LLNL-PRES-501654

FASTMath SciDAC Institute Overview and First Year Technical Progress

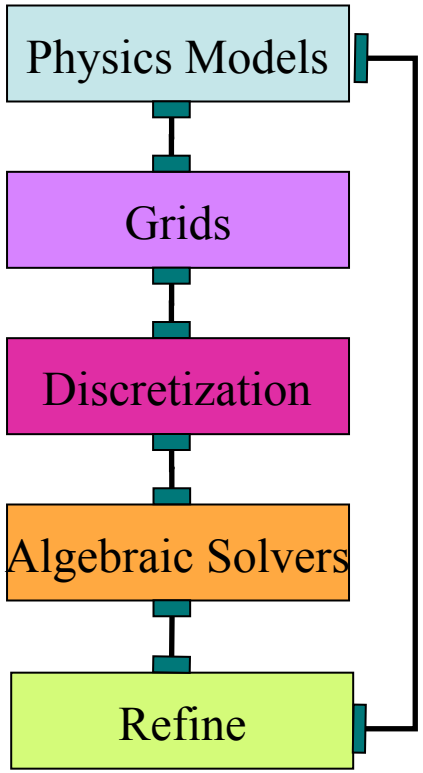
FASTMath Team

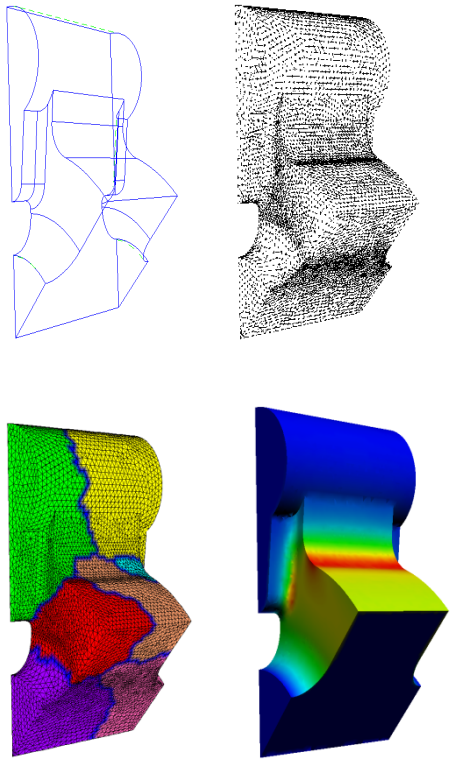
Lori Diachin, Institute Director

FASTMath SciDAC Institute

Foundational to HPC simulations are mathematical algorithms and software

- Develop a mathematical model of the phenomenon of interest
- Approximate the model using a discrete representation
- Solve the discrete representation
- Adapt and refine the mesh or model
- Couple different physics, scales, regions together



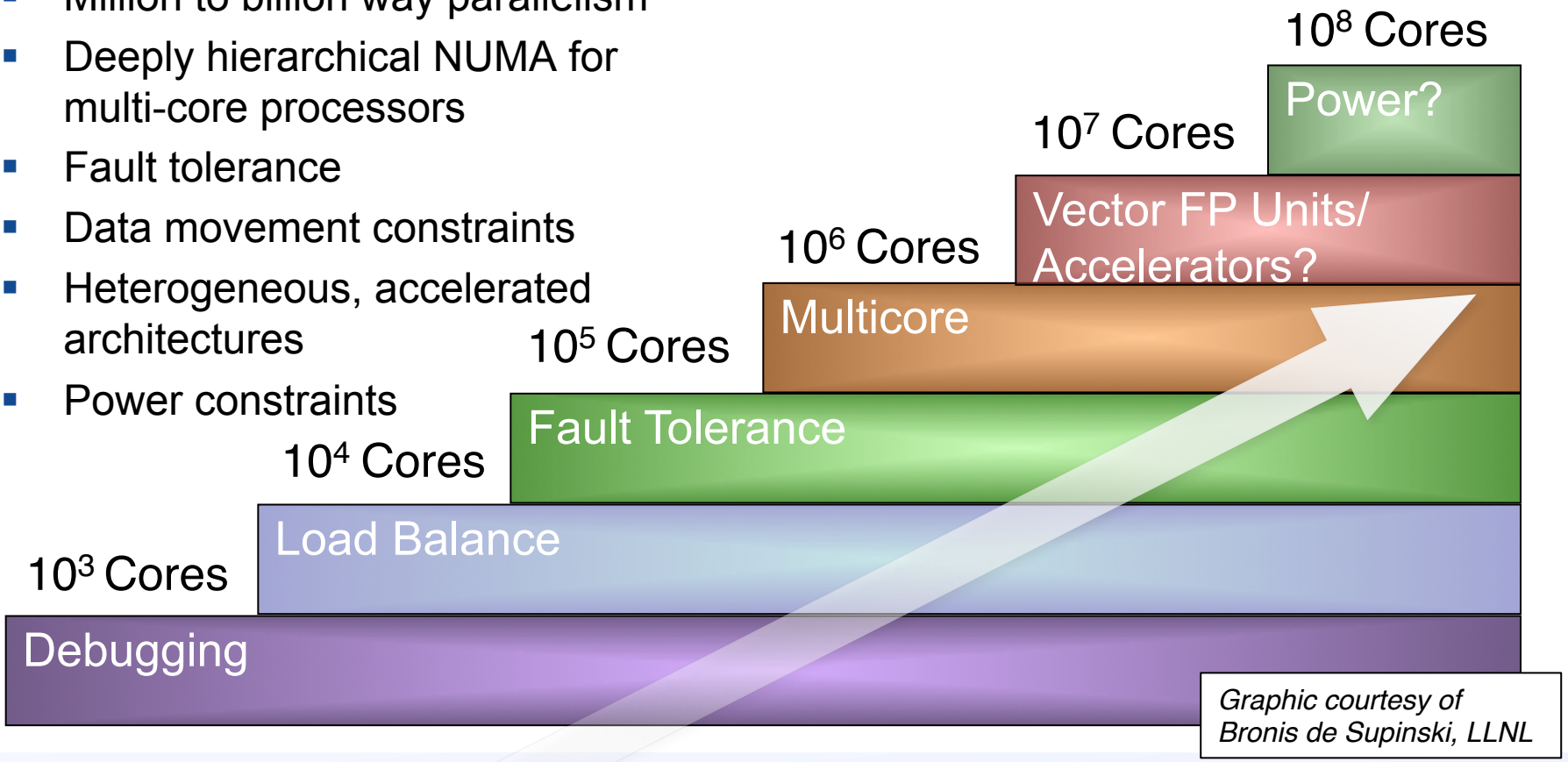


These steps require: CAD models, grid generation, high order discretizations, time integration techniques, linear and nonlinear solution of algebraic systems, eigensolvers, mesh refinement strategies, physics coupling methods, particle techniques, etc…

Modeling and simulation is significantly complicated by the change in computing architectures

Scientific computing software must address ever increasing challenges:

- Million to billion way parallelism
- Deeply hierarchical NUMA for multi-core processors
- Fault tolerance
- Data movement constraints
- Heterogeneous, accelerated architectures
- Power constraints



Graphic courtesy of Bronis de Supinski, LLNL

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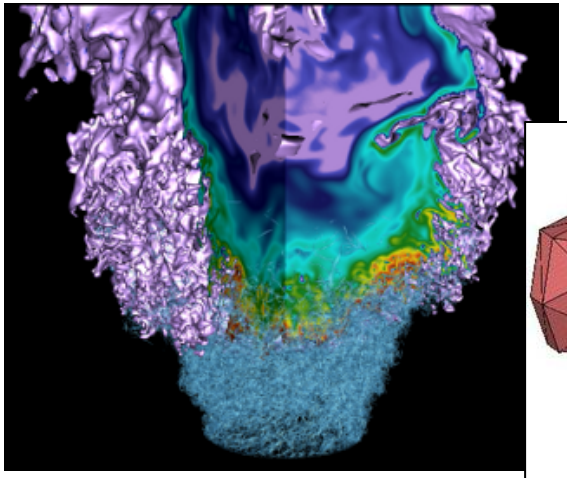
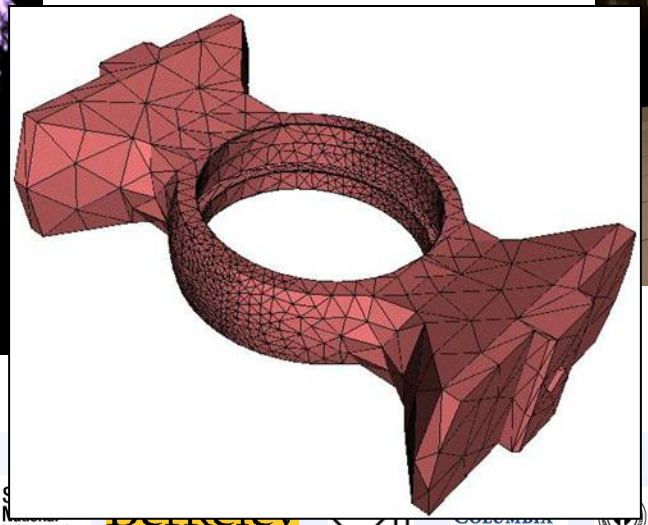
The FASTMath SciDAC project addresses these challenges for mathematics software libraries

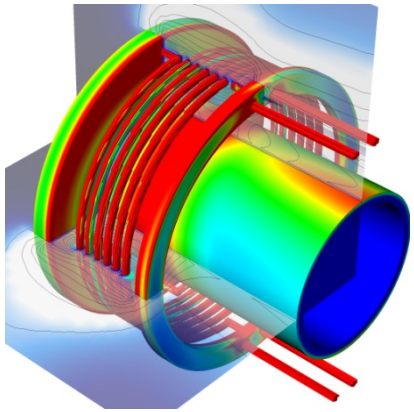
The FASTMath SciDAC Institute develops and deploys scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena and collaborates with DOE domain scientists to ensure the usefulness and applicability of FASTMath technologies





FASTMath will help application scientists overcome two fundamental challenges

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

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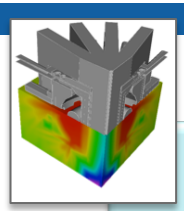
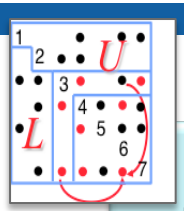
FASTMath encompasses three broad topical areas



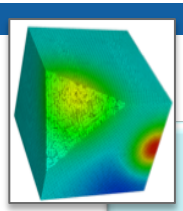
Tools for Problem Discretization

- 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

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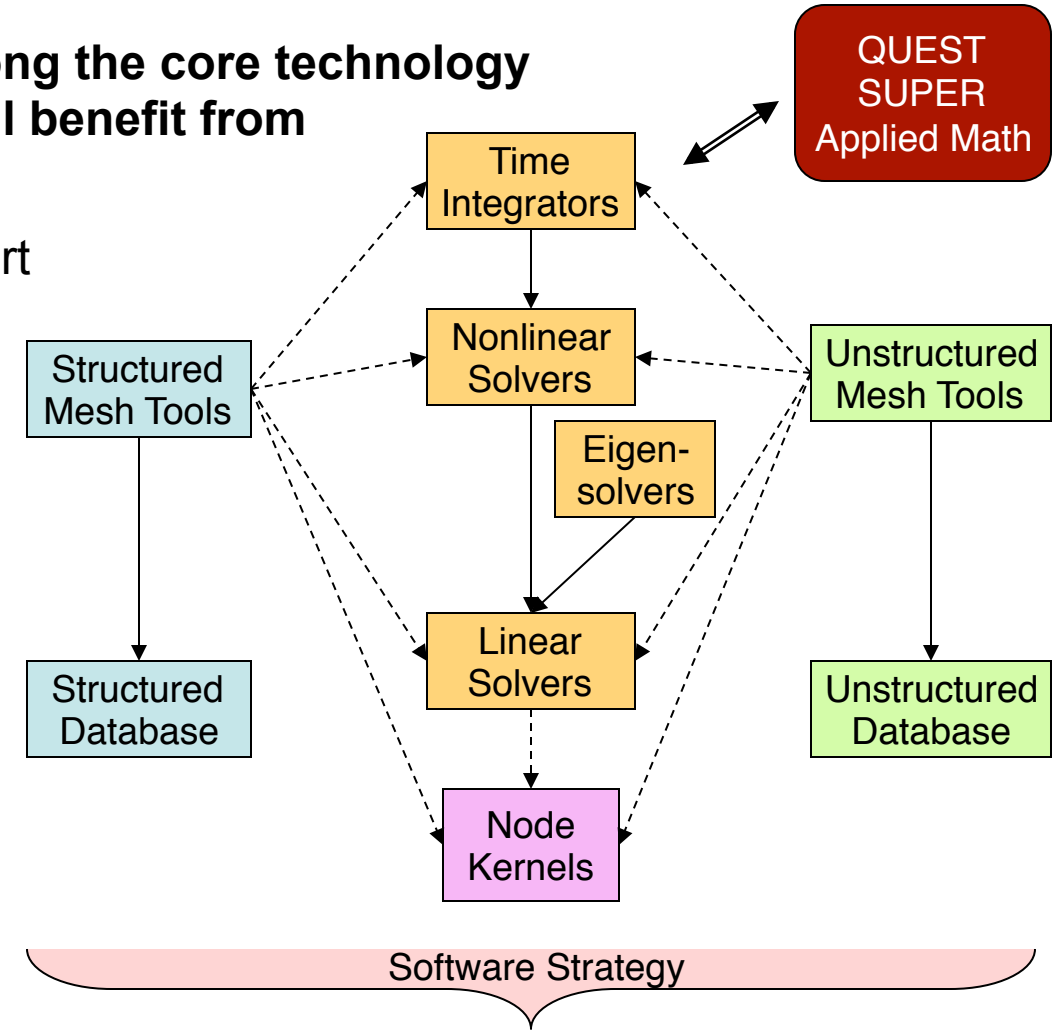
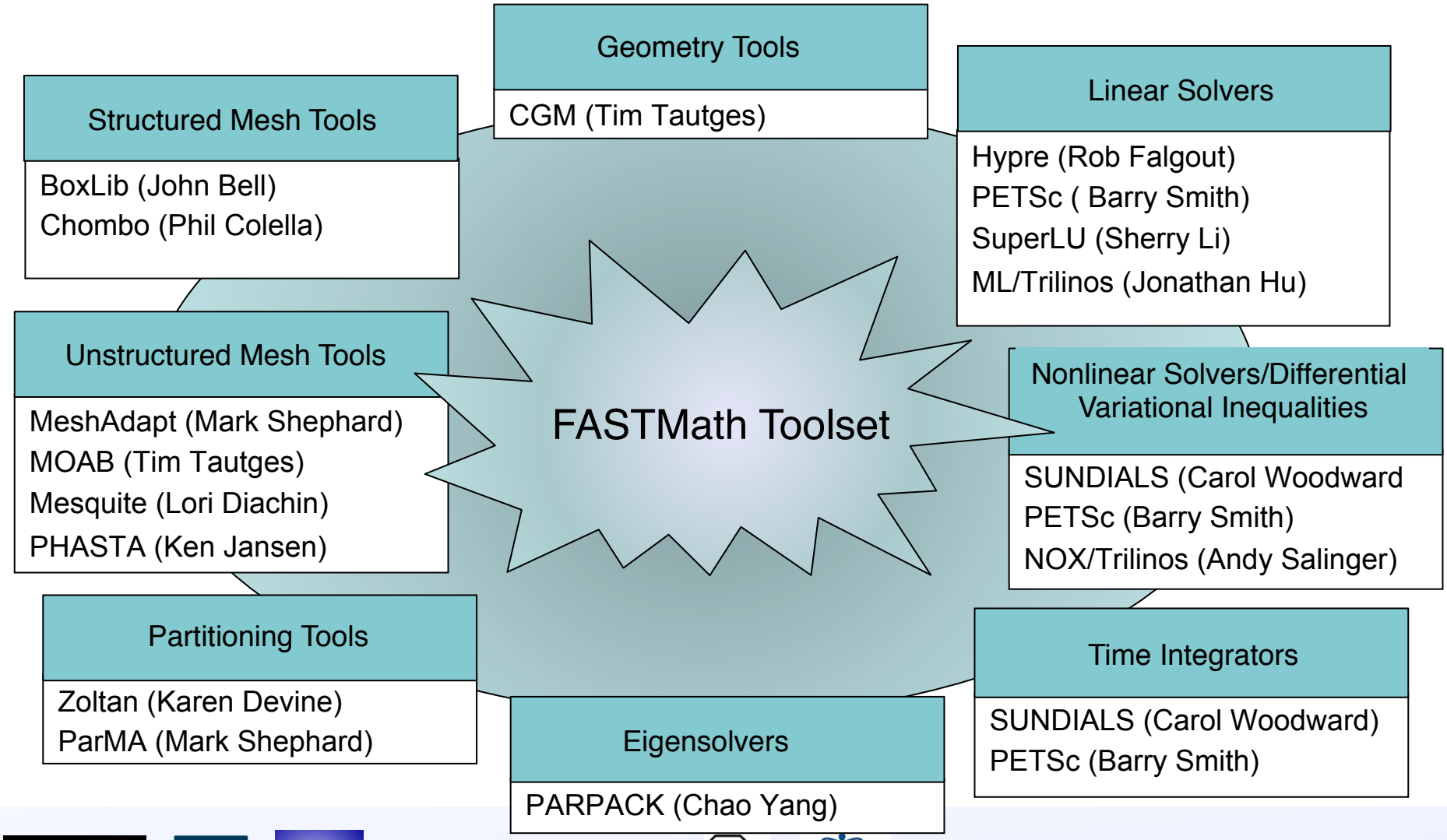
FASTMath provides a unique opportunity to develop integrated capabilities

- **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
  - Field data and manipulation
  - Coupling strategies for multi-physics applications
  - Architecture-aware compute node kernels
  - Unified software strategy

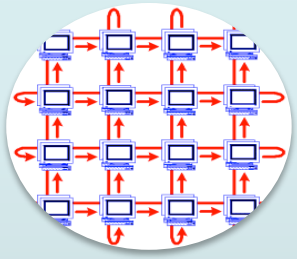


FASTMath brings a spectrum of software tools in these areas to the SciDAC Program



All FASTMath technologies focus on performance engineering for multi-/many-core architectures

MPI Level Parallelism



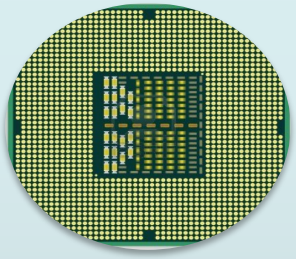
Operate efficiently at 10^5 to 10^6 cores

Architecture-aware and multi-objective load balancing

Communication avoiding and latency tolerant algorithms

Synchronization reducing algorithms

Node Level Parallelism

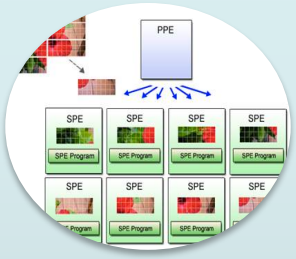


Use of threading techniques

Multi-core kernels and data ordering

Exploit compilers, code transformation tools, programming models and run-time systems as they become available

Data Locality



Hierarchical partitioning and local data ordering methods

Shared efficient data layouts in software packages to prevent re-organization

Code transformation systems, domain specific language extensions to gain performance while maintaining reusability

Coordinated parallelism between different levels (MPI, node, instruction)

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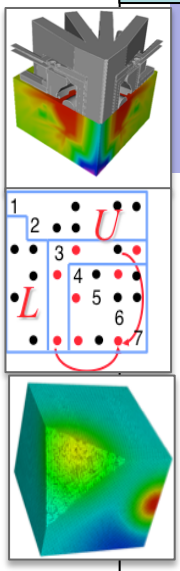
FASTMath technologies are used in 16 of 18 SciDAC application partnerships

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
Predictive Computing for Condensed Matter	So Hirata, UIUC	None	BES	
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	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	Panaggiotis 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	Esmong Ng, Rob Falgout	NP	Algebraic
Nuclear Computational Low-energy Initiative	Joseph Carlson, LANL	Esmond Ng, Chao Yang	NP	Algebraic
Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics	Frithjof Karsch, BNL	None	NP	

FASTMath has made considerable progress in the first year

Topical Areas



- Tools for problem discretization
- Solution of Algebraic systems
- High level integrated capabilities

Progress Categories

- New solution techniques
- Massive parallelism and mixed mode programming models
- Tool interoperability
- Demonstration in applications

Remainder of the talk highlights a few key examples of FASTMath progress; see the poster session for more details

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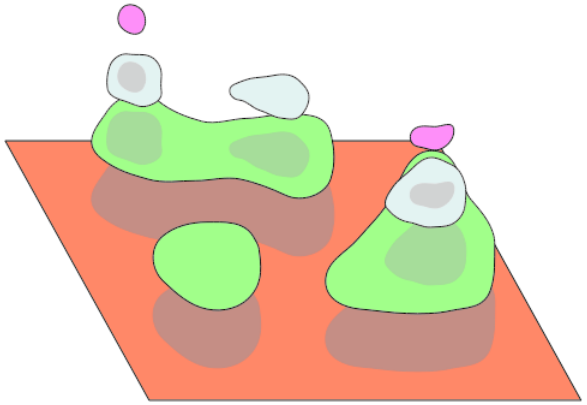
FASTMath is developing a new block-structured mesh refinement paradigm called region-based AMR

Goal: Improve efficiency and generality of AMR for block-structured grids by allowing different regions at the same level of spatial refinement to have different temporal refinement, as determined by optimal subcycling criteria

Technical Challenges:

- Redesign underlying software framework
- Modify time-advancement algorithms for grid-based and particle-mesh methods

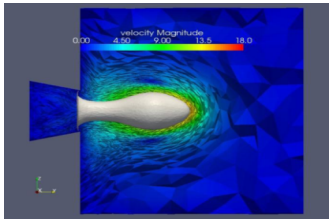


Progress to date:

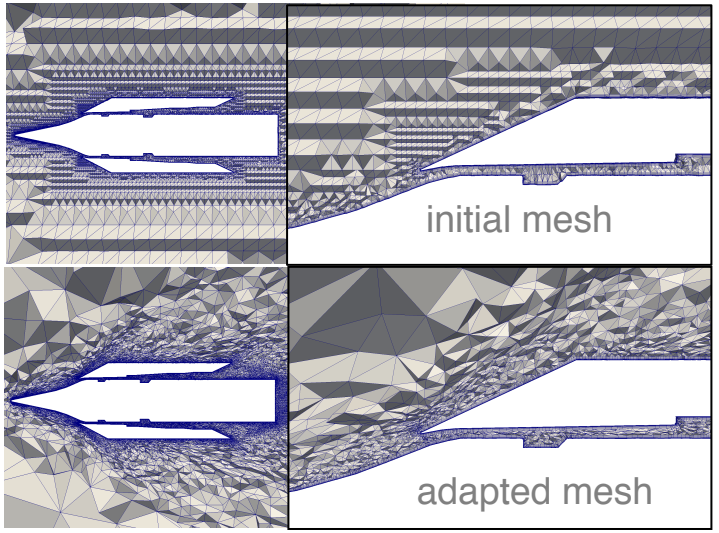
- New branch of BoxLib supports RAMR for non-adjacent regions
- New branch of Nyx (BoxLib-based cosmology code) now runs with RAMR for non-adjacent regions

Unstructured, high-order, anisotropic mesh adaptation tools now scale up to 64K processors

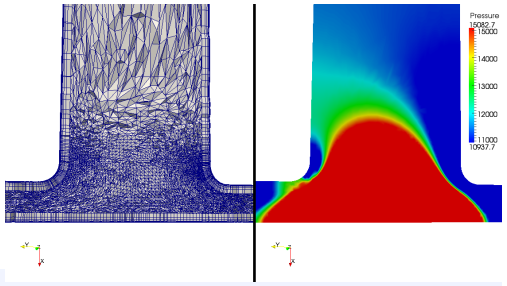
- **Goal**: A general tool for parallel anisotropic mesh adaptation, including curved elements that takes full account of geometry



- **Technical Challenges**:
  - Gaining scalability
  - Meeting specific application needs without loss of generality



- **Progress to date**:
  - Parallel execution up to 64K cores
  - Accepts general anisotropic mesh metric field
  - Full interaction with geometry
  - Support of semi-structured boundary layers

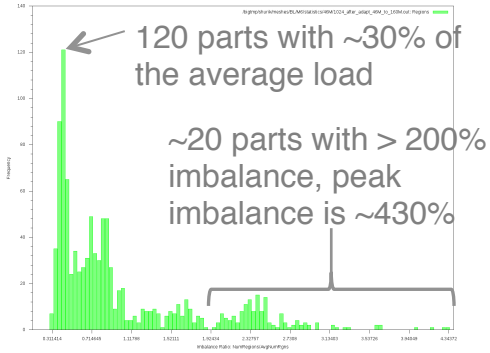


New massively parallel partitioning methods use mesh adjacencies to improve operational efficiency

Goal: Take advantage of the adjacency information in an unstructured mesh representation to control mesh partitions

Technical Challenges:

- Performing parallel graph type operations on a mesh topology
- Fast parallel methods to best partitions



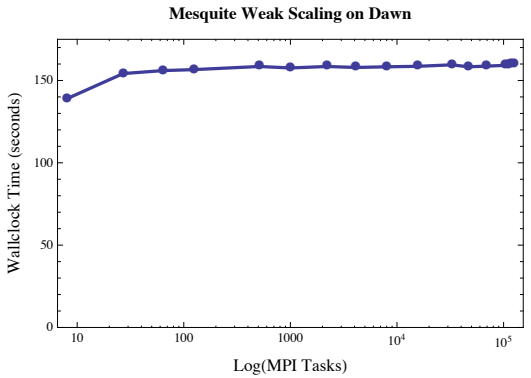
Histogram of estimated part imbalance after adaptation.

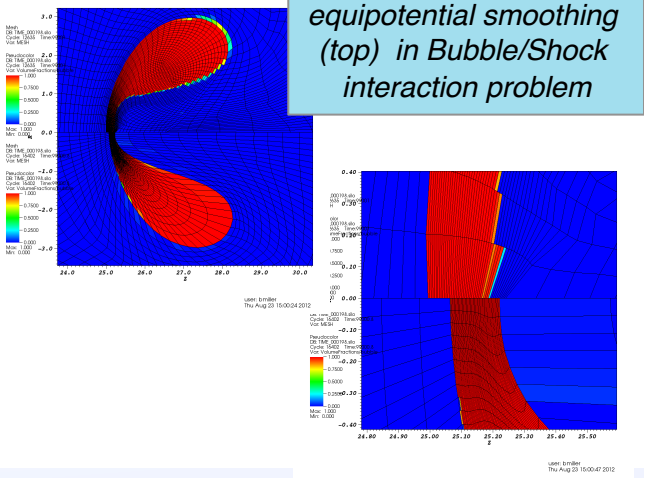
Progress to date:

- Multi-criteria partition improvement operational – strong scaling of 1B element mesh on 288K cores from 0.88 to 0.95
- An approach for fast predictive load balancing underway
- Additional fast partition improvements requested

FASTMath mesh quality tools have new material interface-preserving capabilities

- **Goal:** Provide mesh quality improvement through the *Mesquite* library
- **Technical Challenges:**
  - Use optimization to solve the problem for problem dependent element characteristics (e.g. vector field alignment, boundary meshes, anisotropies)
  - Use for structured, unstructured, hybrid grids in 2 & 3D
- **Progress:**
  - Parallel solution algorithms in Mesquite scale well up to 125,000 cores on BG/P
  - New parallel interface smoothing capabilities are effective on difficult bubble/shock interaction problem in ALE simulation
  - Currently working on mixed programming model approaches for next generation architectures





Side-by-side comparison of Mesquite (bottom) with equipotential smoothing (top) in Bubble/Shock interaction problem

FASTMath is developing a multi-rate time integration solver suite

- **Goal**: Time integration solver suite for multi-scale and multi-physics systems of equations having dynamics that evolve on multiple time scales.
- **Technical Challenges:**
  - Support for the broad array of operating modes inherent to DOE scientific computing applications: implicit, explicit and mixed implicit-explicit (IMEX), at varying orders of accuracy.
  - Determination of default error indicators and solver parameters that provide optimal solvers for a broad range of applications; or automated 'discovery' of such parameters at runtime.

- **Progress to date:**
  - Implemented time-adaptive implicit, explicit and IMEX Runge-Kutta solver infrastructure (ARKode) in SUNDIALS library.
  - Designed initial suite of multi-rate ODE and PDE test problems.
  - Constructed automated regression testing and parameter optimization utilities.

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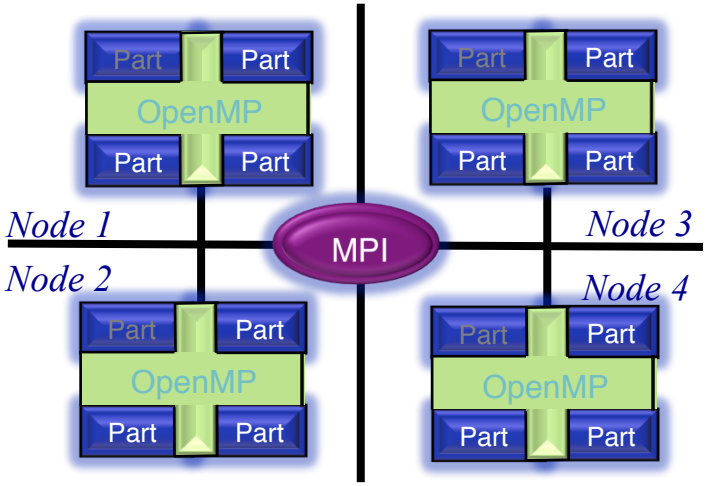
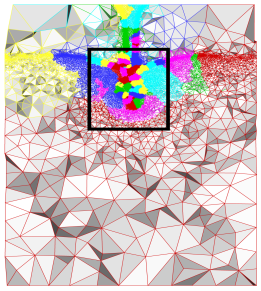
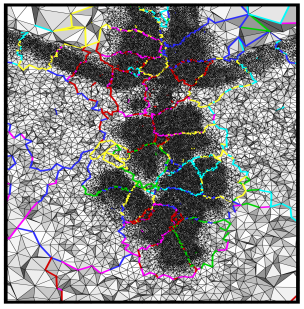
Interoperability of unstructured mesh tools at the exascale requires development of new interfaces

- **Goal**: Develop iMeshP to be an unstructured mesh interface that meets the needs of applications going to exascale
- **Technical Challenges**:
  - Effectively accounting for the expected architectures of exascale computers
  - Meeting the specific needs of the PDE solvers using iMeshP
- **Progress to date**:
  - Developing an architecture-aware two level partition approach
  - Migration (entity, set, tags), ghosting, partitioning supported
  - Multiple parts per process fully supported

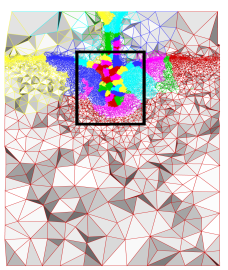


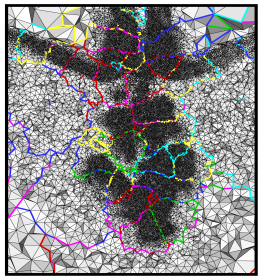




PHASTA demonstrates massively parallel unstructured mesh implicit PDE solver technologies

Goal: A finite element based implicit code that demonstrates excellent strong scaling on general ansiotropic meshes



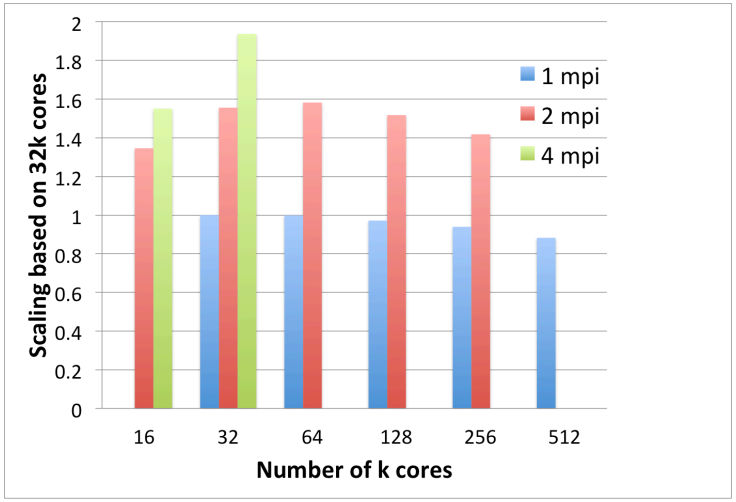


Technical Challenges:

- Methods to structure the parallel solve for partitioned unstructured meshes
- Scaling when using a broader set of FASTMath solvers

Progress to date:

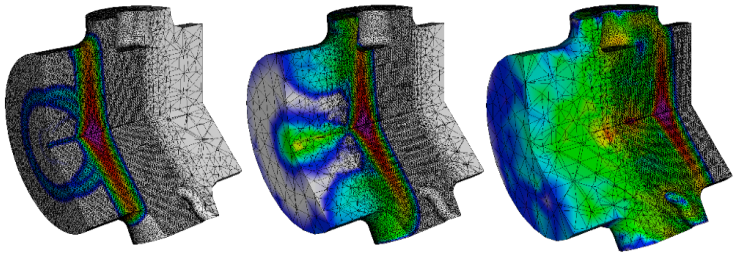
- Strong scaling on Mira
- Variable MPI processes per core
  - 1/core 88% scaling 32K to 512K
  - 2/core 135%-159% scaling
  - 4/core 150%-193% scaling



Application use of in-memory unstructured adaptive mesh tools

- **Goal**: Couple unstructured mesh solvers with mesh adaptation with focus on high performance and low development costs

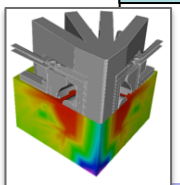
- **Technical Challenges:**
  - File-based methods have unacceptable parallel performance
  - Tight integration very costly to develop



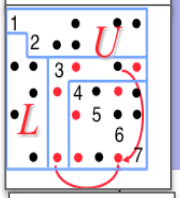
- **Progress to date:**
  - Defined an in-memory approach that requires minimal modification of the solver based on unstructured mesh API's
  - Addresses memory management issues with temporary copies
  - Implemented in PHASTA
  - Implementation started with Albany (Trilinos), ACE3P, FUN-3D

First year progress in FASTMath in the solution of algebraic systems

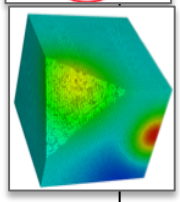
Topical Areas



Tools for problem discretization



Solution of Algebraic systems



High level integrated capabilities

Progress Categories

- New solution techniques
- Massive parallelism and mixed mode programming models
- Tool interoperability
- Demonstration in applications

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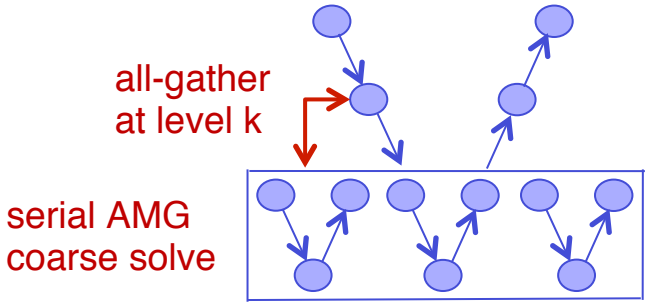
FASTMATH

New algorithms for reducing communication in algebraic multigrid (AMG) methods improve performance

Goal: Significantly speed up AMG on modern multicore architectures

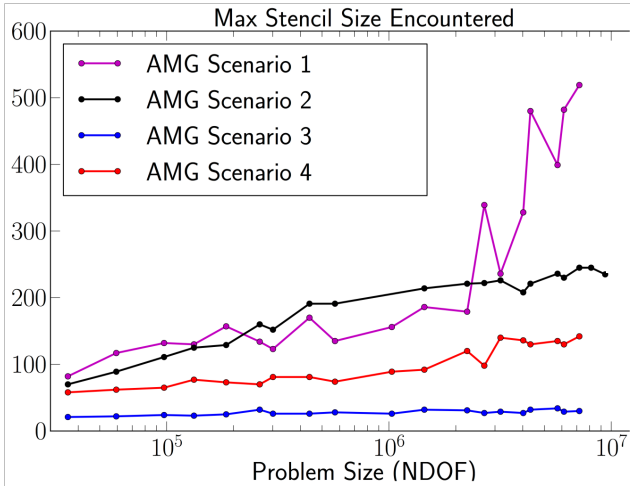


Main Technical Challenge:

- Reduce communication without destroying convergence properties

Progress to date:

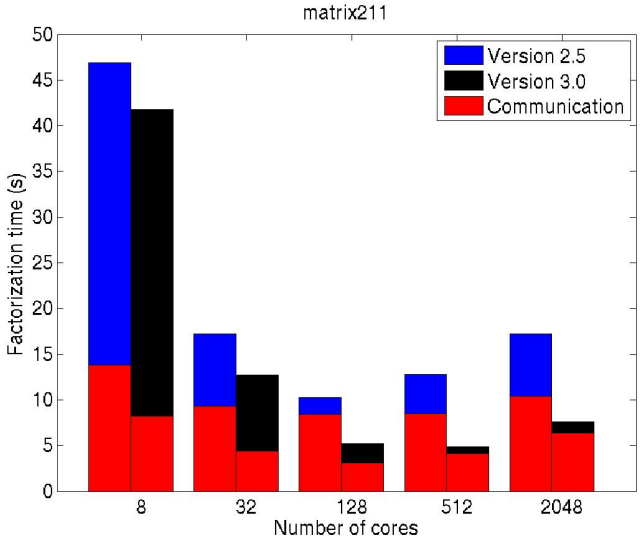
- Redundant coarse grid solve approach has produced speedups of up to 2x
- Method for defining non-Galerkin coarse-grid operators substantially reduces stencil size without sacrificing convergence



SuperLU work has optimized for communication and multicore architectures

Goal: Develop scalable sparse direct linear solvers that are essential in the simulations of the numerically challenging problems, e.g., accelerator, fusion, quantum chemistry, and fluid mechanics.

New scheduling:
Fusion Tokmak Sim. M3D-C1



Technical Challenges:

- High degree of task & data dependency (DAG), irregular data access & communication patterns.
- Memory and bandwidth constraints on many nodes and many cores per node.

Progress to date:

- Tighter scheduling algorithm for DAG execution reduced processes idle time -- 3x faster on 1000s cores.
- Light-weight OpenMP threads in MPI processes reduced memory footprint -- 2x memory reduction.

FASTMath is developing multithreaded kernels for sparse matrix operations

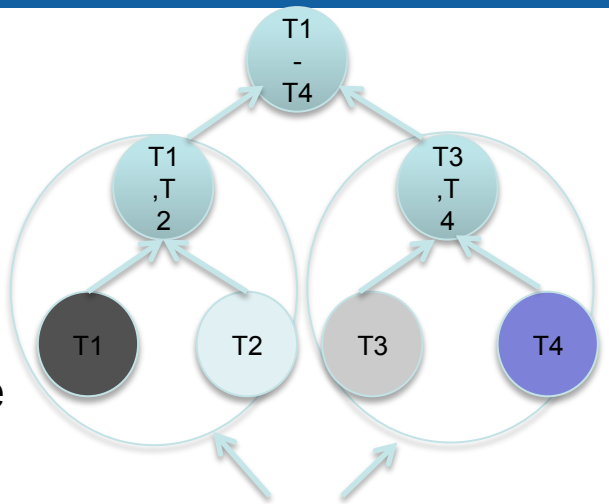
Goal: To design an abstract model/framework and implement various sparse matrix kernels within the framework

Technical Challenges:

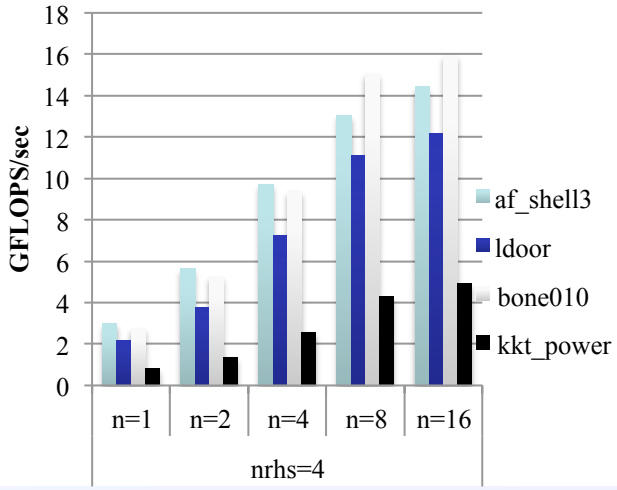
- Reducing the requirements of various kernels to a common framework and ensuring the framework can be supported by various multithreaded runtimes.

Progress to date:

- Designed a task based abstract model that can handle the various algorithms for sparse linear solvers.
- Used graph ordering techniques to extract tasks that map to the hierarchy of the machine.
- Implemented sparse matrix vector multiplication kernel with the task-based framework. (More details in the linear solver poster)



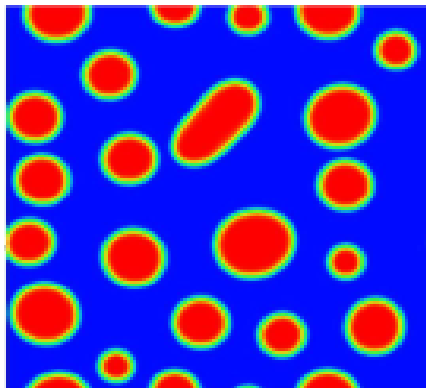
UMA Regions



FASTMATH

Scalable differential variational inequality (DVI) solvers show promise in void formation simulations

Goal: Create scalable DVI solvers to enable consistent and efficient modeling of transitional phenomena (phase changes, free boundaries, hybrid discrete-continuum)



Radiation-generated voids in nuclear fuel

Technical Challenges:

- Overcome physical and numerical inconsistencies; enable larger time steps and higher fidelity simulations

Progress to date:

- Developed semi-smooth and reduced-space active set VI solvers in PETSc (leveraging experience in TAO and PATH);
- Achieved mesh-independent convergence rates for Allen-Cahn system using Schur complement preconditioner (with algebraic and geometric multigrid)
- Validated DVI modeling approach against baseline results of CMSNF for void formation and radiation damage in nuclear fuel: Can use larger time steps than conventional methods, more stable than clamping. Extending to more complex models.

CMSNF
Center for Materials Science of Nuclear Fuel

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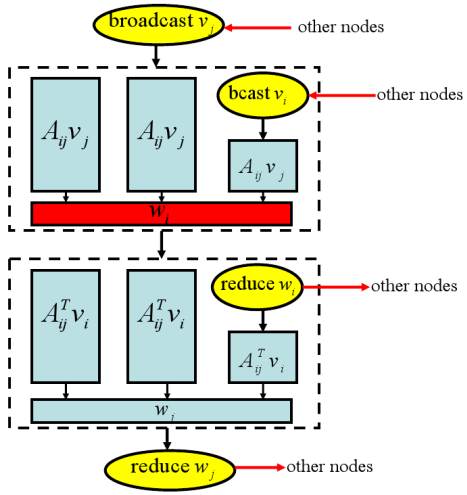
FASTMath will develop new eigensolvers for use in eight different SciDAC application partnerships

Goal: Develop efficient eigensolvers for large-scale linear and nonlinear eigenvalue problems



Algorithmic Challenges:

- Convergence rate
- Reduce complexity (orthogonalization, Rayleigh-Ritz)
- Maintain stability and reliability (early deflation, multiplicity etc.)

Progress to date:

- Developed a preliminary implementation of a penalty-based trace minimization algorithm for computing a large number of eigenpairs for sparse matrices
- Initiated the development of spectrum slicing algorithms that are based on shift-invert Lanczos and contour-integral projection method.

FASTMath eigensolvers work has already significantly improved scalability

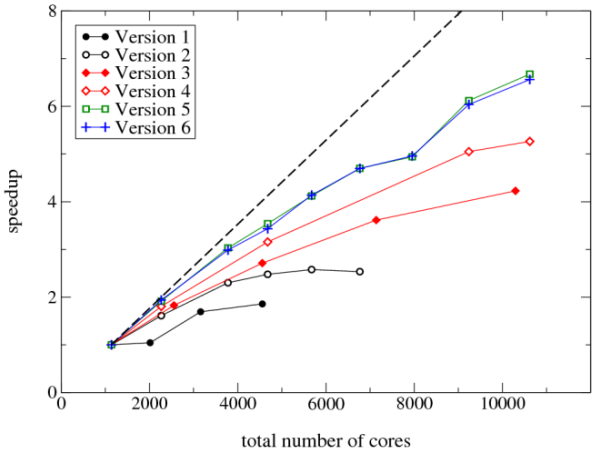
Goal: Develop efficient eigensolvers for large-scale linear and nonlinear eigenvalue problems

Scalability Challenges:

- Exploit concurrency for leadership class machines
- Reduce communication overhead
- Leverage highly efficient computational kernels (e.g. BLAS3)

Progress to date:

- Developed an efficient way to overlap MPI communication with OpenMP thread-based computation in the Lanczos algorithm;
- Use topology-aware task distribution scheme to reduce communication overhead



FASTMath nonlinear solvers enable larger time steps with the ParaDiS dislocation dynamics code

Goal: Improve time integrators and nonlinear solvers within ParaDiS so that larger time steps can be taken

Technical Challenges:

- Expensive force calculations
- Discontinuous topological events
- Problem size changes rapidly

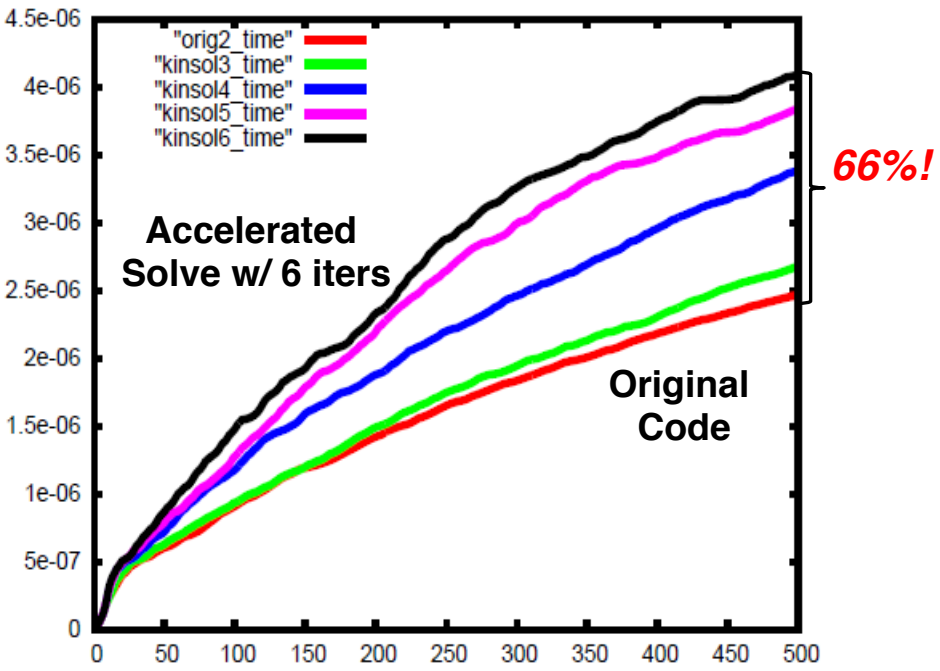
Progress to date:

- Interfaced ParaDiS to SUNDIALS suite
- Added acceleration to nonlinear solve
- Jacobian verification for Newton solver

Results:

- Initial results show significant increase in time step size

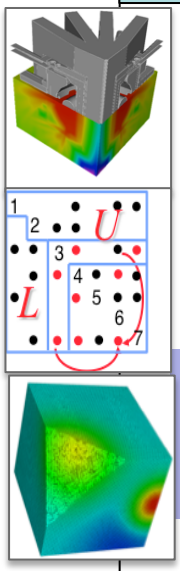
Acceleration allowed longer simulation times for set number of time steps



Observed 45% decrease in runtime for a set simulation time

First year progress in FASTMath in high-level integrated capabilities

Topical Areas



- Tools for problem discretization
- Solution of Algebraic systems
- High level integrated capabilities

Progress Categories

- New solution techniques
- Massive parallelism and mixed mode programming models
- Tool interoperability
- Demonstration in applications

Remainder of the talk highlights a few key examples of FASTMath progress; see the poster session for more details

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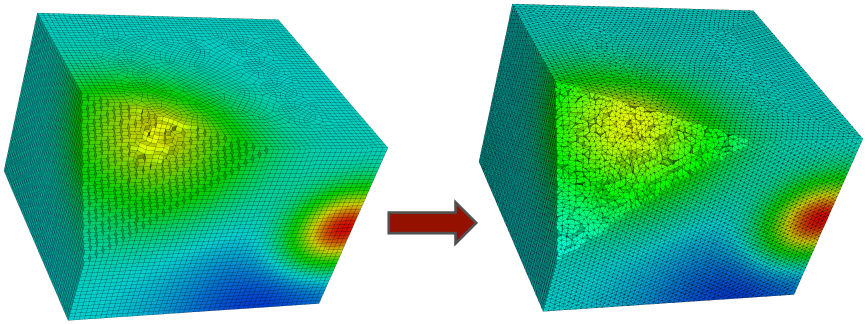
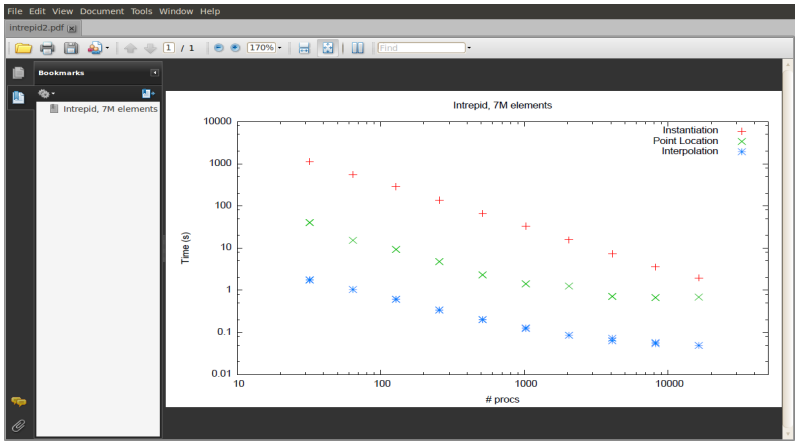
New software capabilities for coupling existing codes for multi-physics applications

- *MBCoupler* tool provides parallel point location, solution interpolation, and various constraint enforcement schemes (e.g. global conservation) for a variety of discretization (FE, SE) and element types (tet, hex)
- *Coupe* driver for various loose and tight coupling schemes, coordinating calls to physics modules, solution transfer, and convergence/time stepping



7M Hexes 28M Tets



Mesh-Solver Chombo/PETSc Interoperability improves robustness of application simulations

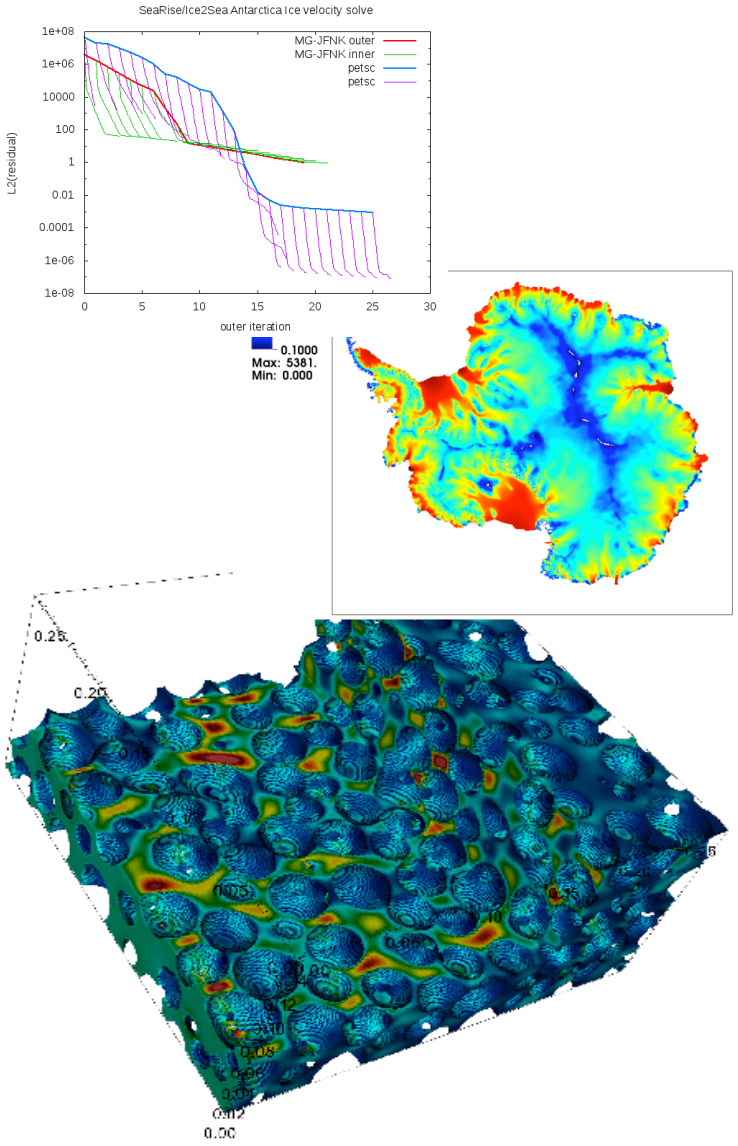
Goal: Facilitate the combination of Chombo discretization support and the PETSc solvers to improve robustness for porous media and climate applications

Technical Challenges:

- Complex geometry and boundary conditions
- Viscous tensor nonlinear equations
- Large jumps in material coefficients

Progress to date:

- Map AMR sparse index space to global equation for sparse solver.
- Able to solve porous media problems using hypre, GAMG, ML and PETSc wehre geometric multigrid method failed
- Used PETSc nonlinear JFNK level solver with AMG solvers for more robust solution to BISICLES ice sheet modeling code



Automating interoperability of Chombo mapped multiblock modules and Hypre solvers for fusion app

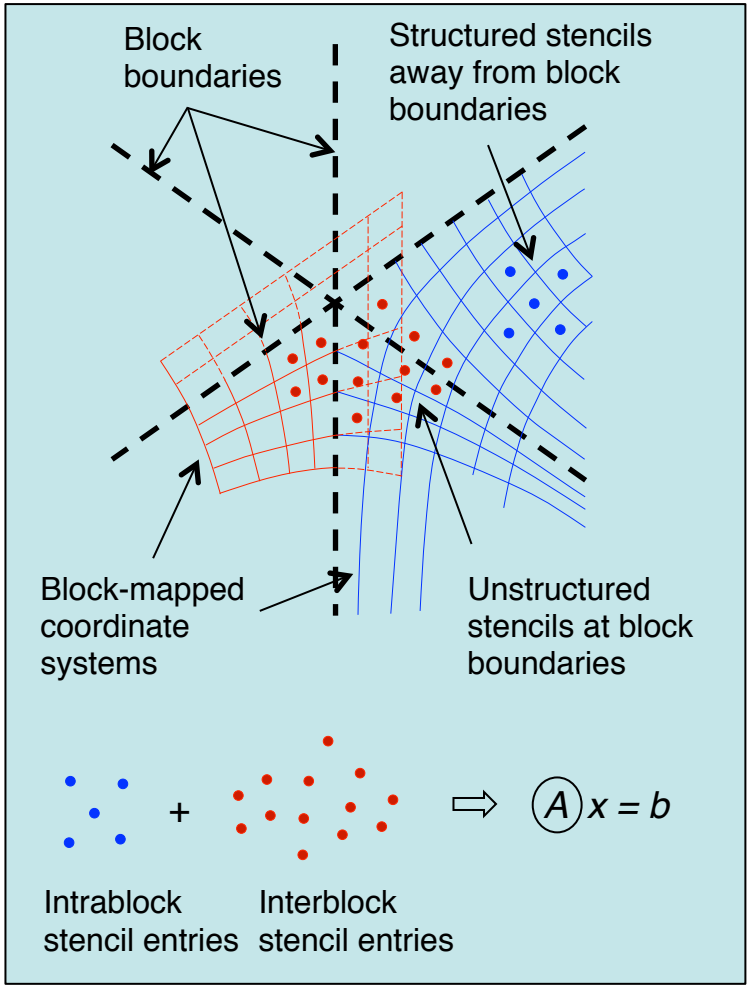
Goal: Combine Chombo mapped-multiblock discretization and Hypre semi-structured (SStruct) interface

Technical Challenges:

- High-order interpolation used in mapped-multiblock finite-volume discretizations yields unstructured stencils at block boundaries
- Hypre SStruct interface accommodates multiple blocks ("parts") and manual specification of arbitrary stencil couplings at block boundaries, but *this is tedious and error-prone, especially for high-order discretizations*

Progress to date:

- Developing an interface to automate matrix construction given (structured) intrablock stencils and Chombo-generated (unstructured) interblock stencils
- Testing new interface with the Hypre BoomerAMG solver in the Chombo-based COGENT gyrokinetic edge code



Extending mapped multiblock infrastructure to support Chombo-SUNDIALS combined use

Goal:

1. Improve Mapped Multiblock Infrastructure for AMR
2. Enable use of SUNDIALS solvers in Chombo AMR simulation codes

Technical Challenges:

- Inter-block communication infrastructure to support conservation at block boundaries
- Mapping between LevelData and NVector data structures
- Interfaces to Chombo's AMR solvers

Progress to date:

- BlockRegister classes implemented and tested
- Single-level NVector/LevelData interface implemented and tested (J. Dahm)

Interoperability of FASTMath unstructured mesh tools used in ice sheet modeling application

Goal: Provide adaptivity across the software stack

Technical Challenges:

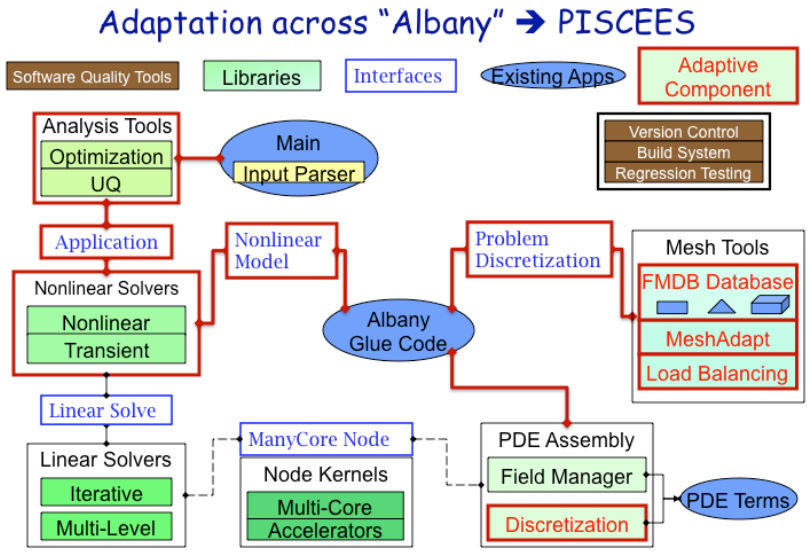
- Solution transfer
- Load balancing

Progress to date:

- Re-load balance with STK/Zoltan
- Reform Albany state data structures and develop/rework interfaces

Applications:

- PISCEES ice sheet modeling
- Leverage for weld deformation and failure/ fracture applications



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

Lawrence Berkeley National Laboratory

- Ann Almgren
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- Dan Graves
- Sherry Li
- Terry Ligocki
- Mike Lijewski
- Peter McCorquodale
- Esmond Ng
- Brian Van Straalen
- Chao Yang

Sandia National Laboratories

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- Vitus Leung
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- Mark Miller
- Carol Woodward
- Ulrike Yang

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- Jim Demmel

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- Mark Adams

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- Lois Curfman McInnes
- Todd Munson
- Barry Smith
- Tim Tautges

Rensselear Polytechnic Institute

- Mark Shephard
- Onkar Sahni

Southern Methodist University

- Dan Reynolds

Colorado University at Boulder

- Ken Jansen

FASTMath posters provide more details

1. **Block Structured AMR: Algorithms and Applications**
   POC: Ann Almgren, LBNL
2. **FASTMath Unstructured Mesh Technologies**
   POC: Mark Shephard, RPI
3. **Data Partitioning for Scientific Applications and Emerging Architectures**
   POC: Karen Devine, SNL
4. **Linear system solution in FASTMath Software**
   POC: Ulrike Yang, LLNL
5. **FASTMath Nonlinear Solvers and Time Integrators**
   POC: Andy Salinger, SNL
6. **Numerical Algorithms for Large-Scale Eigenvalue Calculation**
   POC: Chao Yang, LBNL
7. **Architecture-aware themes in FASTMath Algorithms and Software**
   POC: Jed Brown, ANL
8. **Mesh and Solver Interoperability in FASTMath**
   POC: Mark Adams, Columbia

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FASTMATH

In Memorandum

Francisco Xabier Garaizar

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