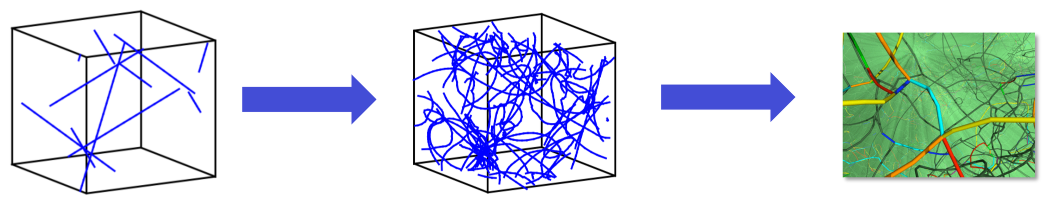
Impact of FASTMath Solver Technologies on Scientific Applications

Linear, nonlinear, and eigenvalue solvers are at the heart of many scientific applications. FASTMath is developing and deploying state-of-the-art solver and time integration technologies that lead to significant performance improvements in application codes and enable scientific discoveries at scale

ParaDiS: Parallel Dislocation Dynamics

A. Arsenlis, S. Aubry, G. Hommes, C. Woodward (LLNL); D. Gardner, D. Reynolds (SMU)

ParaDiS is a massively PARAllel Dislocation Simulator. It models strain hardening by simulating the collective motion and interactions of dislocations. Each dislocation line defect is discretized into segments ended by nodes where forces, velocities, positions, and topological operations are calculated. In particular, positions are obtained by time-integrating the velocities of dislocation nodes. A limiting factor to computational efficiency within ParaDiS is the need to integrate stiff systems in time with expensive force calculations. ***We are working to incorporate faster solvers and higher order time integrators.***



Simulations start with a small number of segments. Dislocation segments multiply under increasing loading, eventually colliding, joining, and separating. Problem configurations grow quickly and change rapidly during a run.

We accelerate the native fixed point solver with Andersen Acceleration (AA) implemented in the SUNDIALS suite of nonlinear solvers and time integrators.

Initialize $x^{(0)}$

For $k = 0, 1, \ldots,$ until $\left\| x^{(k)} - G(x^{(k)}) \right\| < \tau$

  Set $x^{(k+1)} = G(x^{(k)})$

end

Set $m^{(k)} = \min\{m, k\}$

Set $F^{(k)} = (f^{(k-m^{(k)})}, \ldots, f^{(k)})$, where $f^{(i)} = G(x^{(i)}) - x^{(i)}$

Solve $\min_\alpha \left\| F^{(k)} \alpha \right\|_2 \; s.t. \sum_{i=0}^{m^{(k)}} \alpha_i = 1$

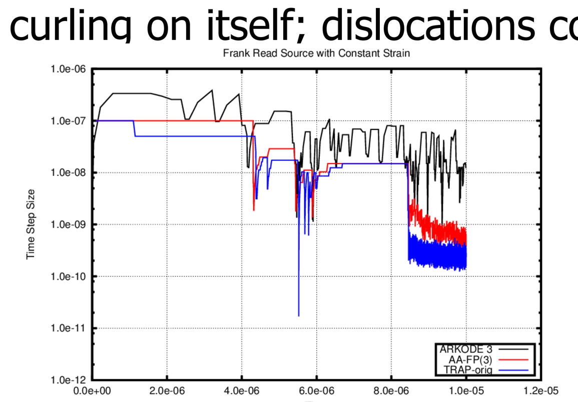
Set $x^{(k)} = \sum_{i=0}^{m^{(k)}} \alpha_i^{(k)} G(x^{(k-m^{(k)}+i)})$

Solve least square problem to find minimal residual over prior iterates

We are testing higher order implicit Runge-Kutta integrators through the ARKODE package in SUNDIALS.

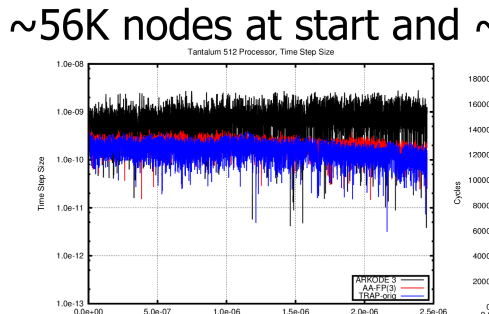
Frank-Read source: Single segment curling on itself; dislocations collide and merge

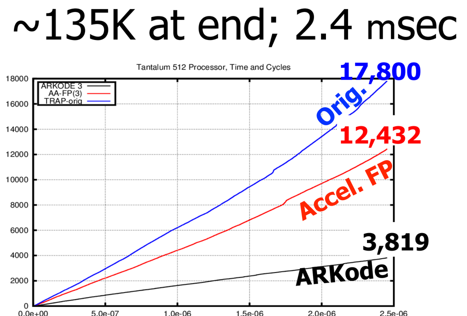
Method	# Steps	Time (s)	SpeedUp
Original (2)	6,284	1,118	-----
Original (3)	4,990	895	20%
AA (2 , m=1)	6,447	1,177	-5%
AA (3 , m=2)	2,359	436	61%
ARKODE 3	257	74	93%
ARK3(3,m=2)	273	61	95%
ARKODE 5	280	92	92%



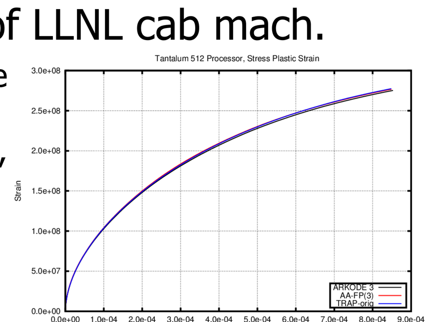
The higher order integrator allows for significantly larger time steps providing large benefits in run time

Tantalum single crystal BCC, 4.25 mm^3 cube; constant strain of 1,000/s along x-dir.; ~56K nodes at start and ~135K at end; 2.4 msec on 512 cores of LLNL cab mach.





Solutions with the new solvers give similar properties, as seen with the stress Plastic strain curve here.



On this more complex test, the accelerated fixed point solver shows definite gains even with a single saved residual. The new integrators provide substantially larger time steps, but each step now requires multiple nonlinear solves.

These results use a finite difference Newton-Krylov nonlinear solver and no preconditioning for the stage solves. Continuing work is in tuning integrator parameters and developing an analytic Jacobian and an effective preconditioner.

Method	# Steps	Run Time (s)	SpeedUp
Original	17,800	6,030	-----
AA (2its, m=1)	17,126	5,550	8%
AA (3its, m=2)	12,432	4,678	22%
ARKODE ord. 3	3,819	12,644	-110%
ARKODE ord. 5	3,716	20,231	-235%

Preliminary results

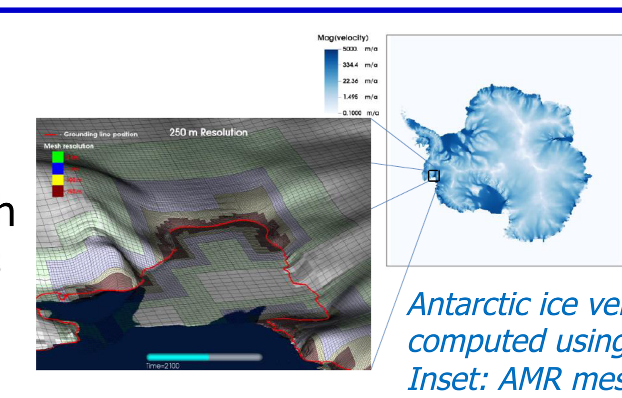
PISCEES Ice Sheet Modeling

S. Price (LANL); M. Adams, D. Martin, E.G. Ng (LBNL); S. Cornford (Bristol), I. Kalashnikova, M. Perego, A. Salinger, R. Tuminaro (SNL); P. Worley (ORNL)

- The Greenland and Antarctic ice sheets are expected to be dominant contributors to 21st-century sea-level rise, and could affect other parts of the climate system through increased freshwater discharge to high-latitude oceans.
- **PISCEES** (Predicting Ice Sheet and Climate Evolution at Extreme Scales) is a BER/ASCR SciDAC Application Partnership focusing on developing the next generation of ice sheet models (see other PISCEES-related posters in this session).
- Development of 2 ice-sheet dynamical cores:
  - **BISICLES**: a finite-volume block-structured AMR dycore built on the FASTMath-supported Chombo framework,
  - **FELIX**: a finite-element unstructured-mesh dycore which uses the FASTMath-supported Trilinos libraries.
- Largest computational expense: Solving a coupled nonlinear elliptic system for the ice velocity field, making PISCEES a natural FASTMath solver customer.

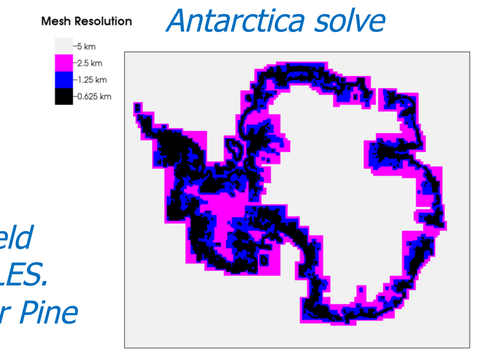
BISICLES:

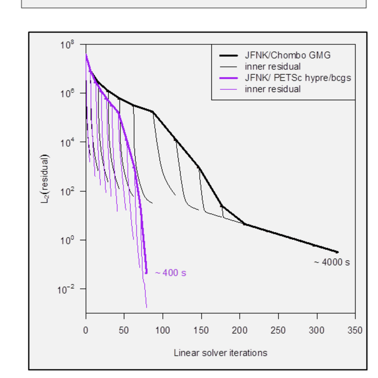
- Parallel, scalable, block-adaptive mesh refinement resolves the *grounding line* (Ice/Land/Ocean interface).
- Block-structured AMR results in complicated discretization stencils at coarse-fine interfaces.
- Native Chombo GMG solvers stall on many realistic problems due to large variations in coefficients.
- Collaboration with FASTMath's Mark Adams enabled coupling to PETSc and access to robust and efficient GAMG solvers.
- **Time-to-solution reduced by 1 order of magnitude.**



Antarctic ice velocity field computed using BISICLES. Inset: AMR meshing for Pine Island Glacier. Grounding line shown in red.

Below: Mesh resolution for Antarctica solve

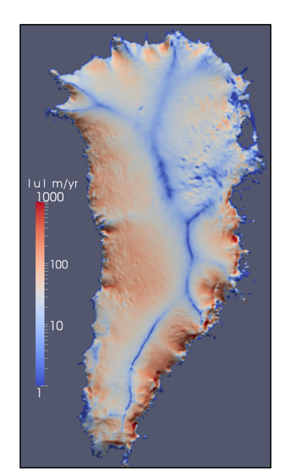


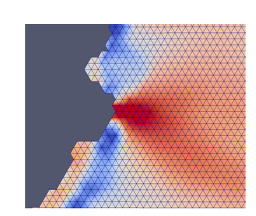


Above: solver performance for Antarctica velocity solve

FELIX:

- FASTMath Trilinos solver libraries enabled development of parallel and robust implicit 3D unstructured-grid finite element PDE code born with advanced analysis tools, all in 1 FTE time, including verification.
- 2km Greenland grid (182M dofs), steady-state solve requires less than 1 minute on 9,600 cores thanks to:
  - Scalable linear solver with algebraic multigrid preconditioner (Trilinos: Belos, ML),
  - Robust nonlinear solver with homotopy continuation (Trilinos: NOX, LOCA).

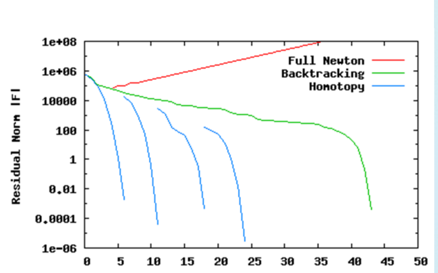




Above: detail of tetrahedral FEM mesh.

Left: Greenland test problem computed ice velocity.

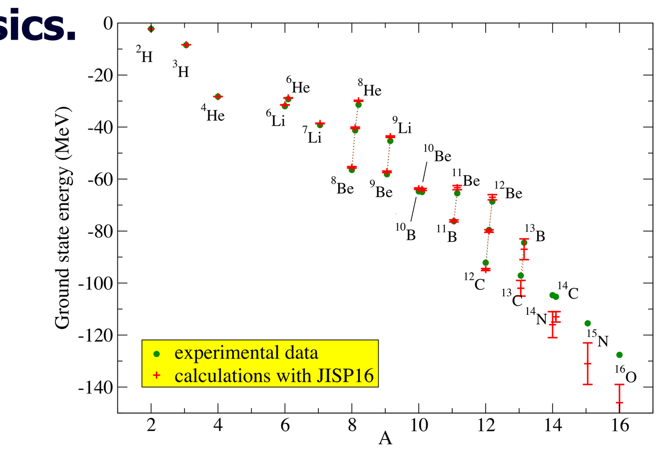
Right: Nonlinear solver performance for Greenland test problem. Increased robustness and efficiency with novel homotopy continuation technique.

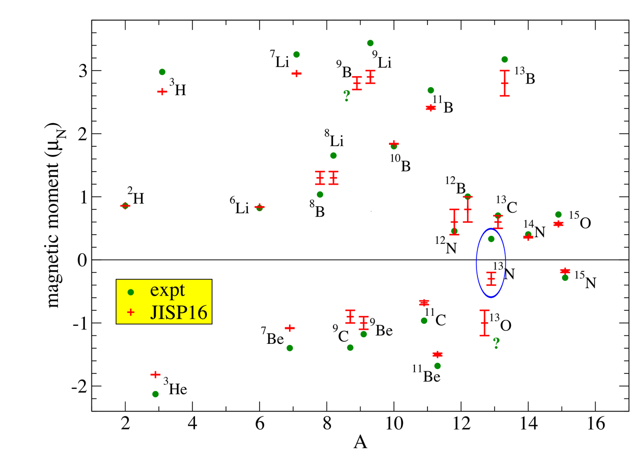


NUCLEI/MFDn

H.M. Aktulga, C. Yang, E.G. Ng (LBNL); P. Maris, J.P. Vary (ISU)

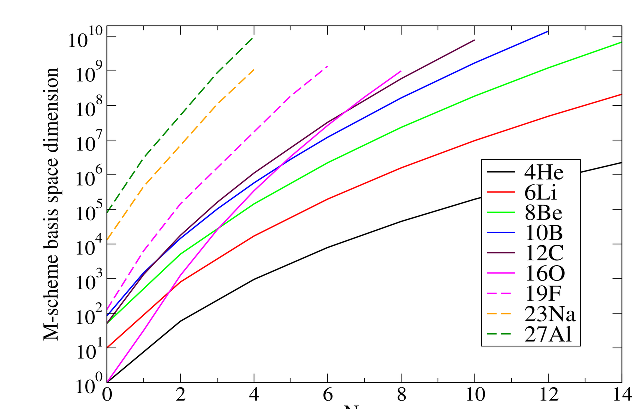
Successful description of the structure of nuclei is a long-standing goal of nuclear physics.

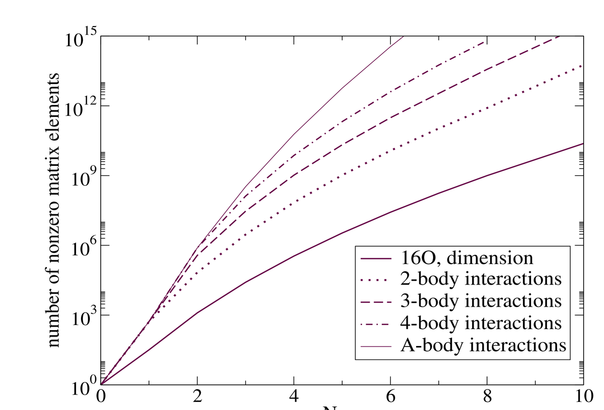




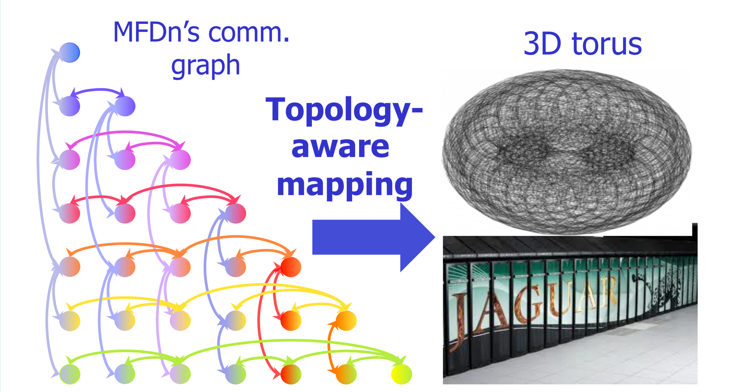
Ab initio no core full configuration approach used in MFDn (Many Fermion Dynamics nuclei) produces remarkably good agreement with experiment, not only for energies, but also for other observables such as magnetic moments.

Main computational kernel in MFDn is the solution of the standard eigenvalue problem. Extremely large size of the matrices, both in terms of matrix dimensions and number of nonzero matrix elements, creates challenges in achieving efficiency and scalability.





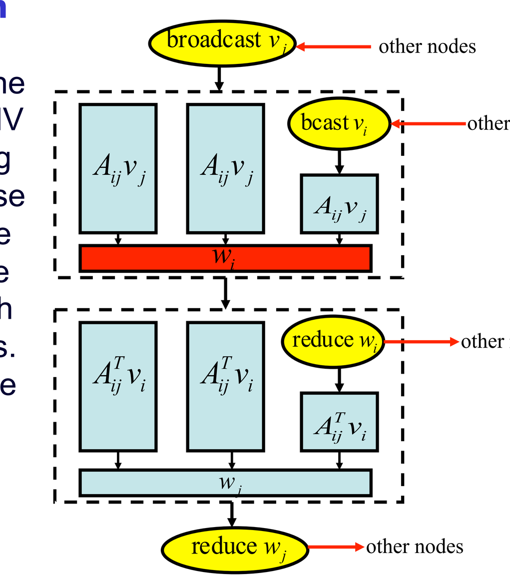
Two key techniques for almost perfect scaling on up to 260,000 cores on Jaguar/Titan:

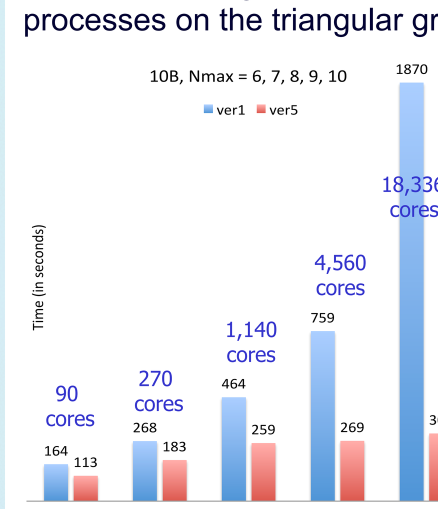


Topology-aware mapping of processes to the physical processors becomes more important as the gap between computational power vs. communication bandwidth of modern supercomputers continues to widen. Column communication groups in MFDn are optimized through a column-major ordering of processes on the triangular grid.

Communication Hiding

The flow-chart for the multi-threaded SpMV computations during the eigensolver phase of MFDn. Expensive communications are fully overlapped with useful computations. Communications are carried out over topology-optimized communication groups.

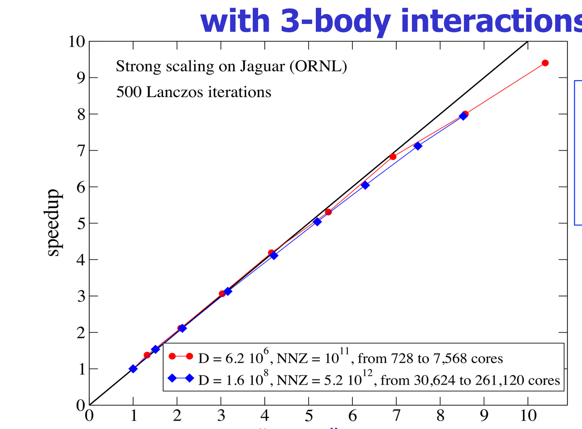




Speed-up on Hopper

Speed-up achieved using the latest version (ver5) of the Lanczos-based eigensolver in MFDn over the previous version (ver1). Using 18,336 cores on Hopper, we observe up to 6.2x speed-up.

Strong scaling on Jaguar with 3-body interactions



Over 90% strong scaling efficiency on 261,120 cores of Jaguar (ORNL)

red: ^{7}Li, N_{max}=8
base = 728 cores

blue: ^{10}Be, N_{max}=8
base = 30,624 cores

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