U.S. DEPARTMENT OF ENERGY | Office of Science

FASTMath: Frameworks, Algorithms and Scalable Technologies for Mathematics

Lori Diachin, LLNL

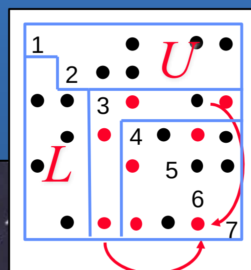
Institute Director

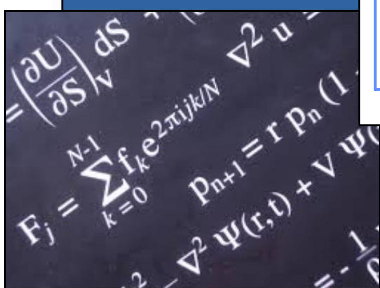
FASTMATH

The FASTMath project brings leading edge computational mathematics technologies to the SciDAC Program

Develop advanced numerical techniques for DOE applications

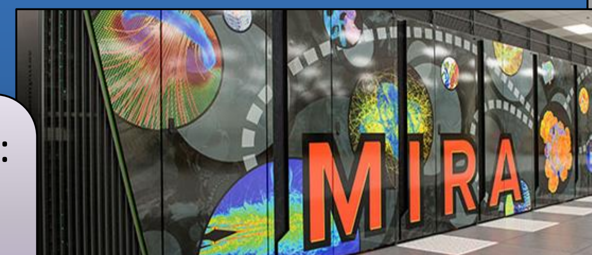
- Eight focused topical areas based on application needs
- High level synergistic techniques



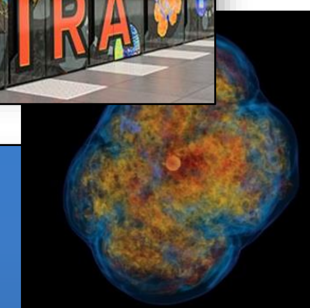


Deploy high-performance software on DOE supercomputers

- Algorithmic and implementation scalability
- Performance Portability
- Interoperability of libraries



FASTMath Objective: Reduce the barriers facing application scientists



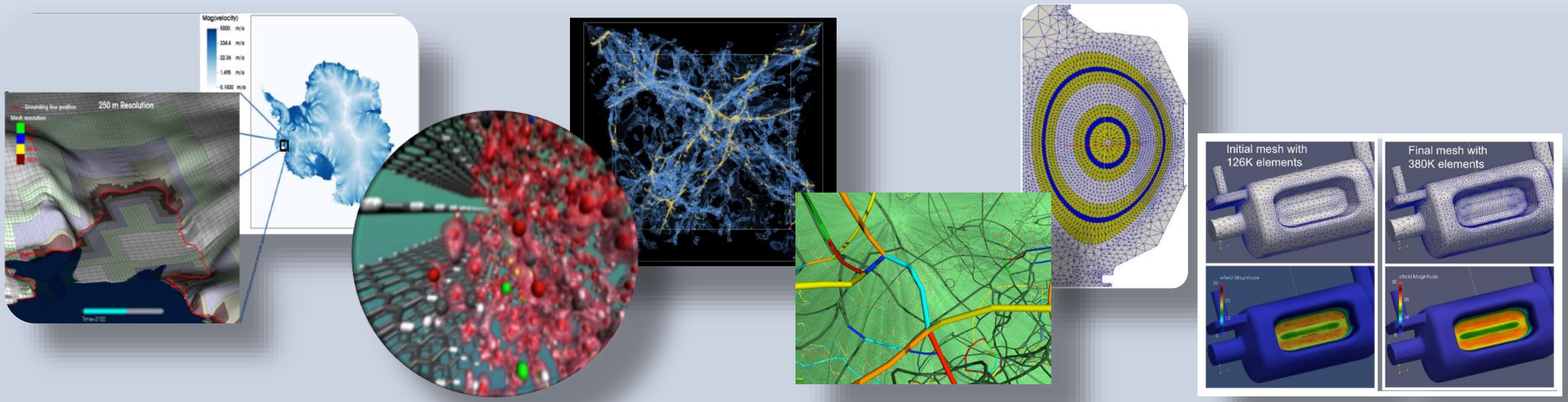
Demonstrate basic research technologies from applied mathematics

- Build from existing connections with basic research
- Focus on research results that are most likely to meet application needs

Engage and support of the computational science community

- Publications and presentations in highly visible venues
- Team tutorials
- Workforce pipeline and training
- Web presence

The FASTMath team has a proven record of advancing application simulation codes



Next Generation Application Codes

- Created unique DOE capabilities in ice sheet modeling
- First ever, self consistent solution of continuum gyrokinetic system in edge plasmas
- Unprecedented resolution for Nyx cosmology code

Faster Time to Solution

- New eigensolvers 2X faster for quantum chemistry software
- Parallel PEXSI software enabled electronic structure calculations with 10,000 atoms (compared to 1000's)
- Accelerated nonlinear solver enabled largest dislocation dynamics simulation with ParaDiS

More Robust Simulations

- Dramatically decreased time to generate meshes for fusion tokamak codes
- Adaptive mesh refinement and discretizations to resolve ELM disruptions in tokamaks
- Order of magnitude improvement in accuracy of integral calculations in material chemistry

There are still a large number of advances to made through strong partnerships between mathematicians and application scientists

The SciDAC-4 FASTMath Institute leverages and builds on the successes of SciDAC-3 to meet application needs

FASTMATH 3 + QUEST

+ Time Discretization
+ Numerical Optimization =
+ Data Analytics

FASTMATH 4

FASTMath brings together an exceptional team of researchers and software library capabilities

Our team comprises over 50 researchers from 5 national laboratories and 5 universities

BERKELEY LAB

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

Sandia National Laboratories

Boulder

USC

MIT

Rensselaer

SMU

Our software has 100s of person years of development behind it

SuperLU

sundials

PETSc

mfem

ZOLTAN

PUMi Parallel Unstructured Mesh Infrastruc

hypre high performance preconditioners

PEXSI

AMReX

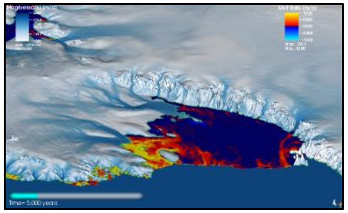
UQTk

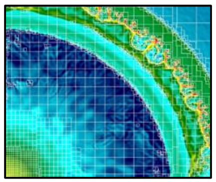
Trilinos

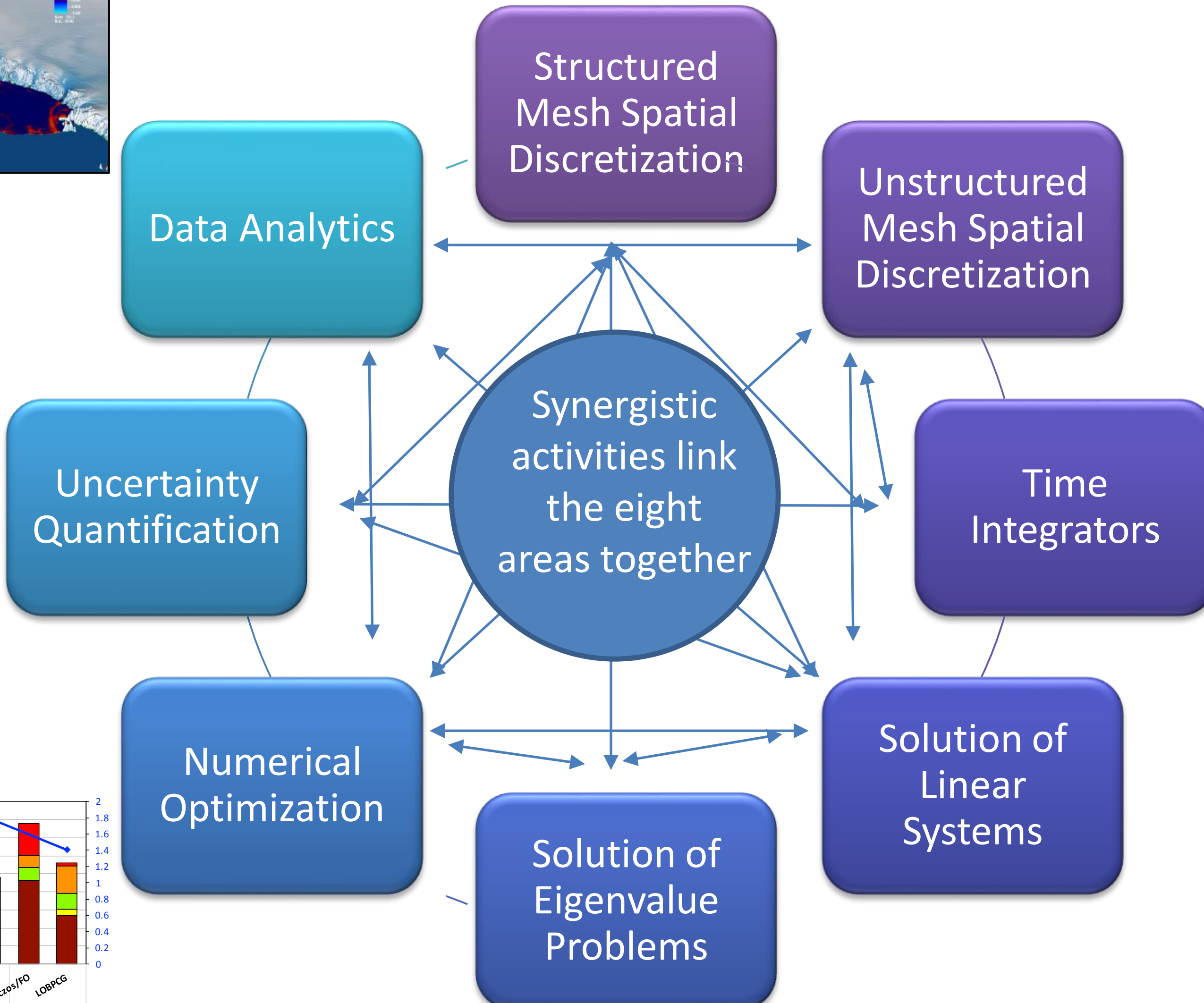
Albany

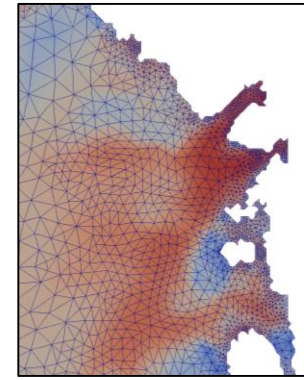
DAKOTA

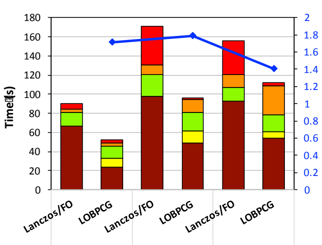
FASTMath is focused on eight core technology areas and the synergies among them

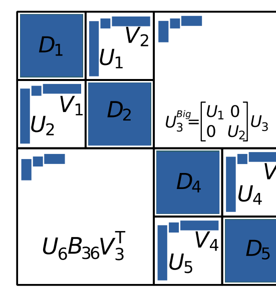










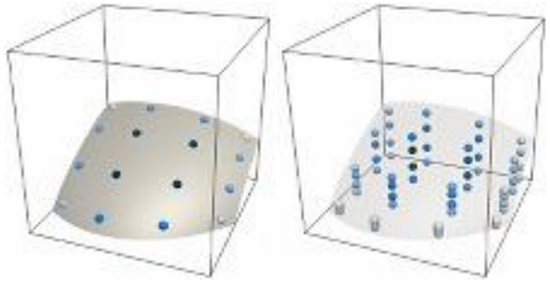


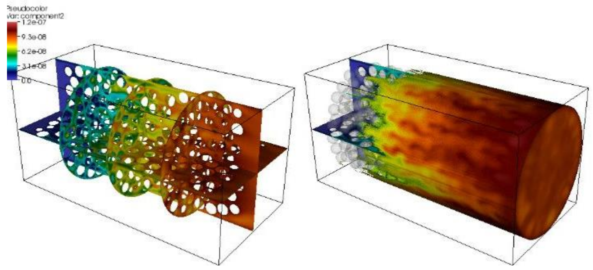
U.S. DEPARTMENT OF ENERGY | Office of Science

FASTMATH

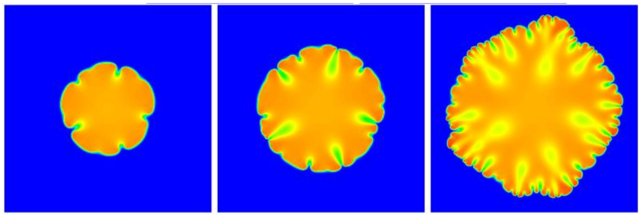
Structured Mesh Discretization Tools

- **Goal:** Provide software support for efficient parallel solution of a large variety of problems in science and engineering using block-structured adaptive mesh approaches
- **Software frameworks:** AMReX, Chombo
- **FASTMath Tasks:**



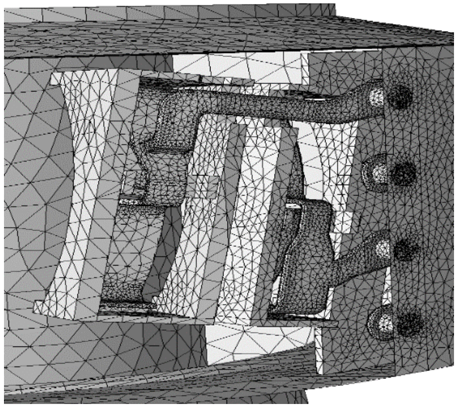


  - High-order representations of fixed and moving interfaces in structured grid simulations
  - Improved mapped multi-block methods
  - Support for higher-order time stepping based on spectral deferred corrections
  - Improved interoperability with SUNDIALS and hypre



- **For more information:** Ann Almgren(ASAlmgren@lbl.gov)

Unstructured Mesh Discretization tools



- **Goal:** Scalable and performant unstructured mesh tools to support complex geometry applications
- **Software tools:** Albany, EnGPar, MeshAdapt, MFEM, PHASTA, PUMI, Zoltan/Zoltan2
- **FASTMath Tasks:**

Mesh Adaptation
- Conforming and non-conforming adaptation
- High-order curved mesh adaptation
- Anisotropic adaptivity
- Adaptation in UQ space
- Parallel meshes with particles methods
- Combined mesh motion and adaptation
- Effective in-memory integration methods

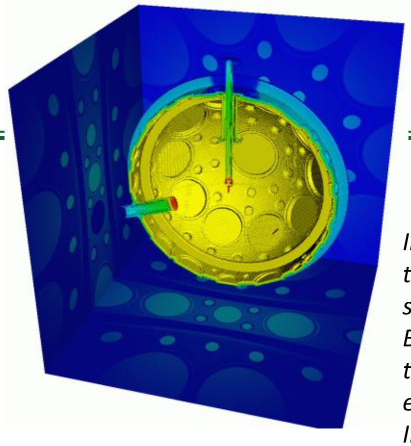
Scalable & Performant
- Performant on latest many core and hybrid systems nodes
- Robust and fast dynamic multi-criteria load balancing
- Architecture aware load balancing
- Performant portability using latest tools
- In situ visualization and problem modification

Discretization Technologies
- High-order FEM
- Stabilized FEM for complex flow problems
- Non-linear coupled mechanics
- Error estimation procedures
- Conservative field transfer
- Scalable and performant on the latest systems

- **For more information:** Mark Shephard (shephard@scorec.rpi.edu)

FASTMATH

Time Integrators



Intensity in NOVA test chamber; solution of Boltzmann transport equation using IDA

- **Goal:** Efficient and robust time integration methods and software for stiff implicit, explicit, and multirate systems in DOE applications
- **Software tools:** SUNDIALS, PETSc, AMReX
- **FASTMath Tasks:**

Time Integrators for Multirate Systems in SUNDIALS

- Implement 4th order 2-rate explicit integrator
- Implement variable step two-rate IMEX methods
- Develop 3-rate IMEX multirate methods and implement for a reaction-advection-diffusion problem in the AMReX package

Spectral Deferred Correction Methods for AMReX

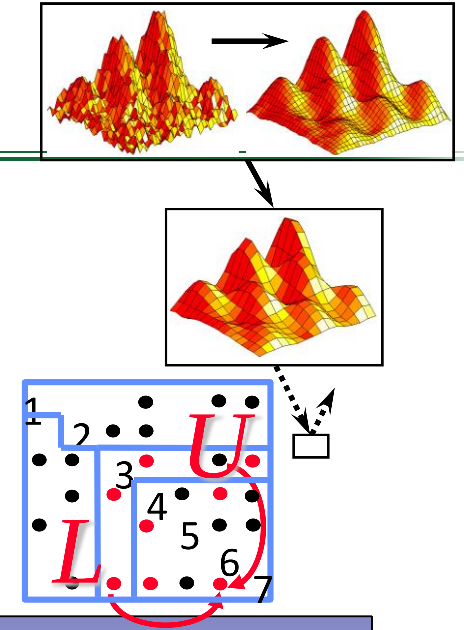
- Develop high-order spectral deferred correction (SDC) method in AMReX
- Addition of high-order multiple-level SDC in AMReX
- Enhance the SDC in AMReX to include dynamic AMR with error estimation

Enhancements to Time Integrators in SUNDIALS and PETSc

- Parallel-in-time capability added to SUNDIALS
- Efficiency additions for multiple forward integrations in single integrator in PETSc
- Solution constraint handling added to SUNDIALS ODE integrators

- **For more information:** Carol Woodward (woodward6@llnl.gov)

FASTMath Linear Solvers



- **Goals:** Providing efficient direct and iterative linear solvers and preconditioners for large scale parallel computers.
- **Associated software packages:** hypre; PETSc; MueLu, ShyLU (Trilinos); KokkosKernels; SuperLU; STRUMPACK; symPACK
- **FASTMath Tasks:**

Efficient kernels and solvers

- On-node and GPU kernels for iterative solvers
- Develop efficient linear solvers for systems with multiple right hand sides
- Improve scalability for hierarchical low-rank preconditioners
- Design and deploy local discrete convolution methods (LDCMs)

Develop multigrid methods

- Design and implement semi-structured multigrid methods that effectively use grid structures
- Implement efficient Schur complement-based multilevel algorithms for strongly coupled multi-physics systems
- Develop fast hybrid geometric/algebraic multigrid solvers for elliptic and hyperbolic systems

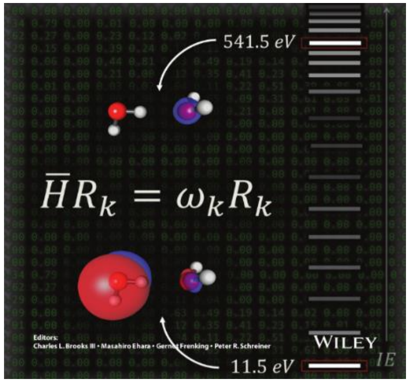
Deploy highly efficient direct linear solvers

- Investigate and implement butterfly-based data-sparse methods
- Decrease communication in symmetric indefinite solvers
- Improve structural and data sparsity through scalable ordering and symbolic factorization algorithms

- **For more information**: Ulrike Yang (yang11@llnl.gov)

FASTMath Eigenvalue Toolset

- **Goal:** Scalable eigenvalue computation tools for linear and nonlinear eigenvalue problems in DOE applications
- **Software tools:** FASTEig (a collection of eigensolvers for a variety of eigenvalue problems)
- **FASTMath Tasks:**



Efficient algorithms for eigenvalue computation
- Spectrum slicing for many eigenpairs
- Pade approximation and linearization, compact rational Krylov for nonlinear problems
- Algorithms for tensor eigenvalue problems
- Structure preserving algorithms for linear response and spectroscopy

Scalable implementation for distributed many-cores and GPUs
- Increase concurrency though multilevel algorithms and randomization
- Load balancing
- Overlap computation with communication

Deploy solvers in software packages used in DOE SciDAC and other applications
- Linear eigensolver for Quantum Espresso, PARSEC, NWChemEX
- Structure eigensolver for BerkeleyGW
- Linear response eigensolver for Chronus-Q
- Solvers for iTensor

- **For more information:** Chao Yang (CYang@lbl.gov)

Numerical Optimization Tools

- **Goal:** Develop methods for numerical optimization problems with constraints and for sensitivity analysis using adjoint capabilities.
- **Software tools:** MATSuMoTo, MINOTAUR, ORBIT, ROL, TAO
- **FASTMath Tasks:**

Dynamic Optimization

- Deliver new capabilities for problems with PDE constraints that include:
  - Dynamics and controls
  - State and design constraints
  - Discrete variables
  - Multiple objectives
- Support a range of derivative requirements

Sensitivity Analysis

- Develop iterative sampling methods that employ sensitivity analysis and surrogate models to determine the most important parameters
- Explore multilevel approach that uses a low-fidelity model to predict parameter sensitivities

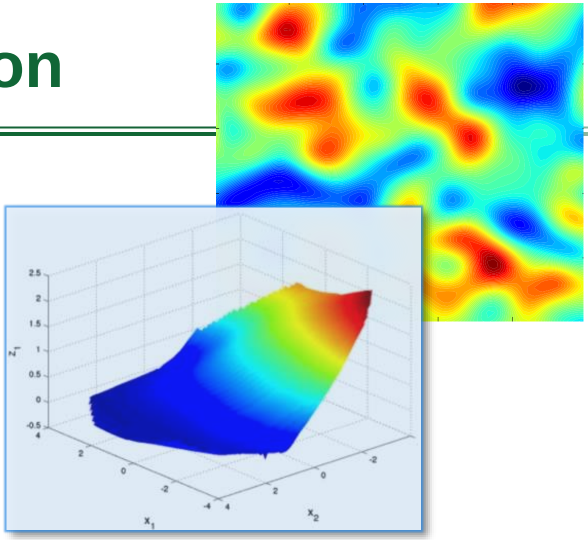
Adjoints

- Develop advanced adjoint and forward sensitivity capabilities to provide essential derivative information
- Provide methods for computing the action of second-order adjoints
- Support calculations involving many quantities of interest arising from constraints and multiple objectives

- **For more information:** Todd Munson (tmunson@mcs.anl.gov)

FASTMATH

Uncertainty Quantification



- **Goal:** Provide robust and efficient capabilities for uncertainty quantification in large-scale computations of physical systems.
- **Software tools:** DAKOTA, UQTk
- **FASTMath Tasks:**

Deploy advanced algorithms in UQ tools
- Functional low rank decompositions on mixed spaces
- MCMC methods focused on likelihood informed subspaces
- Adaptive basis
- Multilevel multifidelity
- Regression and classification
- Model error

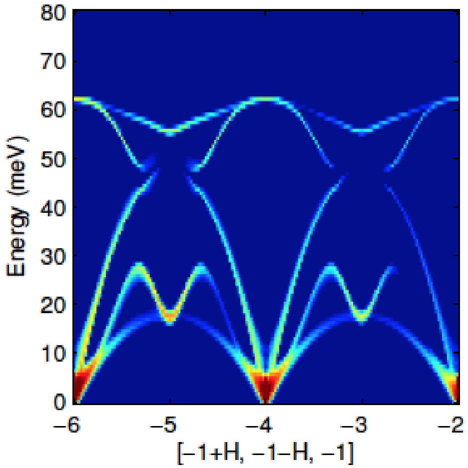
Advance UQ methods
- Adaptive low rank sparse constructions
- Parallel SDE sampling on manifolds
- Multilevel UQ based on sparse low rank emulators
- Online local surrogate refinement coupled with data driven dimension reduction

Tools for optimization under uncertainty
- Recursive trust-region model management for optimization across deep model hierarchies
- Advanced methods for probability of failure estimation
- Reliability based OUU for design in the presence of rare events

- **For more information:** Habib N. Najm (hnnajm@sandia.gov)

FASTMATH

Data Analytics



- **Goal:** Sparse functional representation of data, to enable faster IO and analysis of big datasets
- **Software tools:** Tasmanian, PUMI, TAO
- **FASTMath Tasks:**

Sparse IO of Big Data
- Advanced sampling techniques for distributed data
- Research adaptive methods for sparse representation
- Build accurate uncertainty estimates for sparse representations of data

Fast Estimation & Evaluation
- Develop and design high order regularizers that optimize functional representations of data
- Surrogate models that accelerate estimation and evaluation of sparse data approximation

Streaming Data Ranking
- Algorithms that maximize information transfer
- Ordered sparse functional representations of data
- Parallel methods for streaming distributed datasets

- **For more information:** Rick Archibald (ArchibaldRK@ornl.gov)

FASTMATH

Synergystic activities will results in new capabilities or higher efficiencies

New Capabilities

- Optimization under uncertainty
- Discrete and multi-objective optimization for data analytics
- In situ simulation on unstructured meshes

Higher Efficiency

- Leverage multiple right hand sides from optimization and UQ ensembles in linear and nonlinear solvers
- Adaptivity in the spatial and stochastic space in UQ on unstructured grids;
- Dynamic UQ load balancing
- In situ simulation on unstructured meshes

FASTMath Organization and Team

Institute Management
Lori Diachin, LLNL, Director
Esmond Ng, LBNL, Deputy Director

Institutional POCs
T. Munson, ANL
E. Ng, LBNL
L. Diachin, LLNL
R. Archibald, ORNL
M. Shephard, RPI
K. Devine, SNL

Software Strategy
U. Yang, LLNL
C. Smith, RPI
B. Smith, ANL
B. Debusschere, SNL

CS Institute Outreach
S. Wild, ANL
K. Jansen, UCB
R. Archibald, ORNL

Scientific Application Outreach
E. Ng, LBNL
M. Shephard, RPI
H. Najm, SNL
C. Woodward, LLNL
T. Munson, ANL
A. Salinger, SNL

Community Outreach
L. McInnes, ANL
M. Shephard, RPI
X. Li, LBNL
K. Devine, SNL

LCF and NERSC Facility POCs
R. Hartman-Baker, NERSC
J. Hill, OLCF
T. Williams,ALCF

Structured Mesh
A. Almgren, LBNL

P. Colella, LBNL
D. Martin, LBNL
P. McCorquodale, LBNL
R. Saye, LBNL

Unstructured Mesh
M. Shephard, RPI

O. Sahni, RPI
G Slota, RPI
C. Smith, RPI
S. Seol, RPI
K. Jansen, UCB
T. Kolev, LLNL
V. Dobrev, LLNL
K. Devine, SNL
A. Salinger, SNL
D. Ibanez, SNL

Time Integrators
C. Woodward, LLNL

D. Reynolds, SMU
H. Zhang, ANL
B. Smith, ANL
L. McInnes, ANL
D. Gardner, LLNL
J. Loffeld, LLNL
M. Minion, LBNL

Linear Systems
U. Yang, LLNL

R. Falgout, LLNL
J. Schroder, LLNL
M. Adams, LBNL
P. Colella, LBNL
X. Li, LBNL
E. Ng, LBNL
P. Ghysels, LBNL
M. Jacquelin, LBNL
H. Zhang, ANL
B. Smith, ANL
J. Hu, SNL
S. Rajamanickam, SNL

Eigensystems
C. Yang, LBNL

O. Marques, LBNL
E. Ng, LBNL
M. Jacquelin, LBNL

Numerical Optimization
T. Munson, ANL

S. Lyeffer, ANL
S. Wild, ANL
H. Zhang, ANL
J. Mueller, LBNL
M. Perego, SNL

Uncertainty Quantification
H. Najm, SNL

R. Ghanem, USC
Y. Marzouk, MIT
B. Debusschere, SNL
M. Eldred, SNL
J. Jakeman, SNL
C. Safta, SNL
K. Sargsyan, SNL

Data Analytics
R. Archibald, ORNL

H. Tran, ORNL
K. Jansen, UCB

FASTMath is actively engaged with 18 SciDAC-4 application partnerships

BER (5)

- Structured grid AMR
- Unstructured grid AMR
- Time integration
- Linear/Nonlinear solvers, Preconditioners
- Optimization
- Verification / UQ

FES (5)

- Unstructured meshes
- Discretization technologies
- Iterative Linear solvers
- UQ

HEP (3)

- Direct solvers
- Structured Grid AMR
- Optimization
- Sensitivity Analysis
- Inference and machine learning

NP (2)

- Structured grid AMR
- Eigenvalue problems
- Inference and Machine Learning

BES (2)

- Nonlinear and tensor eigenvalue problems
- Linear solvers and Preconditioners

NE (1)

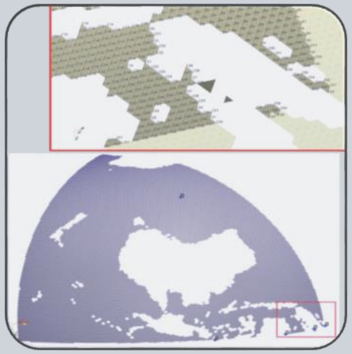
- UQ

FASTMath and RAPIDS will actively collaborate to continue to improve math libraries and application experience

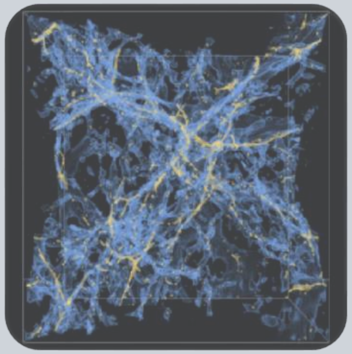
RAPIDS + FASTMATH

- **Performance improvements to math library software**
  - Improved scaling (identify performance bottlenecks, find ‘performance bugs’, eliminate unnecessary communication)
  - Improved on-node performance (programming models, memory)
- **Using performance models to improve foundational understanding of algorithms**
- **Advanced visualization tools for FASTMath tools (e.g., AMR)**
- **In situ visualization tools for unstructured mesh simulation workflow**
- **Use CS abstractions to improve/accelerate application development**
  - Domain Specific Language compilers/tools
  - Leverage abstractions developed by RAPIDS for I/O to unify application experience

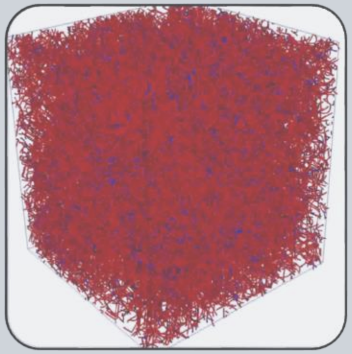
Math-CS collaborations led to significant advances in SciDAC-3 application sciences



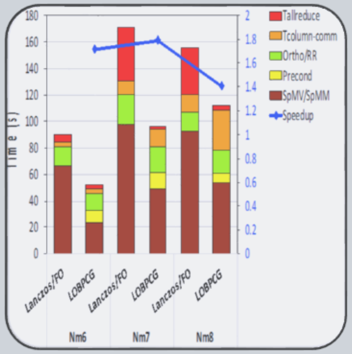
Increased accuracy of MPAS Ocean modeling system through improved scaling and improved partitioning algorithms



Development of highly-scalable, many core-aware multigrid solver increased ability of cosmologies to simulated evolution and fate of the universe (HPGMG in BoxLib)



New nonlinear solver and evaluation of OpenMP performance enabled largest dislocation dynamics simulation using ParaDiS



Improved efficiency of eigensystem solution reduced time to solution in large, sparse ab initio calculations in nuclear structure

FASTMath will leverage the software integration strategy adopted by the ECP math libraries area

- **FASTMath software products have varying degrees of interoperability, maturity, robustness, user support**
- **Goals: Build a more integrated, high-performing software base for applications; share software development best practices internally and across DOE**
  - *Deployment and Distribution*: All FASTMath products are required to meet a mall set of software quality requirements (versioning/ documentation); leverage xSDK and IDEAS efforts
  - *Integration* of three or more FASTMath products together; focus on deployment and usability; testing and documentation of combined use
  - *Ease of adoption* through a web based portal providing links to our software; SPACK FASTMath module; maintain installations on DOE LCFs

For more information…

- **Contacts:**
  – Lori Diachin, Director (diachin2@llnl.gov)
  – Esmond Ng, Deputy Director (egng@lbl.gov)
  – Any of the numerical components leads
- **Web site:**
  – www.fastmath-scidac.org