FASTMath: An overview of mathematical algorithms and software

FASTMath Team
Lori Diachin, Institute Director

FASTMath SciDAC Institute
Mathematical algorithms and software are foundational to HPC simulations

- 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…
First consider a very simple example

- 1D rod with one end in a hot water bath, the other in a cold water bath
- Mathematical Model

$$\nabla^2 T = 0 \in \Omega$$

$$T(0) = 180^\circ \quad T(1) = 0^\circ$$

Hot Water Bath  |  |  Cold Water Bath
Discretizing the equations

- Approximate the derivatives in the continuous equations with a discrete representation that is easier to solve.
- One approach: Finite Differences

\[ \nabla^2 T \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{h^2} = 0 \]

\[ T_0 = 180^\circ \quad T_n = 0^\circ \]
Solve for the unknowns $T_i$

- Set up a matrix of the unknown coefficients
  - include the known boundary conditions
- Solve the linear system for $T_i$

\[
\begin{bmatrix}
2 & -1 & 0 & \ldots & 0 \\
-1 & 2 & -1 & 0 & \ldots & 0 \\
0 & -1 & 2 & -1 & 0 & \ldots & 0 \\
\vdots & & & & \ddots & & \vdots \\
0 & \ldots & 0 & -1 & 2
\end{bmatrix}
\begin{bmatrix}
T_1 \\
T_2 \\
T_3 \\
\vdots \\
T_{n-1}
\end{bmatrix}
= 
\begin{bmatrix}
180 \ h^2 \\
0 \\
0 \\
\vdots \\
0
\end{bmatrix}
\]

- Visualize and analyze the results
As problems get more complicated so do the steps in the process

- Different discretization strategies exist for differing needs
  - Efficiency
  - Flexibility

- Most problems are time dependent and nonlinear
  - Need higher algorithmic levels than linear solvers

- Increasingly combining multiple physical processes
  - Interactions require careful handling

- Goal-oriented problem solving required optimization, uncertainty quantification
As problems grow in size so do the corresponding discrete systems

- Targeting applications with billions grid points and unknowns
- Most linear systems resulting from these techniques are LARGE and sparse
- Often most expensive solution step
- Solvers:
  - Direct Methods (e.g. Gaussian Elimination)
  - Iterative Methods (e.g. Krylov Methods)
    - Preconditioning is typically critical
    - Mesh quality affects convergence rate
- Many software tools developed at DOE labs deliver this functionality as numerical libraries
  - PETSc, Hypre, SuperLU, etc.
Modern scientific application development involves many different tools, libraries, and technologies

Observation: Exascale computing will enable high-fidelity calculations based on multiple coupled physical processes and multiple physical scales

- Adaptive algorithms
- Composite or hybrid solution strategies
- High-order discretization strategies
- Sophisticated numerical tools
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

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

Graphic courtesy of Bronis de Supinski, LLNL.
These complexities result in common challenges facing application scientists

- **Reliability**
  - Accurate, stable discretizations
  - Robust solution algorithms
  - Error minimization

- **Software Complexity**
  - Interoperating numerical software
  - New algorithms (e.g., interactive/dynamic techniques, algorithm composition)
  - New programming models

- **Performance**
  - Load balancing (perhaps dynamic)
  - Portability across architectures
  - Massive scale

**Application life cycle costs are increasing**
- Require the combined use of software developed by different groups
- Difficult to leverage expert knowledge and advances in subfields
- Difficult to obtain portable performance

**Too much energy focused on too many details**
- Little time to think about modeling, physics, mathematics
- Fear of bad performance without custom code
- Even when code reuse is possible, it is far too difficult
The FASTMath SciDAC project focuses on the development and use of 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 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
Structured grid capabilities focus on high order, mapped grids, embedded boundaries, AMR and particles.

Application to cosmology, astrophysics, accelerator modeling, fusion, climate, subsurface reacting flows, low mach number combustion, etc.
Our unstructured grid capabilities focus on adaptivity, high order, and the tools needed for extreme scaling.

Parallel mesh infrastructures
Dynamic load balancing
Mesh adaptation and quality control
Parallel performance on unstructured meshes
Architecture aware implementations

Application to fusion, climate, accelerator modeling, NNSA applications, nuclear energy, manufacturing processes, etc.
Our work on algebraic systems provides key solution technologies to applications.

Linear system solution using direct and iterative solvers.

Nonlinear system solution using acceleration techniques and globalized Newton methods.

Eigensolvers using iterative techniques and optimization.

Architecture aware implementations.

Application to fusion, nuclear structure calculation, quantum chemistry, accelerator modeling, climate, dislocation dynamics etc.
Integrating technologies is a key value added by the FASTMath Institute

Mesh/solver interactions
Mesh-to-mesh coupling methods
Unstructured mesh technologies into simulation workflows
Software unification strategies

Application to climate, plasma surface interactions, structural mechanics, nuclear energy, cosmology, fluid flow, etc.
FASTMath encompasses our algorithm development in widely used software

**Structured Mesh Tools**
- BoxLib (Ann Almgren)
- Chombo (Phil Colella)

**Linear Solvers**
- Hypre (Rob Falgout)
- PETSc (Barry Smith)
- SuperLU (Sherry Li)
- ML/Trilinos (Jonathan Hu)

**Unstructured Mesh Tools**
- PUIMI (Seegyoung Seol)
- MeshAdapt (Mark Shephard)
- MOAB (Vijay Mahadevan)
- Mesquite (Lori Diachin)
- PHASTA (Ken Jansen)
- APF (Cameron Smith)

**Partitioning Tools**
- Zoltan (Karen Devine)
- ParMA (Mark Shephard)

**FASTMath Software**

**Eigensolvers**
- PARPACK (Chao Yang)

**Nonlinear Solvers/Differential Variational Inequalities**
- SUNDIALS (Carol Woodward)
- PETSc (Barry Smith)
- NOX/Trilinos (Andy Salinger)

**Time Integrators**
- SUNDIALS (Carol Woodward)
- PETSc (Barry Smith)
Our research to improve performance on HPC platforms focuses on both inter- and intra-node issues:

**Inter-node: Massive Concurrency**
- Reduce communication
- Increase concurrency
- Reduce synchronization
- Address memory footprint
- Enable large communication/computation overlap

**Intra-node: Deep NUMA**
- MPI + threads for many packages
- Compare task and data parallelism
- Thread communicator to allow passing of thread information among libraries
- Low-level kernels for vector operations that support hybrid programming models
We are developing new algorithms that address key bottlenecks on modern day computers

**Reduce communication**
- AMG: develop non-Galerkin approaches, use redundancy or agglomeration on coarse grids, develop additive AMG variants (hypre) (2X improvement)
- Hierarchical partitioning optimizes communication at each level (Zoltan) (27% improvement in matrix-vector multiply)
- Relaxation and bottom solve in AMR multigrid (Chombo) (2.5X improvement in solver, 40% overall)
- HSS methods

**Increase concurrency**
- New spectrum slicing eigensolver in PARPACK (Computes 10s of thousands of eigenvalues in small amounts of time)
- New pole expansion and selected inversion schemes (PEXSI) (now scales to over 100K cores)
- Utilize BG/Q architecture for extreme scaling demonstrations (PHASTA) (3.1M processes on 768K cores unstructured mesh calculation)

**Reduce synchronization points**
- Implemented pipelined versions of CG and conjugate residual methods; 4X improvement in speed (PETSc) (30% speed up on 32K cores)

**Address memory footprint issues**
- Predictive load balancing schemes for AMR (Zoltan) (Allows AMR runs to complete by maintaining memory footprint)
- Hybrid programming models

**Increase communication and computation overlap**
- Improved and stabilized look-ahead algorithms (SuperLU) (3X run time improvement)

Used in PFLOTRAN applications

Used in PHASTA extreme scale applications

Used in Omega3P accelerator simulations
We have helped the application teams significantly reduce time to solution in their simulations.

Sparse direct solves improve time to solution 20X for accelerators allowing 8 cavity simulation (Spentzouris).

Acceleration-based nonlinear solvers speed up dislocation dynamics 35-50%; multistage Runge-Kutta methods reduce time steps by 94% (Arsenlis).

Sped up flux surface creation to improve 2D mesh generation in fusion application from 11.5 hours to 1 minute (Chang).

Sophisticated eigensolvers significantly improve materials calculations in many domains including ions in solution (Car), excited state phenomenon (Chelikowsky, Head-Gordon).
We have helped the application teams achieve unprecedented resolution and increased reliability.

- Astrophysics Lyman-α forest simulation at 4096^3 in an 80Mpc/h box; produced statistics at 1% accuracy for first time (Habib)
- Predictions of grounding line match experiment for first time in ice sheet modeling due to AMR (Price)
- Implicit ODE integrators combined with AMG linear solvers enables solution of 4D reaction-diffusion eqns for plasma surface interactions (Wirth)
- High-order unstructured meshes for particle accelerators overcome mesh generation/adaptation bottlenecks (Spentzouris)
We are addressing key package management issues targeting interoperability software

Issues Addressed:

- Inconsistent installation processes
- Inconsistent or missing configuration information
- Copying sources as a means of managing dependencies
- Spoofing sources (e.g. MPI) as a means of simplifying package code
- Inconsistent or missing versioning
- Managed installations

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

**Lawrence Berkeley National Laboratory**
- Mark Adams
- Ann Almgren
- Phil Colella
- Anshu Dubey
- Dan Graves
- Sherry Li
- Lin Lin
- Terry Ligocki
- Mike Lijewski
- Peter McCorquodale
- Esmond Ng
- Brian Van Straalen
- Chao Yang
- Subcontract: Jim Demmel (UC Berkeley)

**Lawrence Livermore National Laboratory**
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- Rob Falgout
- Mark Miller
- Jacob Schroder
- Carol Woodward
- Ulrike Yang
- Subcontract: Carl Ollivier-Gooch (Univ of British Columbia)
- Subcontract: Dan Reynolds (Southern Methodist)

**Barna Bihari**

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- Vijay Mahadevan
- Barry Smith
- Subcontract: Jim Jiao (SUNY Stony Brook)
- Subcontract: Paul Wilson (Univ of Wisconsin)

**Sandia National Laboratories**
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- Glen Hansen
- Jonathan Hu
- Vitus Leung
- Siva Rajamanickam
- Michel Wolf
- Andrew Salinger

**Rensselaer Polytechnic Inst.**
- E. Seegyoung Seol
- Onkar Sahni
- *Mark Shephard*
- Cameron Smith
- Subcontract: Ken Jansen (UC Boulder)
FASTMath Tutorial Goals

- Provide a basic understanding of a variety of applied mathematics algorithms for scalable linear, nonlinear, and ODE solvers as well as discretization technologies (e.g., adaptive mesh refinement for structured and unstructured grids)

- Provide an overview of FASTMath software tools available to perform these tasks on HPC architectures

- Practice using one or more of these software tools on basic demonstration problems
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<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Presenter(s)</th>
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</thead>
<tbody>
<tr>
<td>11:00</td>
<td>An Overview of Mathematical Algorithms and Software</td>
<td>Lori Diachin, LLNL</td>
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<tr>
<td>11:40</td>
<td>Algebraic Solvers in FASTMath: An Introduction</td>
<td>Barry Smith, ANL</td>
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<tr>
<td>12:00</td>
<td>Lunch and Hands-on Exercises</td>
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<tr>
<td>1:00</td>
<td>PETSc: Portable, Extensible Toolkit for Scientific Computing</td>
<td>Barry Smith, ANL</td>
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<tr>
<td>2:00</td>
<td>HYPRE: High Performance Preconditioners</td>
<td>Rob Falgout, LLNL</td>
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<td>2:30</td>
<td>Break</td>
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<tr>
<td>3:00</td>
<td>SuperLU: Parallel Direct Solvers</td>
<td>Xiaoye (Sherry) Li, LBNL</td>
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<tr>
<td>3:30</td>
<td>Sundials: Suite of Nonlinear and Differential/Algebraic Equation Solvers</td>
<td>Carol Woodward, LLNL</td>
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<tr>
<td>4:00</td>
<td>Intro to Unstructured Mesh Technologies (Part 1)</td>
<td>Vijay Mahadevan, ANL, Mark Shephard and Cameron Smith, RPI, and Glen Hansen, SNL</td>
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<tr>
<td>4:30</td>
<td>Panel: Challenges in Extreme Scale Solvers</td>
<td>FASTMath Team</td>
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<td>5:30</td>
<td>Dinner Talk: &quot;Perspectives on Teaming from the DOE National Labs&quot;</td>
<td>Lori Diachin, LLNL</td>
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<td>6:30</td>
<td>FASTMath Hands-on Exercises</td>
<td>Mark Miller, LLNL and the FastMath Team</td>
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<tr>
<td>9:30</td>
<td>Wrap-up</td>
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### FASTMath Tutorial Schedule: Saturday, August 9

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<thead>
<tr>
<th>Time</th>
<th>Activity</th>
<th>Speakers</th>
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<tbody>
<tr>
<td>7:30 AM</td>
<td>Continental Breakfast</td>
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<tr>
<td>8:30</td>
<td>Unstructured Mesh Technologies (Part 2)</td>
<td>Vijay Mahadevan, ANL, Mark Shephard and Cameron Smith, RPI, and Glen Hansen, SNL</td>
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<tr>
<td>9:30</td>
<td>Block Structured AMR Libraries and Their Interoperability with Other Math Libraries</td>
<td>Mark Adams and Anshu Dubey (LBNL)</td>
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<tr>
<td>10:30</td>
<td>Break</td>
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<tr>
<td>11:00</td>
<td>FASTMath Hands-on Exercises for meshing, AMR</td>
<td>Mark Miller, LLNL and FASTMath Team</td>
</tr>
<tr>
<td>12:00 PM</td>
<td>Lunch and Hands-on Exercises</td>
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<tr>
<td>1:00</td>
<td>Wrap-up</td>
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FASTMath Executive Council
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- Andy Salinger, Integrated Technologies agsalin@sandia.gov, 505-845-3523
- Mark Shephard, Unstructured Mesh Tools shephard@scorec.rpi.edu, 518-276-8044
- Barry Smith, Linear Solvers, bsmith@mcs.anl.gov, 630-252-9174

For more information, please contact any of the following or visit our web site http://www.fastmath-scidac.org
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