titan cores in Drekar simulations



SARANS turbulence*

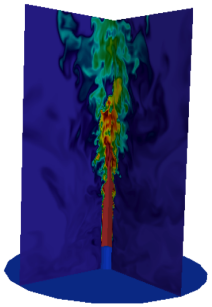


MHD generator*



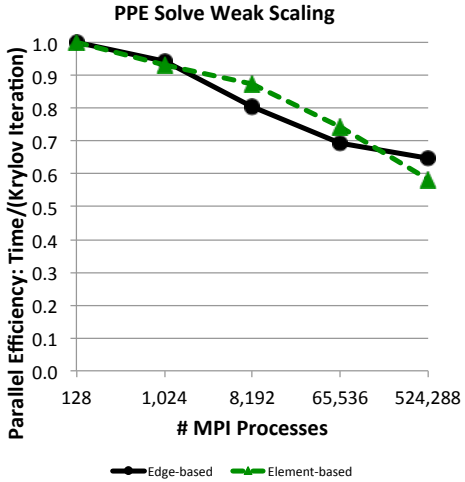
Tokamak*

*courtesy E. Cyr/SNL



Turbulent OpenJet (Re=6600)
(courtesy P. Lin/SNL)

MueLu scales up to 524K BG/Q cores in Sierra/Nalu simulations



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:**

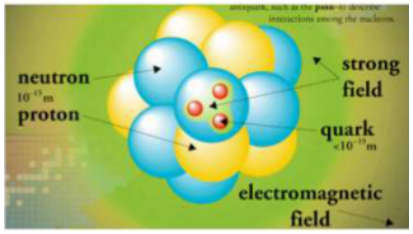
  http://www.caam.rice.edu/software/ARPACK/
- **Further information:** beyond PARPACK
  - EIGPEN (based on penalty trace minimization for computing many eigenpairs)
  - Parallel multiple shift-invert interface for computing many eigenpairs

PARPACK

- Hybrid MPI/OpenMP implementation
- MATLAB interface available (eigs)

MFDn: Nuclear Configuration Interaction Calculation

- MFDn (Many-body Fermion Dynamics for nuclear physics) is the most robust and efficient configuration interaction code for studying nuclear structure
- Solve the nuclear $\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) \;=\; \lambda\,\Psi(r_1,\ldots,r_A)$



$$\hat{\mathbf{H}} \;=\; \frac{m}{2\,A}\sum_{i<j}\left(\vec{v}_i-\vec{v}_j\right)^2+\sum_{i<j}V_{ij}+\sum_{i<j<k}V_{ijk}+\ldots$$

- PARPACK allows low excitation states to be extracted from a low dimensional Krylov subspace