FASTMath

Frameworks, Algorithms, and Scalable Technologies for Mathematics SciDAC Institute

The FASTMath Team

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SciDAC
Scientific Discovery through Advanced Computing

The FASTMath SciDAC Institute will develop and deploy scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena and will collaborate with DOE domain scientists to ensure the usefulness and applicability of FASTMath technologies.

As the complexity of computer architectures and the range of physical phenomena that can be numerically simulated for important DOE applications continue to grow, application scientists have two fundamental challenges to overcome. First, they must continue to improve the quality of their simulations by increasing accuracy and fidelity of the solution and improving the robustness and reliability of both their software and their algorithms. Second, they must adapt their computations to make effective use of the high-end computing facilities being acquired by DOE over the next five years. This challenge will necessitate million-way parallelism and implementations that are efficient on many-/multi-core nodes. The FASTMath SciDAC Institute will help DOE application scientists address both of these challenges by focusing on the interactions among mathematical algorithms, software design, and computer architectures. Key to addressing the first challenge is a thorough understanding of application needs, and the FASTMath team has a strong and proven track record of doing just this.

FASTMath Topical Areas: FASTMath work is organized around the following broad topical area themes:

- **Structured mesh capabilities:** block structured adaptive mesh refinement, embedded boundary methods, particle techniques, high -order discretization
- **Unstructured mesh capabilities:** complex geometry representations, adaptive mesh refinement, dynamic partitioning, mesh quality improvement, high-order discretization
- **Linear solvers**: geometric and algebraic multigrid, domain decomposition, Krylov iterative techniques, ILU and LU factorizations
- **Nonlinear solvers:** Newton based with various globalization schemes including line search and trust region
- **Time integrators:** implicit/explicit methods, symplectic, multiscale, backward differentiation, generalized linear, differential algebraic equations, error control
- **Variational inequality solvers:** Newton-based active set methods and semi-smooth methods
- **Eigensolvers:** Krylov & non-Krylov subspace methods, optimization-based techniques

Addressing the Challenges of Next Generation Computing: One of the key challenges facing the scientific computing community is the shift to multi-/many-core nodes and million-way parallelism. Thus a pervasive theme in our work is understanding the most effective ways to implement our algorithms at scale on these architectures, with particular emphasis on hybrid programming models, architecture-aware partitioning and data layout techniques, and communication reducing algorithms.

Argonne National Laboratory · Berkeley Lab · Sandia National Laboratories · Berkeley University of California · Columbia University · Rensselaer · SMU · The University of British Columbia

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The FASTMath Toolset

Much of our knowledge and experience in this area is embodied in the FASTMath software capabilities, many of which are DOE landmark packages that are widely available and used by DOE and other application scientists.

Structured meshes:
- BoxLib (Bell)
- Chombo (Colella)

Unstructured meshes:
- MeshAdapt (Shephard)
- MOAB (Tautges)
- Mesquite (Diachin)

Geometry:
- CGM (Tautges)

Partitioning:
- Zoltan (Devine)

Linear systems:
- Hypre (Falgout)
- PETSc (Smith)
- SuperLU (Li)
- ML/Trilinos (Hu)

Nonlinear systems:
- SUNDIALS (Woodward)
- NOX/Trilinos (Salinger)
- PETSc (Smith)

Time Integration:
- SUNDIALS (Reynolds)
- PETSc (Smith)

Eigensystems:
- PARPACK (C. Yang)

Integrated FASTMath Capabilities and Software: The FASTMath Institute will provide advanced algorithms and integrated software technologies for DOE application needs that build on the foundational technologies described above. In particular, FASTMath will provide specific technologies for the construction of reliable multi-physics simulations including 1) integrated software that increases the overall efficiency of adaptive mesh control techniques, 2) managing the communication of the simulation field data throughout the software stack, and 3) mesh-to-mesh and particle-to-mesh coupling techniques. We will also build a more integrated, high performing software base for applications by maximizing the performance of our integrated software on leadership-class platforms. Our software development and distribution strategy is designed to improve the quality, ease of adoption, and integration of the many FASTMath software products, with the ultimate goal of maximizing our impact in the application community.

Building on Success: The FASTMath team has extensive experience and software tools available for DOE application simulations and has already demonstrated significant gains in efficiency and fidelity using our methodologies allowing domain scientists to achieve new scientific results that were previously unobtainable. See the SciDAC-2 web sites associated with the TOPS, APDEC, ITAPS projects for more details. The FASTMath SciDAC Institute will build on this success and provide the mathematical algorithms, software tools, and human expertise to effectively use the future generations of computers to address open scientific questions of importance to them.

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SciDAC-2 Web Sites:
- TOPS: http://www.tops-scidac.org
- APDEC: http://www.apdec.org
- ITAPS: http://www.itaps-scidac.org

Coming soon: FASTMath Web site: http://www.fastmath-scidac.org

For FASTMath help, please contact Lori Diachin or fastmath-help@lists.llnl.gov