



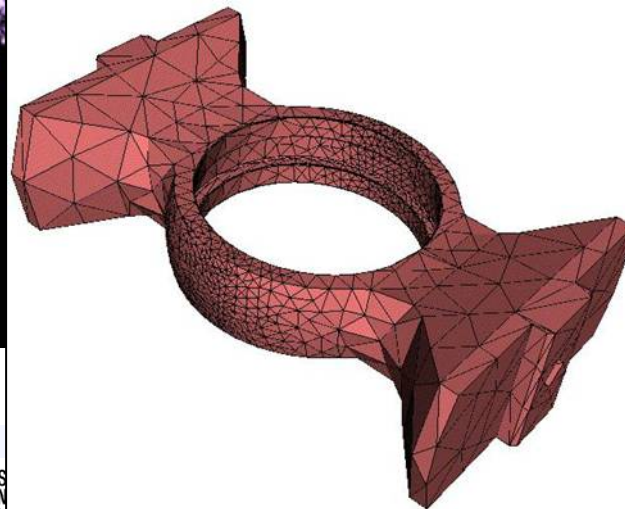
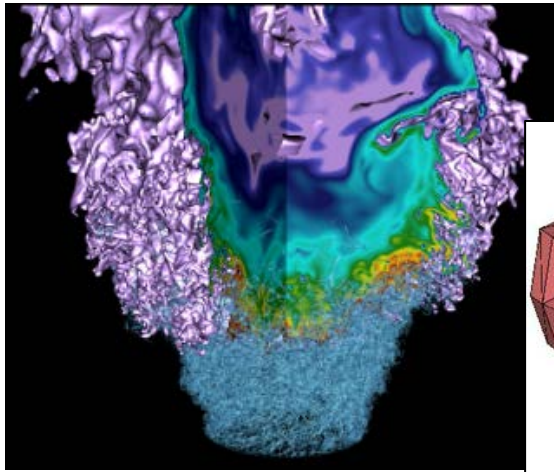
FASTMath Technology Developments and Partnership Activities

FASTMath Team
Lori Diachin, Institute Director

FASTMath SciDAC Institute

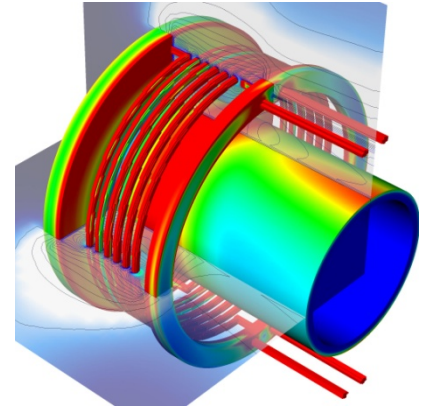


The FASTMath SciDAC Institute develops and deploys scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena and collaborates with DOE domain scientists to ensure the usefulness and applicability of FASTMath technologies



1. Improve the quality of their simulations

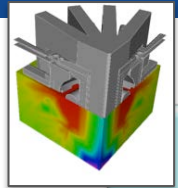
- Increase accuracy
- Increase physical fidelity
- Improve robustness and reliability



2. Adapt computations to make effective use of LCFs

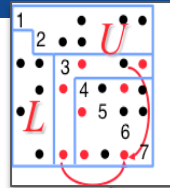
- Million way parallelism
- Multi-/many-core nodes

FASTMath will help address both challenges by focusing on the interactions among mathematical algorithms, software design, and computer architectures



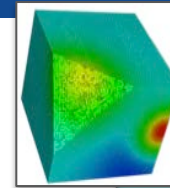
Tools for Problem Discretization

- Structured grid technologies
- Unstructured grid technologies
- Adaptive mesh refinement
- Complex geometry
- High-order discretizations
- Particle methods
- Time integration



Solution of Algebraic Systems

- Iterative solution of linear systems
- Direct solution of linear systems
- Nonlinear systems
- Eigensystems
- Differential variational inequalities



High Level Integrated Capabilities

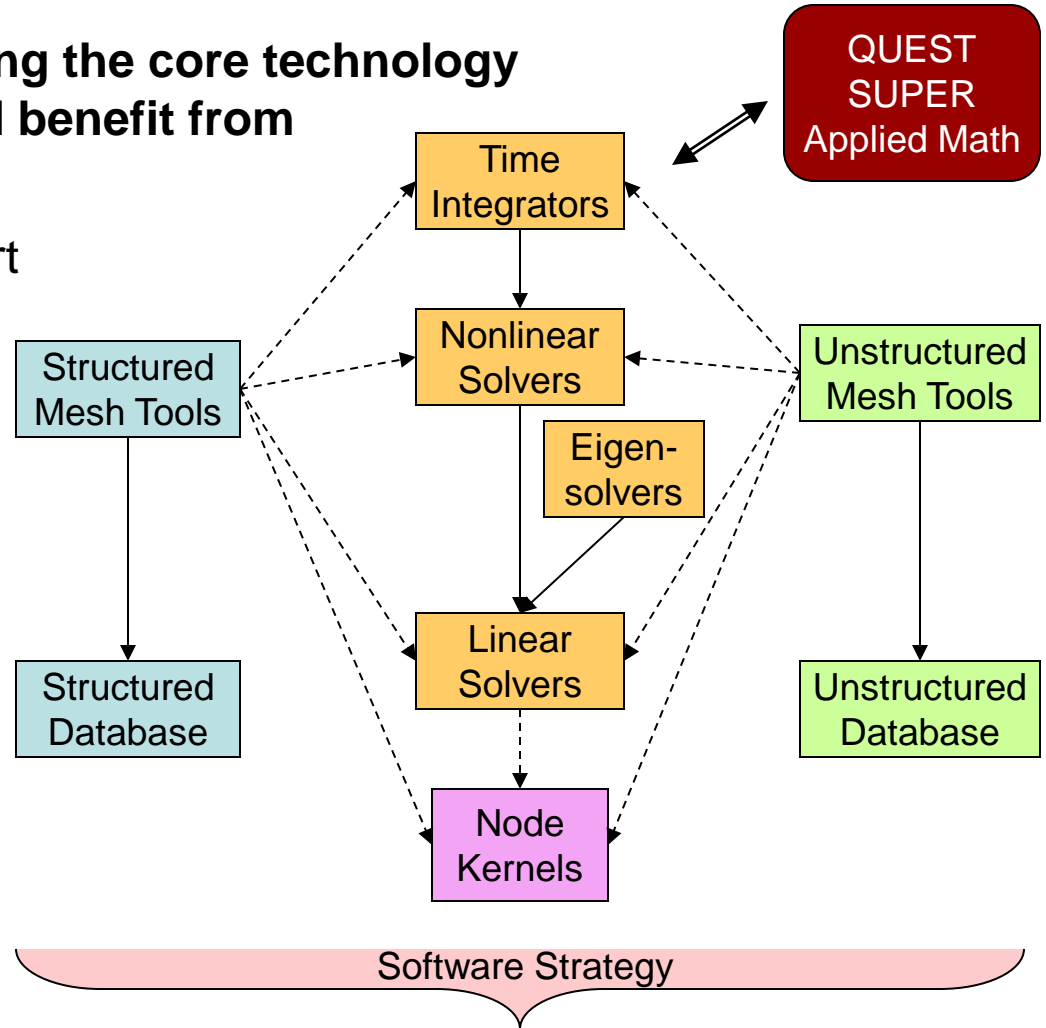
- Adaptivity through the software stack
- Management of field data
- Coupling difference physics domains
- Mesh/particle coupling methods

- As we provide integration among the core technology areas, science applications will benefit from

- Expanded capabilities
- Decreased development effort

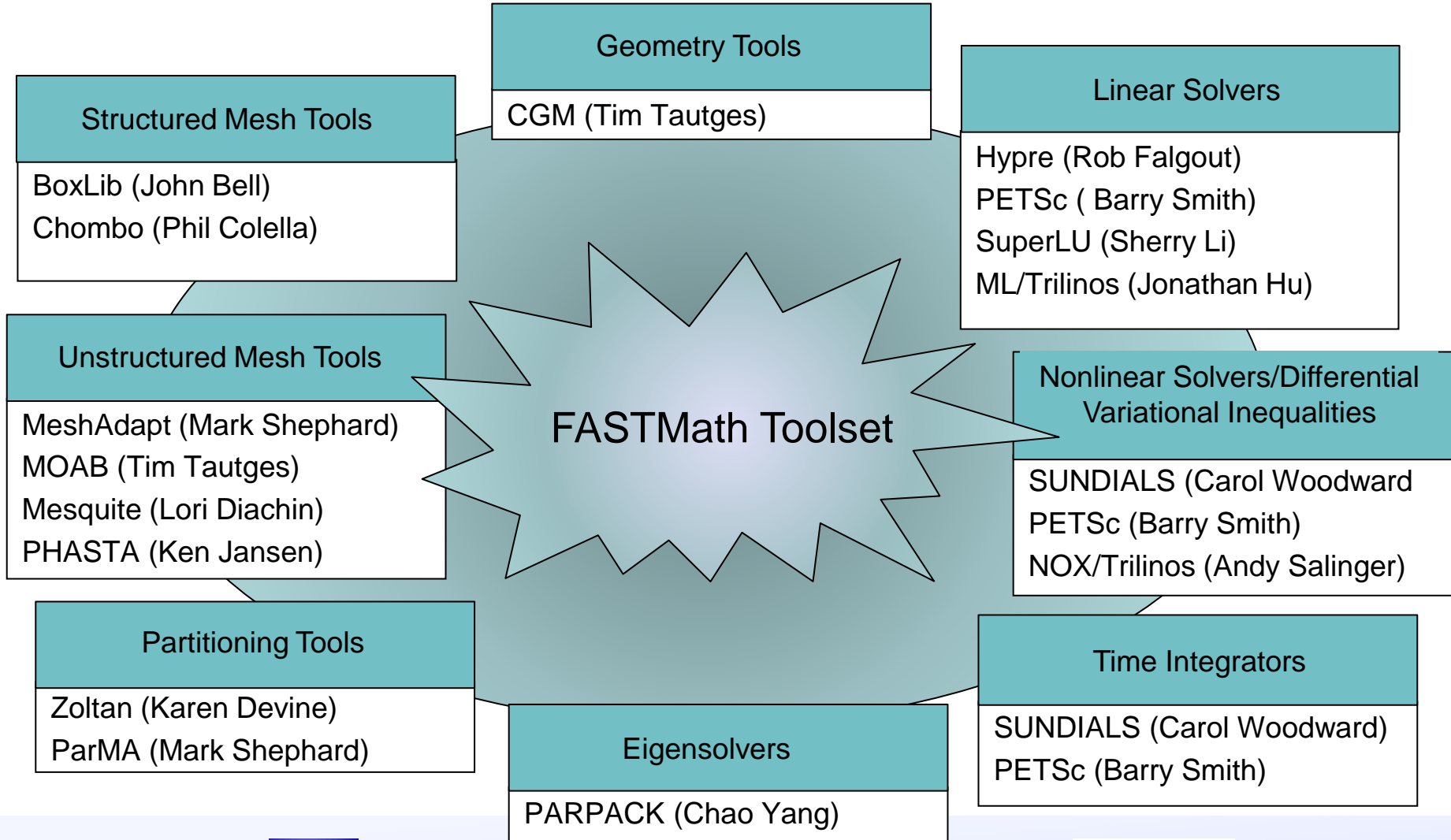
- Development efforts for expanded capability integration:

- Adaptivity through the software stack
- Mesh-solver integration
- Coupling strategies for multi-physics applications
- Architecture-aware compute node kernels
- Unified software strategy





FASTMath brings a spectrum of software tools in these areas to the SciDAC Program







The FASTMath team includes experts from four national laboratories and five universities

 Lawrence Berkeley National Laboratory
Mark Adams Ann Almgren John Bell Phil Colella Anshu Dubey Dan Graves Sherry Li Terry Ligocki Mike Lijewski Peter McCorquodale Esmond Ng Brian Van Straalen Chao Yang


 Berkeley University
Jim Demmel


 Lawrence Livermore National Laboratory
Lori Diachin Milo Dorr Rob Falgout Jeff Hittinger Mark Miller Carol Woodward Ulrike Yang


 Sandia National Laboratories
Karen Devine Jonathan Hu Vitus Leung Andrew Salinger

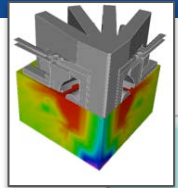
 University of British Columbia
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 Argonne National Laboratory
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 Rensselaer Polytechnic Institute
Mark Shephard Onkar Sahni

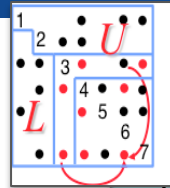
 Southern Methodist University
Dan Reynolds

 Colorado University at Boulder
Ken Jansen



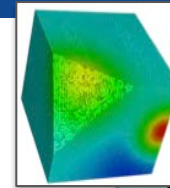
Tools for Problem Discretization

- Robust 4th order convergence for hyperbolic and paraboloid structured grid calculations
- Using discretization eigenstructures to understand stability and accuracy of EB
- Boundary layer thickness unstructured AMR
- New task mapping algorithms in Zoltan
- Optimized parameters for new multi-rate IMEX solver
- ODE system support with non-identity, but still non-singular mass matrices



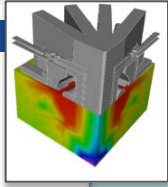
Solution of Algebraic Systems

- Limited stencil growth in Galerkin coarse grid correction in algebraic multigrid
- Advances in smoothed and truncated interpolation schemes give comparable convergence rates in additive AMG compared to multiplicative
- Blocked implementation of Aasen's algorithm for factorizing dense symmetric matrices
- Compared spectral slicing and penalized trace minimization for eigenvalue computations



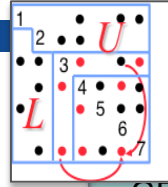
High Level Integrated Capabilities

- Mesh solver interoperability allowed comparison of 3 AMG methods; showed improved convergence of newly available methods compared to original
- CouPE designed to explore four different coupling strategies (operator-split, Picard, n-Richardson, JFNK)



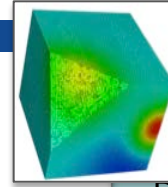
Tools for Problem Discretization

- Chombo ported to ACLF using both coarse- and fine-grained parallelism
- Continued study of MPI+threads in Zoltan up to 64K processors
- ParMA predictive load balancing for AMR
- Experiments show mesh migration runs twice as fast with 64 threads compared to straight MPI
- PHASTA scales to 512K cores
- Replaced MPI AlltoAll calls in BoxLib to improve performance



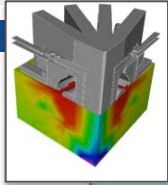
Solution of Algebraic Systems

- GPU support added to PETSc using OpenCL
- Implemented pipelined versions of CG and conjugate residual methods; 4X improvement in speed
- New parallel implementation of energy minimizing multigrid
- Improved and stabilized look-ahead algorithms in SuperLU
- New communication avoiding matrix powers algorithm
- Communication hiding schemes in Lanczos solvers
- Preliminary thread-parallel vector kernel
- New performance model for determining AMG redundant coarse grid solves



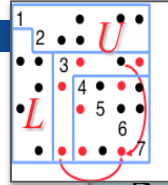
High Level Integrated Capabilities

- Determined canonical set of machines for FASTMath support (ACLF, OCLF, NERSc)
- Developing FASTMath tutorial for the Argonne Extreme Scale computing training program



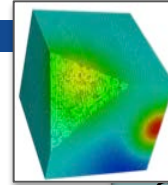
Tools for Problem Discretization

- New interface to PETSc SLEPc package in Chombo
- PHASTA linked directly to PETSc
- Interface between IDA DAE integrator and SUPERLU_MT linear solver
- Fortran interface for ARKODE
- MOAB extended to allow applications direct access to adjacency array information
- MOAB 4.6.0 released
- Released Zoltan and Zoltan2 in Trilinos v11.2
- Improving documentation and usability of ARKODE



Solution of Algebraic Systems

- Developed wrappers for Trilinos NOX nonlinear solvers that are compatible with Tpetra data structures
- SUPERLU_DIST 3.3 and SuperLU_MT 2.1 released
- Trilinos MueLU v11.2 released
- NOX V11.2 released
- Hypre linear solver interface in Chombo tested in COGENT code
- New PETSc linear and nonlinear equations solver interface for EB applications



High Level Integrated Capabilities

- Generalizing the Chombo-SUNDIALS interface to handle full AMR
- New DMMoab data vector to share data with PETSc
- In memory integration of MeshAdapt with SLAC eigensolver component
- Integrated Geometry/model information from FMDB into Albany
- MeshAdapt integrated into Albany and isotropic AMR tested
- Exploring common approach to autoconf-like interface for configure and build



FASTMath technologies are used in most SciDAC application partnerships and an NNSA application

Title	PI	FASTMath involvement	Office	Technology
Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)	William Lipscomb, LANL	Esmond Ng, Andy Salinger	BER	Algebraic
Multiscale Methods for Accurate, Ecient, and Scale-Aware Models of the Earth System	William Collins, LBNL	Carol Woodward	BER	Algebraic
Applying Computationally Efficient Schemes for BioGeochemical Cycles	Forrest Hoffman, ORNL	Tim Tautges	BER	Discretization
Charge Transfer and Charge Transport in Photoactivated Systems	Chris Cramer, Minnesota	Esmond Ng, Chao Yang	BES	Algebraic
Simulating the generation, evolution and fate of electronic excitations in molecular and nanoscale materials with first principles methods.	Martin Head-Gordon	Sherry Li, Esmond Ng, Chao Yang	BES	Algebraic
Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments	Roberto Car, Princeton	Esmond Ng, Chao Yang	BES	Algebraic
Scalable Computational Tools for Discovery and Design -- Excited State Phenomena in Energy Materials	James Chelikowsky, UT Austin	Chao Yang	BES	Algebraic
Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles	John Pask, LLNL	Chao Yang	BES	Algebraic
Optimizing Superconductor Transport Properties through Large-scale Simulation	Andreas Glatz, ANL	Todd Munson	BES	Algebraic
Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing	Brian Wirth, ORNL	Tim Tautges, Emil Constantinescu, Barry Smith	FES	Discretization, Algebraic
Center for Edge Physics Simulation	CS Chang, PPPL	Mark Adams, Mark Shephard	FES	Discretization
Searching for Physics Beyond the Standard Model: Strongly-Coupled Field Theories at the Intensity and Energy Frontiers	Paul Mackenize, Fermilab	Rob Falgout	HEP	Algebraic
Computation-Driven Discovery for the Dark Universe	Salmon Habib, ANL	Ann Almgren	HEP	Discretization
ComPASS: High performance Computing for Accelerator Design and Optimization	Panagiotis Spentzouris, Fermilab	Esmond Ng, Phil Colella, Sherry Li, Todd Munson, Chao Yang	HEP	Discretization, Algebraic
A MultiScale Approach to Nuclear Structure and Reactions: Forming the Computational Bridge between Lattice QCD and Nonrelativistic Many-Body Theory ("CalLAT")	Wick Haxton, LBNL	Esmond Ng, Rob Falgout	NP	Algebraic
Nuclear Computational Low-energy Initiative	Joseph Carlson, LANL	Esmond Ng, Chao Yang	NP	Algebraic
ParaDiS Dislocation Dynamics	Tom Arsenlis, LLNL	Carol Woodward	NNSA	Algebraic





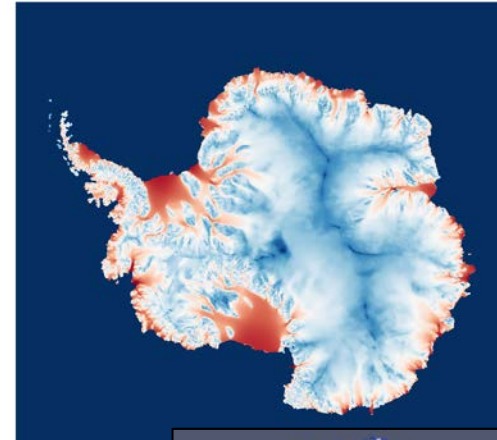
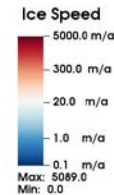
Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)

PI: Bill Lipscomb and Phil Jones, LANL

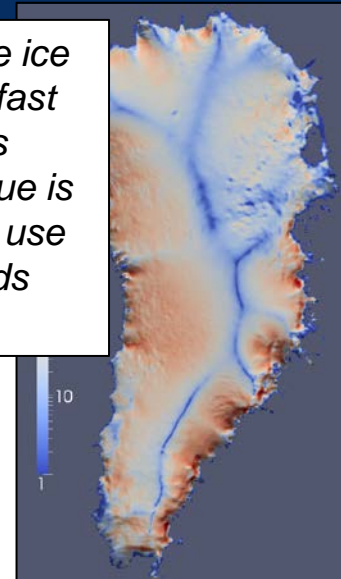
**POCs: Andy Salinger (SNL), Phil Colella (LBNL),
Barry Smith (ANL), Mark Adams (LBNL)**



- **Project Goal:** to develop predictive capability for ice sheet evolution:
 - Future **Land Ice** component of global earth system models
 - Focus primarily on Greenland and Antarctic ice sheets
- Developing a new dynamical core that contains the following new technologies:
 - Adaptive, refined meshes to focus resolution (Chombo, Trilinos)
 - Improved nonlinear solvers for steady and quasi steady state solves using homotopy and FAS multigrid (NOX, Chombo/PETSc)
 - Improved linear solver preconditioners using multigrid (MLU, hypre, PETSc)



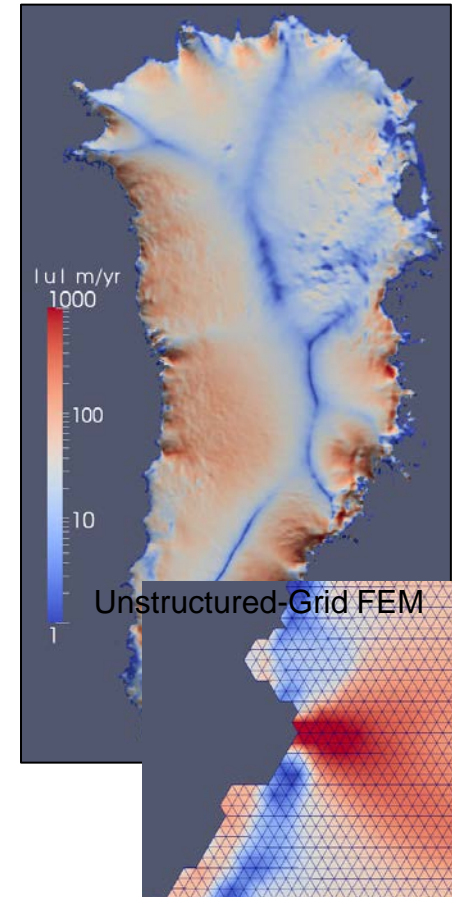
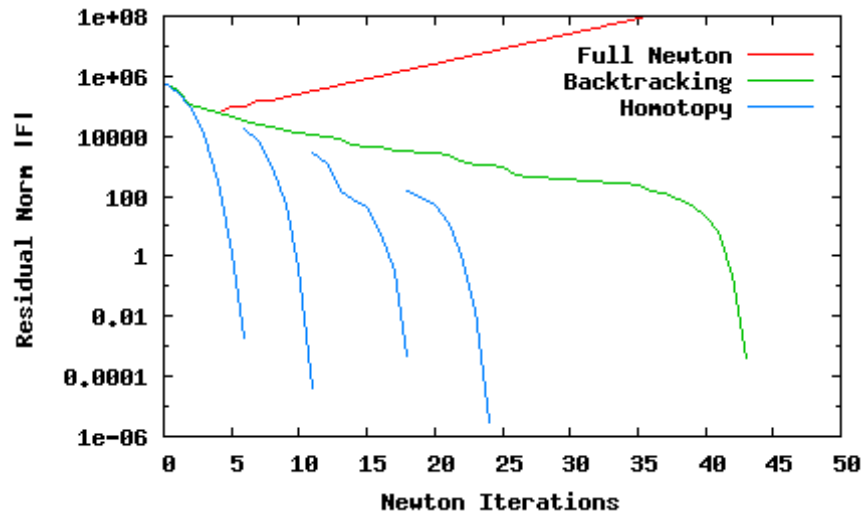
The colors are ice flow – red is fast and needs refinement, blue is slow and can use coarser grids



Parallel, 3D Unstructured-grid FEM, Implicit, Robust, Verified, Tested, PDE code written in less than 1 year:

- **Greenland** & Antarctic simulations
- Scalable Multi-level linear solves (Trilinos/ML)
 - Model problem with 182M unknowns on 4096 cores
 - 2km Greenland grid, steady-state solve, requires less than 1 minute on 9600 cores
- **Robust nonlinear solves using homotopy (Trilinos/NO**

❖ Linked to Dakota for UQ and Calibration

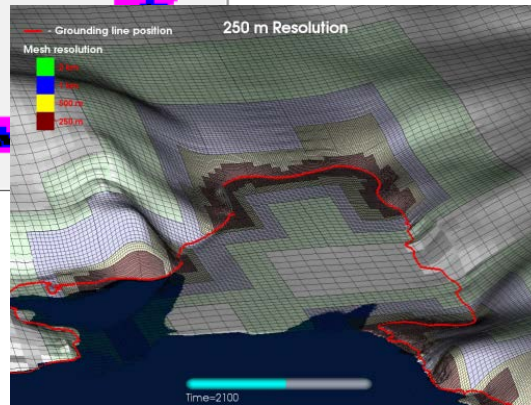
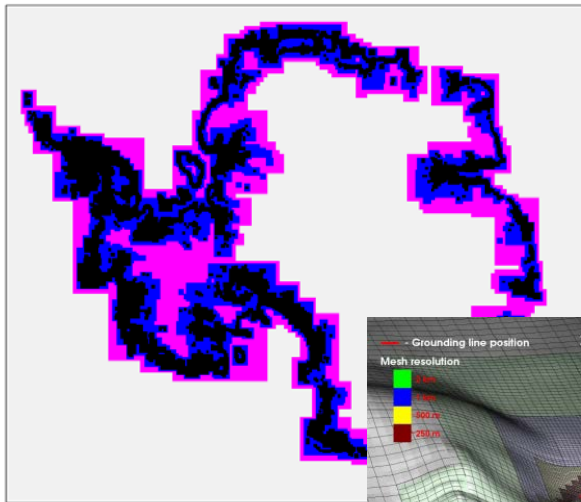


Greenland Ice Sheet Surface Velocities (constant friction model)

[Salinger, Kalashnikova, Perego, Tuminaro, Worley]

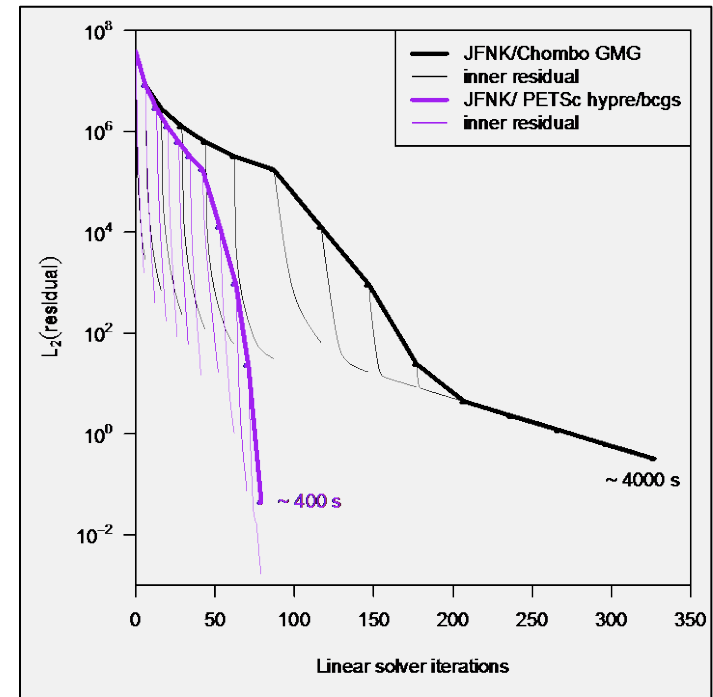
Parallel, scalable, block-adaptive mesh refinement resolves the *grounding line* (Ice/Land/Ocean interface).

Mesh Resolution



JFNK Solver with Algebraic Multi-Grid (AMG) delivers improved convergence

- Nonlinear solution of L1L2 flow model on 5km grid of Antarctica



[Adams, Cornford, Martin]

- **Past: Pre-FASTMath reasons for success...**
 - Inter-disciplinary teams were already formed under ISICLES (FY10-12)
 - Ice Sheet application needs align very well with FASTMath technology
- **Present: What makes this work (in addition to previous slides)**
 - Large pieces of development owned by ASCR computational experts:
 - Partnership, not just hanging solver libraries off of legacy codes
 - Use of more formal Software Engineering processes:
 - E.g., verification, automated testing, continuous integration,...
- **Future: Ongoing FASTMath development that will impact PISCEES...**
 - Mesh adaptivity in unstructured grid FELIX code
 - Albany/FMDB mesh adaptivity effort (see Hansen/Shephard poster)
 - Improved AMG algorithms for Ice Sheet application
 - PETSc/Hypre (Adams), ML (Hu, Tuminaro)
 - Use of DOE's LCFs: porting, tuning, new kernels, ...

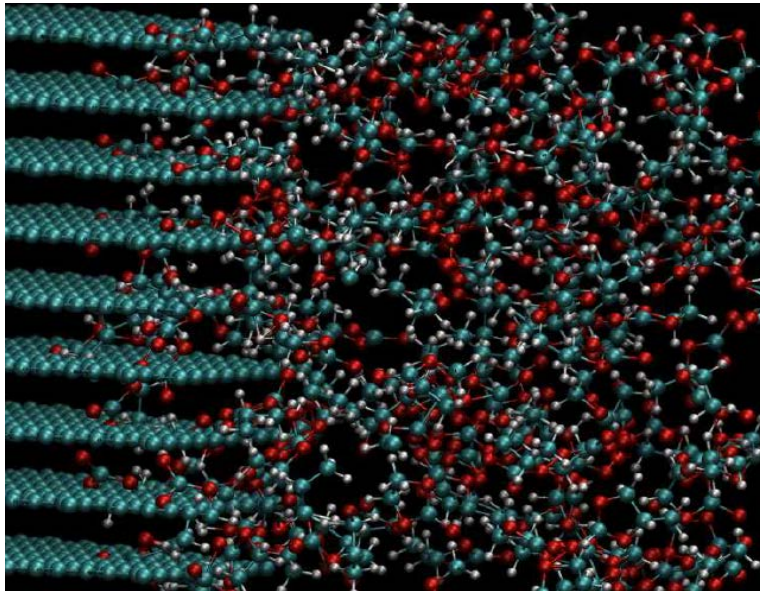


Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles
PI: John Pask, LLNL

POCs: Chao Yang, Esmond Ng
LBNL



- **Project Goal:** Develop fast *quantum* molecular dynamics (QMD) simulation tools for studying the formation and evolution of solid electrolyte interface in Li-ion battery cells



- Requires highly efficient solution of the Kohn-Sham equations
- Exploring use of discontinuous Galerkin discretization schemes

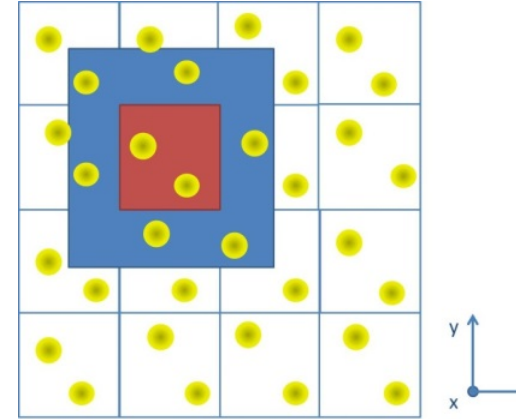
Discretization	DOF/atom	Systematic Improvable?	Chemical environment
Local atomic orbital	10	N	N
Planewave expansion	~1000	Y	Y
Finite difference	>1000	Y	Y
Finite element	>1000	Y	Y

Project Objectives:

- Minimize the number of degrees of freedom (DOF) per atom
- Systematically improvable
- Local basis functions taking into account both the atomic and environmental information

Basic Strategy:

- Domain decomposition to create local problems
- Extended elements to incorporate neighbor information
- Solve Kohn-Sham on extended element
- Restrict back to local problem create the basis functions for the global solve



Advantages:

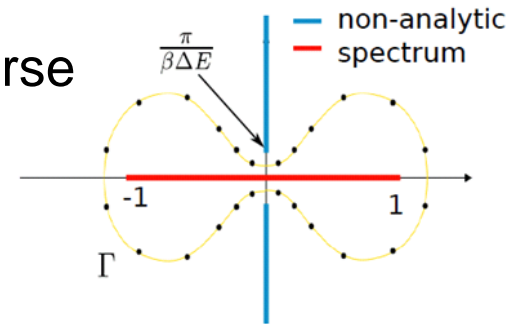
- Embarrassingly parallel local solutions
- Incorporates nearby chemical environment information

Disadvantages:

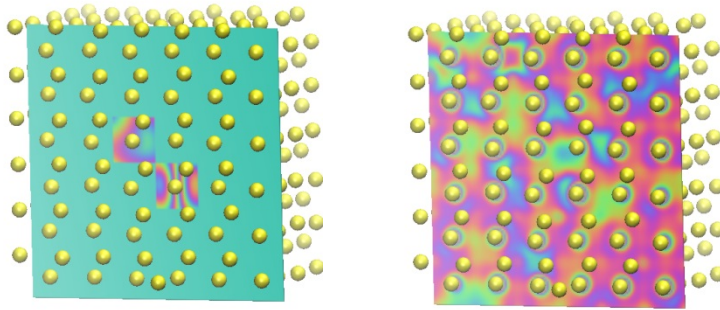
- Discontinuities introduce numerical difficulties
- Requires additional terms in energy functional to represent discontinuous jumps in flux on the boundaries

- Construction of local basis functions do not require full solution of the Kohn-Sham problem
 - No need to solve the nonlinear problem self-consistently
 - Compute a number of eigenfunctions of a reasonable Kohn-Sham Hamiltonian
- *FASTMath is developing an efficient linear iterative eigenvalue solver for the local Kohn-Sham Hamiltonian*
 - Currently using locally optimal blocked preconditioned conjugate gradient algorithm
 - Currently developed a penalized trace minimization algorithm to further reduce the cost of the Rayleigh-Ritz calculations

- Efficient and accurate local basis functions allow representation of the global Kohn-Sham Hamiltonian as a sparse matrix
- Compute energy, electron density, and forces without computing eigenvalues/eigenvectors (PEXSI Scheme)
 - Express relevant quantities as a rational, Fermi operator expansion of the Hamiltonian (Pole Expansion)
 - Carefully choose the pole positions and corresponding weights
 - Less than 100 terms needed to achieve high accuracy
 - At each pole, use selected inversion to compute selected elements without computing the full inverse
 - $O(N^2)$ compared to the $O(N^3)$ required for diagonalization
 - Easy to parallelize over the the poles

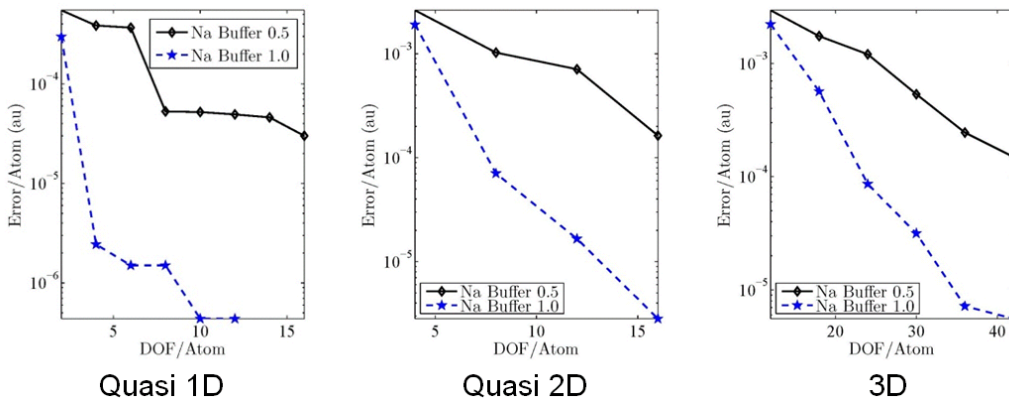


Disordered Sodium System



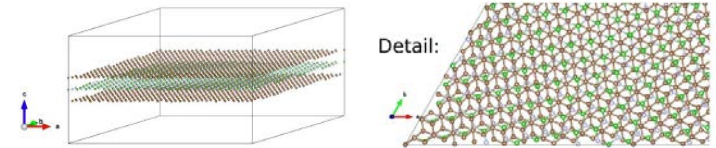
Local basis functions Global electron density

Discretization accuracy and efficiency



C-BN-C layered System

PEXSI performance



One SCF iteration on $40 \times 256 = 10,240$ cores

Number of atoms	Matrix dimension	Time
2532	32916	32
10128	131664	258
20256	263328	554

Comparison with diagonalization:
 ScaLAPACK took 230 sec for 2532 atoms using 768 processors and **does not scale beyond** that many cores

- **Future work:**
 - Parallelization within each local element solve
 - MPI plus threading to achieve 16-24 cores for each local problem
 - Development of more efficient eigensolvers; particularly focused on preconditioning strategies
- **Collaboration:** FASTMath pays for solver development, application pays for discretization and use of solvers
- **What makes this work?**
 - Significant information exchange
 - Strong collaboration with weekly telecons and monthly face to face meetings
 - Value of FASTMath efforts recognized

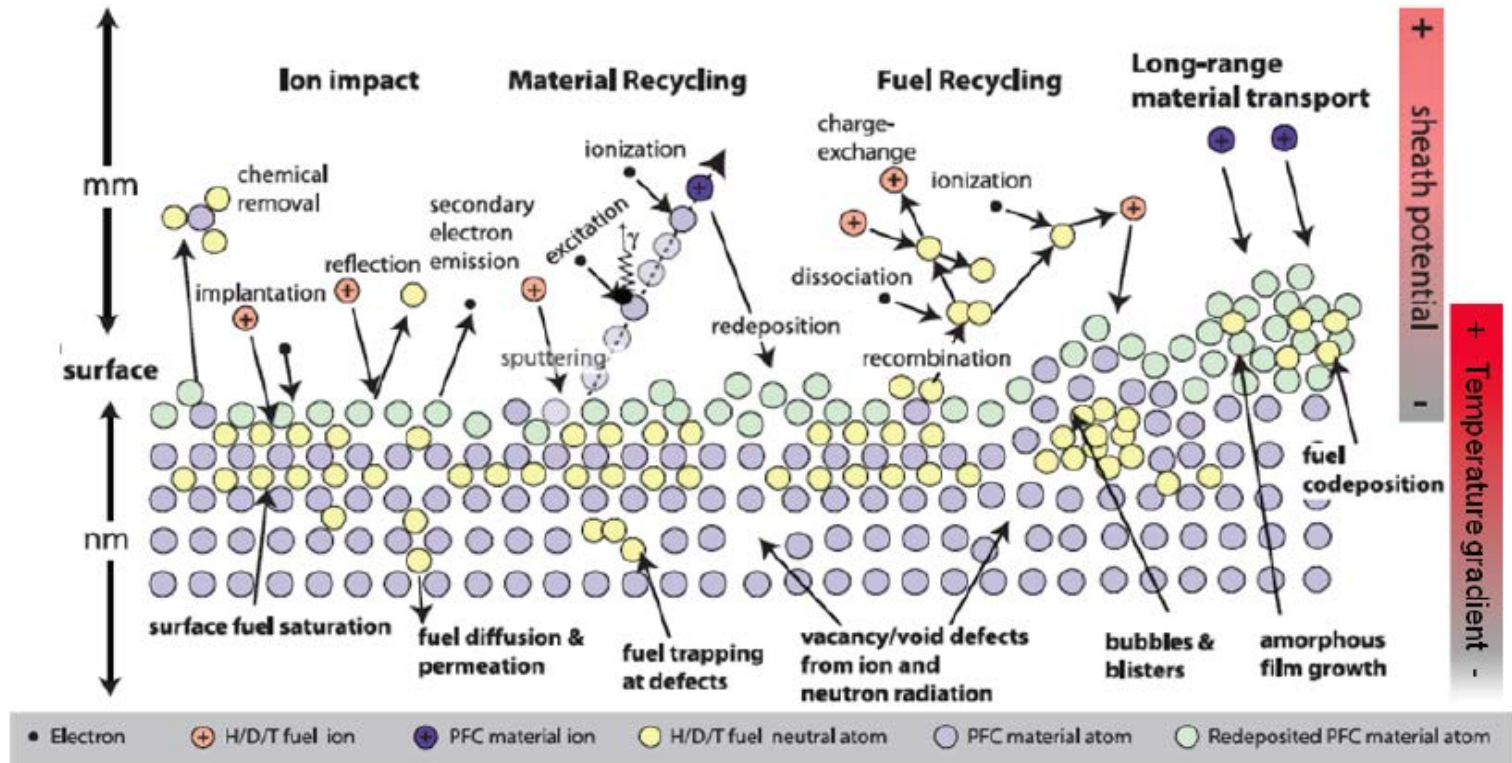


Plasma Surface Interactions: Bridging from the Surface to the Micron
Frontier through Leadership Class Computing
PI: Brian Wirth, ORNL

**POCs: Tim Tautges, Barry Smith,
Emil Constantinescu, Jungho Lee**
ANL



This project aims to model complex, interlinked plasma surface interactions



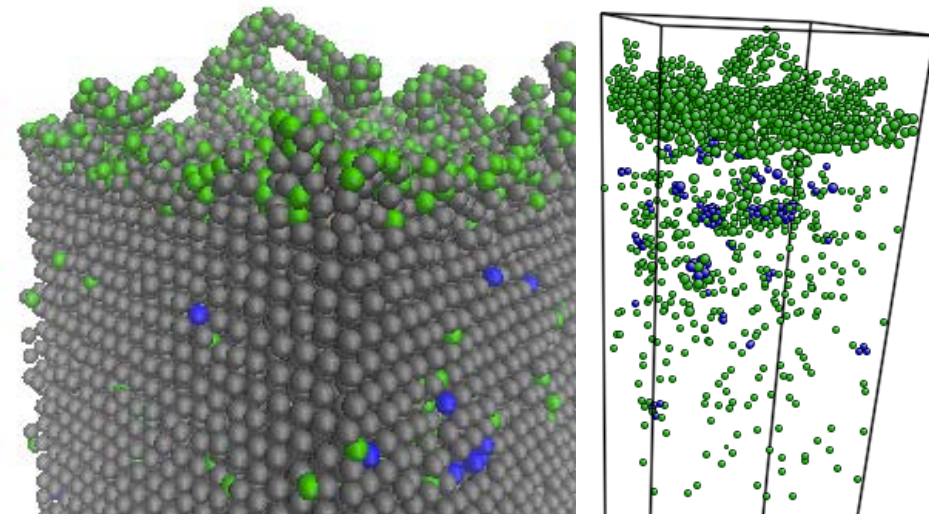
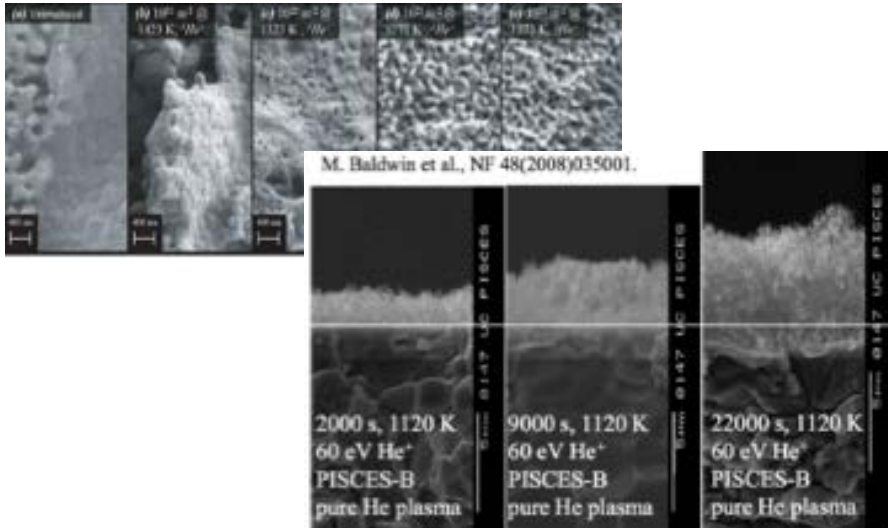
* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* 36 (2011) 216-222

Interesting processes:

- Plasma ions striking and penetrating metal material ($10^{24} \text{ m}^{-2}\text{s}^{-1}$)
 - Causes void defects, bubbles, blisters in the metal
- Material from metal goes into the plasma and impacts the plasma behavior

Fuzz and coral (material defects): investigate adaptive mesh refinement technologies to capture local effects

Fast and slow time scales in ion flux penetration requires sophisticated multi-scale time integration methods



Goal of the FASTMath efforts:

- Improved solvers for the reaction-diffusion continuum models
- Use of unstructured adaptive meshes
- Efficient 4D algebraic and geometric multigrid methods
- More efficient coupled ODE integrators

The Challenge: Reaction equations have 100's of thousands of species

- Each grid point has 100's of thousands of unknowns (compare to 4 or 5 that is typical in other problems)
- Think of this as a 4D problem

$$\frac{\partial C_i(x,t)}{\partial t} = D_i \frac{\partial^2 C_i(x,t)}{\partial x^2} + \sum_{\substack{jk \\ j+k=i}} k_{jk}^+ C_j C_k - C_i \sum_j k_{ik}^+ C_j + \sum_j k^- C_j - k^- C_i$$

C_i Represents Helium atom, vacancy, or interstitial clusters of size i at each grid point

Notes:

- Most species only involved in reaction (off diagonal blocks)
- Need a highly accurate solver for species involves in the diffusion terms
- Large scale nature of the problem $O(10^3 \times 10^3 \times 10^3 \times 10^4)$ drives the need for exascale computing

Solution Strategy: Solved with implicit or semi-implicit ODE integrator, Newton based nonlinear solver and multigrid based linear solver.

- Leverage ODE IMEX infrastructure in PETSc
- Link to hypre multigrid solvers

Research Questions

- Reaction terms:
 - Very large and sparse but some structure; can this be leveraged?
 - Best parallelism strategy still needs to be determined
- Diffusion terms:
 - Unclear if standard multigrid is sufficient for highly accurate solution needed



FASTMath is developing unstructured grid techniques to capture features of interest

This is one of the applications driving the need for closer mesh/solver software interactions in FASTMath

- Simplified interfaces between mesh (MOAB) and vector-matrix (PETSc) versions of ODE system, including MOAB-PETSc memory sharing for solution vectors.
- Eventual MOAB support for moving surface to account for “fuzz” and bubble formation at plasma interface.
- Coupling to lower-length-scale codes, e.g. for material properties



What makes this work?

- PSI willing and interested in using FASTMath developed tools and software
 - Will allow for easy incorporation of advanced FASTMath tools and solvers as they are developed
- FASTMath supports infrastructure and solver development for the large-scale reaction-diffusion problems
- PSI partnership supports the investigation using realistic problems and parameters
 - Without real terms and parameters, this is an academic study



ParaDiS: Dislocation Dynamics

PI: Tom Arsenlis, LLNL

POC: Carol Woodward, LLNL

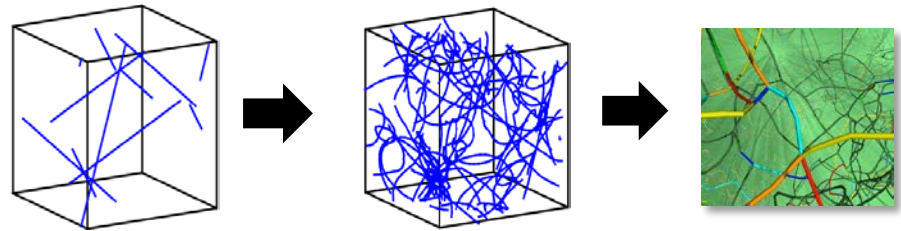
FASTMath SciDAC Institute



ParaDiS: Parallel dislocation dynamics code at LLNL solving very large-scale strain hardening problems on massively parallel computers

Technical Challenges:

- Very stiff systems in time
- Expensive force calculations
- Discontinuous topological events
- Problem size changes rapidly



Goal of the partnership

Improve time integrators and nonlinear solvers within ParaDiS so that larger time steps can be taken *while maintaining accuracy and achieving faster run times*

Key FASTMath Technologies

SUNDIALS: Suite of Nonlinear and Differential / Algebraic Equation Solvers

- Accelerated fixed point solver
- Newton nonlinear solver
- ARKODE higher order time integrators



We have enabled larger time steps with the ParaDiS dislocation dynamics code

Frank-Read source: Single dislocation that curls on itself causing segments to collide and merge.

Observed 94% speedup for single processor Frank-Read source with higher order integrator

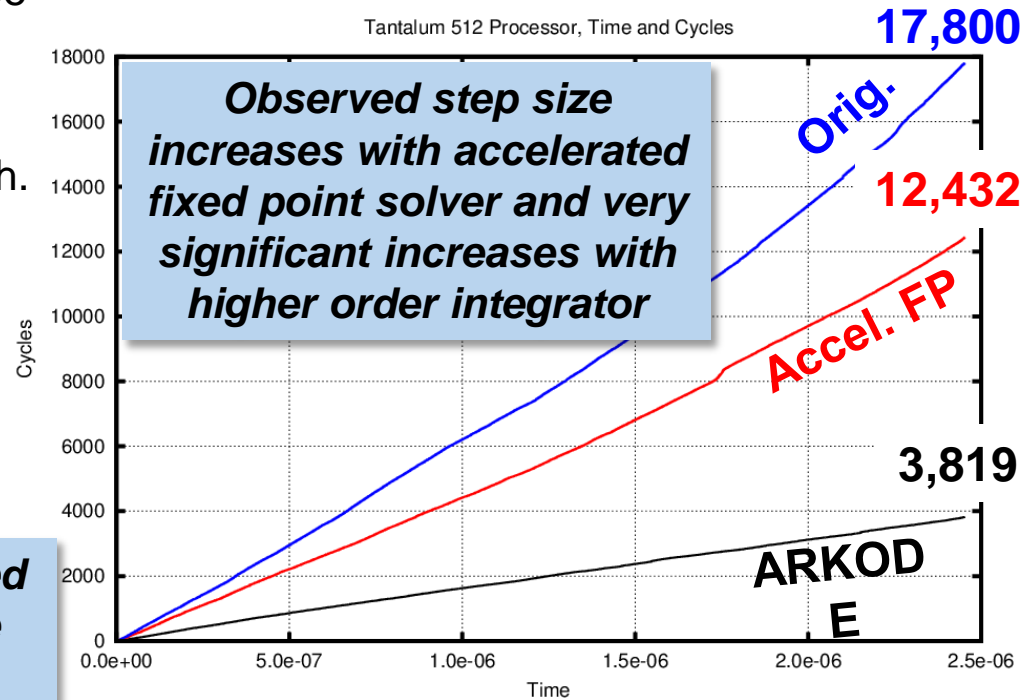
Method	Run Time (m)	Speed Up
TRAP-FP	20.15	-----
ARKODE ord. 3	6.40	68%
ARKODE ord. 4	1.13	94%
ARKODE ord. 5	1.75	91%

Tantalum single crystal BCC, 4.25 μm^3 cube

Constant strain of 1,000/sec along the x-dir
Starts with ~56K and ends with ~135K nodes
Run 2.4 μsec on 512 cores of LLNL cab mach.

Method	Run Time (s)	Speed Up
TRAP-FP	6,030	-----
ARKODE ord. 3	12,644	-110%
ARKODE ord. 5	20,231	-235%
TRAP-Accel 2 its	5,550	8%
TRAP-Accel 3 its	4,678	22%

Observed speed up with accelerated fixed point, ongoing work is in improving the stage solvers for the integrator





NUCLEI: Nuclear Computational Low-energy Initiative

PI: Joe Carlson, LANL

POC: Esmond Ng, LBNL

FASTMath SciDAC Institute



Method

- Configuration Interaction approach: Highly accurate ab-initio method
- MFDn (Many Fermion Dynamics nuclei) code by Vary, et al. ISU

Mathematical Problem

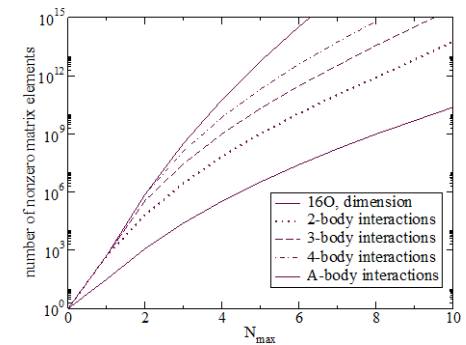
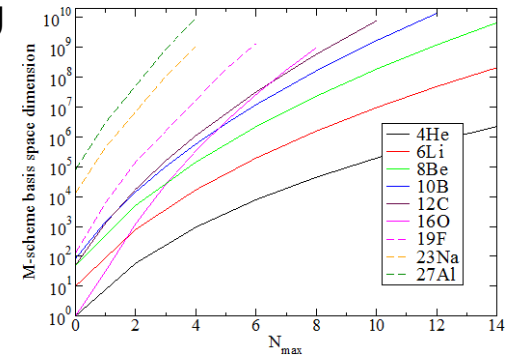
- Eigenvalue problem for A nucleons

$$\hat{H}\Psi(r_1, \dots, r_A) = \lambda\Psi(r_1, \dots, r_A)$$

- \hat{H} describes the nuclear interactions - symmetric
- Few lowest eigenvalues λ give ground-state energy levels of the nuclei
- Eigenvectors Ψ allow us to compute physical observables

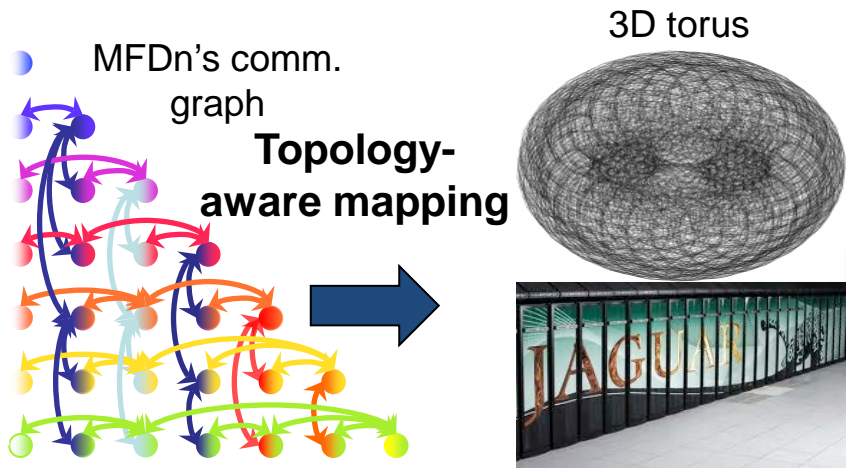
Challenges

- The extremely large size of the matrices – in terms of dimensions and number of nonzeros
 - Unique 2D triangular processor topology – only half the matrix is stored
 - How to get the Lanczos algorithm to run efficiently and scale to 100,000s of cores

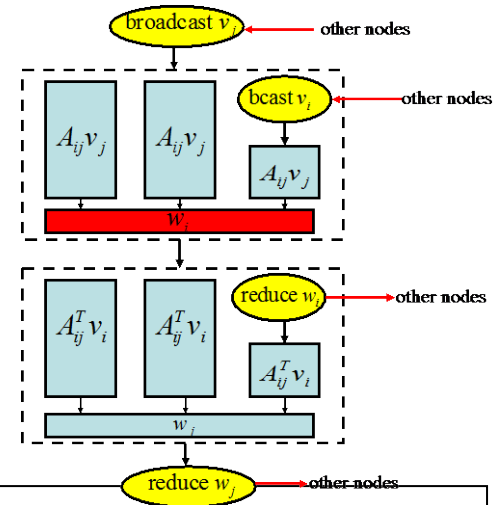


Topology-aware mapping: Column communication groups in MFDn are optimized through a column-major ordering of processes on the triangular grid

Communication hiding: Overlap expensive communication with computation and utilize topology-optimized communication groups



The flow-chart for the multi-threaded SpMV computations during the eigensolve phase of MFDn.



- Impact**
- Drastically reduced communication overheads in the eigensolver
 - Significant speed-ups over an earlier version of MFDn (up to 6x on 18,000 cores)
 - Almost perfect strong scaling on up to 260,000 cores on Jaguar

- 1. FASTMath Structured Meshing Technologies**
POC: Phil Colella, LBNL
- 2. FASTMath Unstructured Mesh Technologies**
POC: Mark Shephard, RPI
- 3. New FASTMath Iterative Solver Technologies**
POC: Barry Smith, ANL
- 4. FASTMath Direct Solver Technologies**
POC: Sherry Li, LBNL
- 5. FASTMath Integrated Technologies**
POC: Glen Hansen, SNL
- 6. Impact of FASTMath Structured Mesh Technologies**
POC: Phil Colella, LBNL
- 7. Impact of FASTMath Unstructured Mesh Technologies**
POC: Tim Tautges, ANL
- 8. Impact of FASTMath Solver Technologies on Applications**
POC: Esmond Ng, LBNL

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