SIGMA: Scalable Interfaces for Geometry and Mesh based Applications

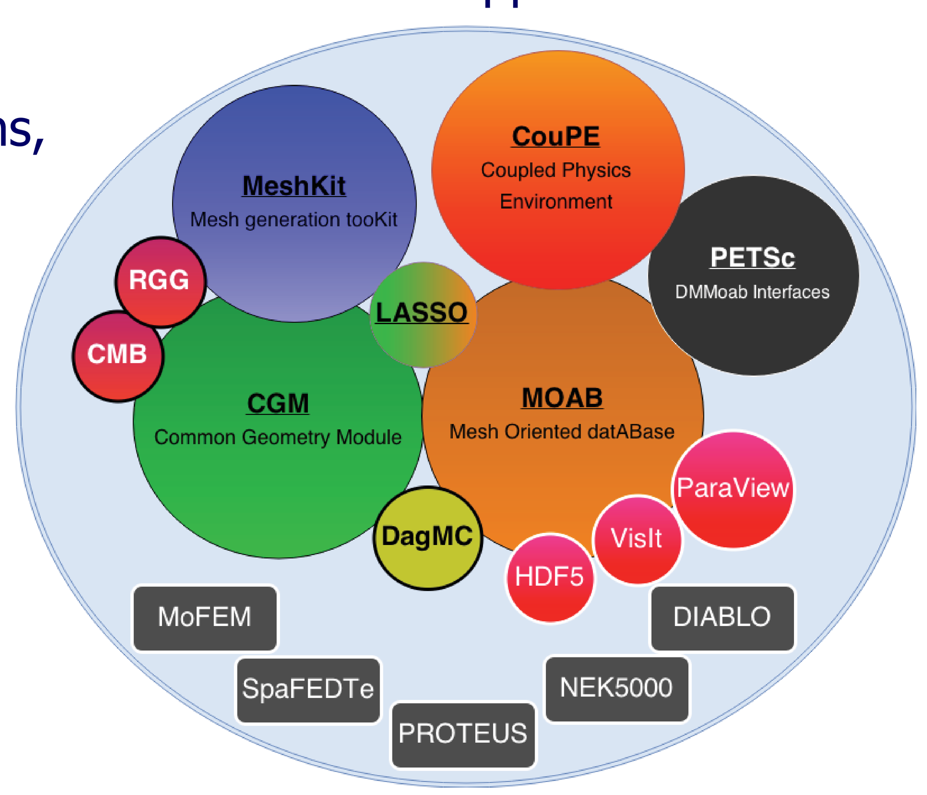
FASTMath Team Members: V. S. Mahadevan, I. Grindeanu, R. Jain, N. Ray, D. Wu, E. Vanderzee, P. Shriwise and P. Wilson

HPC applications need robust modeling workflows to resolve spatio-temporal scales on complex geometric domains, with high-quality unstructured meshes that interoperate optimally with several scalable solvers. The FASTMath team is developing components to improve scientific productivity without sacrificing accuracy or efficiency (reduced memory/communication overhead) on emerging architectures.

Simplifying computational modeling workflow

An open-source simulation workflow for SciDAC applications

- ★ CGM: accurate API for geometry representations,
- ★ MeshKit: seamlessly generate high-quality computational mesh,
- ★ MOAB: load, handle, manipulate parallel unstructured meshes
- ★ DMMoab: optimal interoperable MOAB-PETSc interfaces

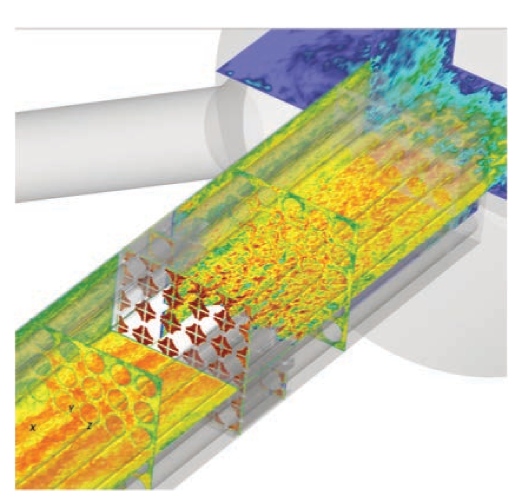


- ★ CouPE: enable robust coupled multi-physics simulations

Parallel mesh infrastructures

Goal: Enabling *strongly* scalable application support through *loosely* connected software component architectures.

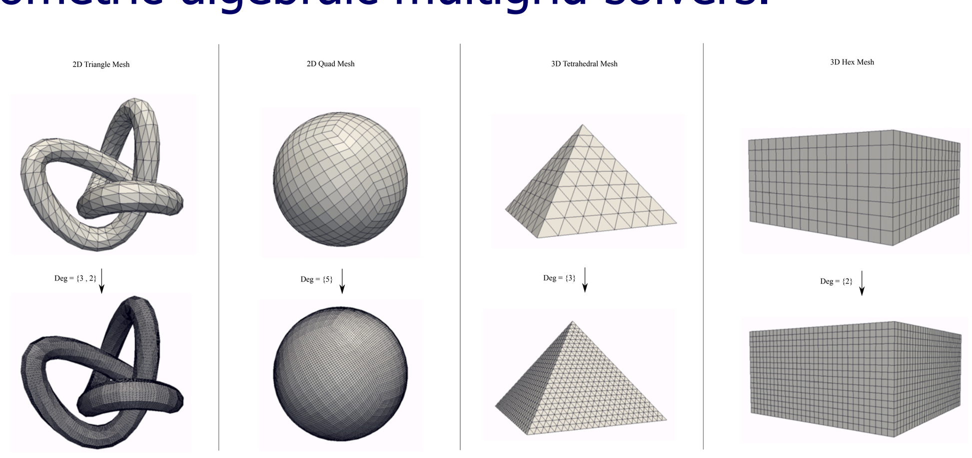
- ★ Scalable implementations for petascale class machines with focus on portability,
- ★ Common topological model access to solid geometry engines (ACIS/OCC),
- ★ Efficient (discrete) geometry and array-based unstructured mesh representations
- ★ Scalable HDF5 I/O and in-situ visualization to improve scientific productivity



Uniform refinement and geometric multigrid

Goal: Template-based arbitrary degree UMR hierarchy generation to support parallel hybrid geometric-algebraic multigrid solvers.

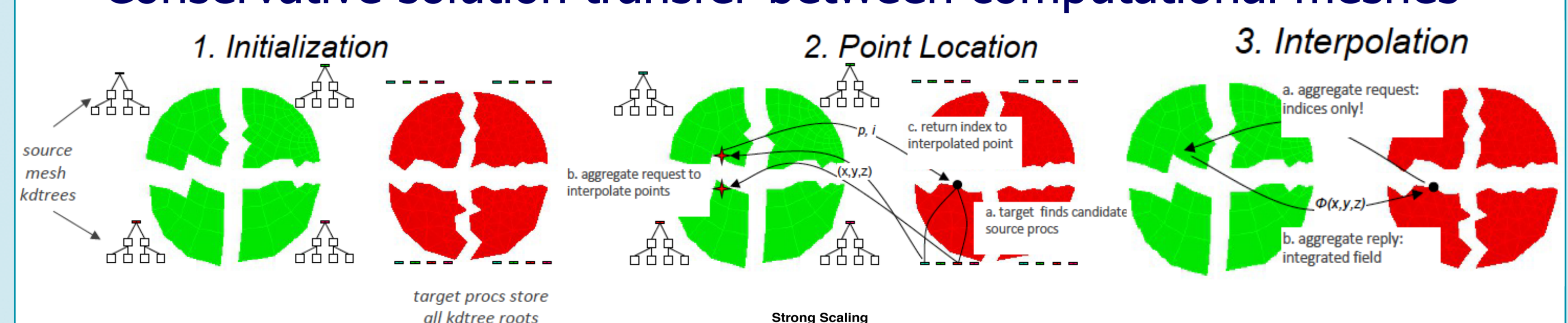
- ★ Parent-child queries
- ★ Ghost layer exchange
- ★ Array-based adjacency for optimal assembly
- ★ Inter-level projection operator computation



Parallel Point Location for Solution Transfer

Goal: Simplify geometry searches and unified discretization kernels.

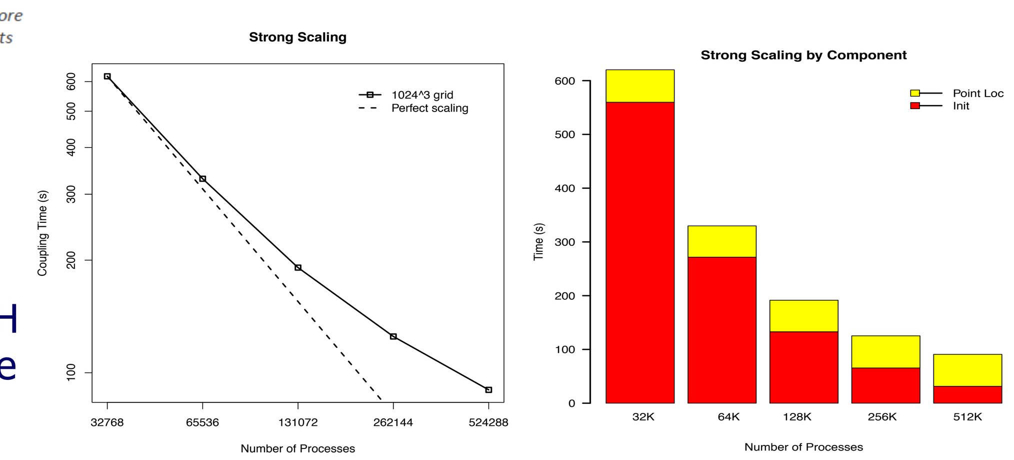
- ★ Geometry search: parallel point-in-element query for arbitrary topologies (edge,tri/quad/polygon,tet/hex/prism/pyramid)
- ★ Discretization: support transformations, higher-order basis (lagrange, spectral) for optimized local FE/FV computations
- ★ Conservative solution transfer between computational meshes



4. Global normalization

5. Subset Conservation

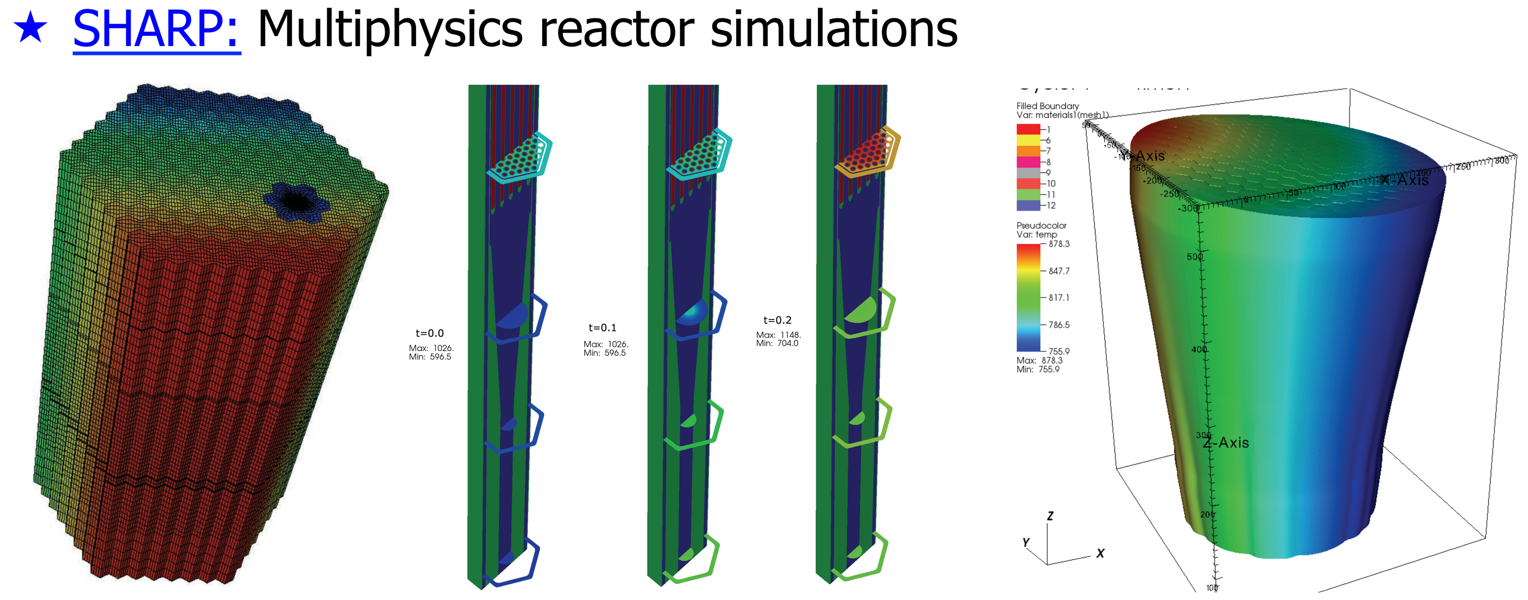
Bottleneck: *Kd*-tree scales as O(nlog(n)); consider BVH tree to attain O(log(n)) time complexity.



Coupled multi-physics simulations

Goal: Provide a flexible coupled multi-physics library to integrate together existing and new computational solvers robustly.

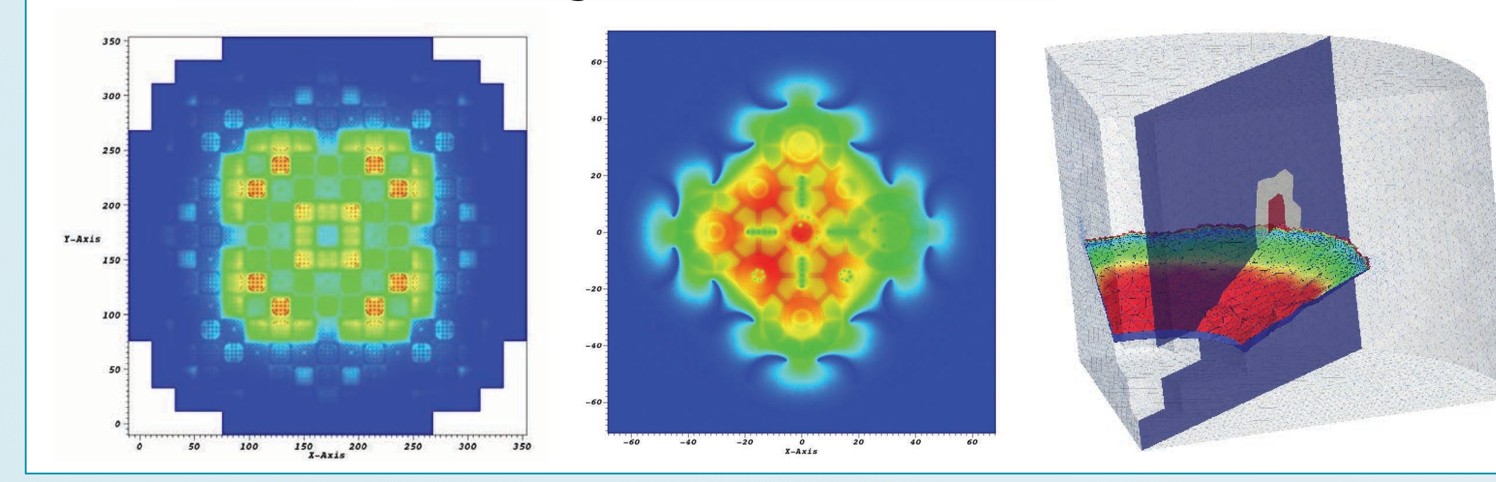
- ★ Leverage scalable mesh (MOAB) and nonlinear solver (PETSc) implementations to build CouPE,
- ★ Plug-and-play with existing physics modules enabled through conservative solution transfer between disparate meshes.
- ★ Provide several Operator-Split and tightly coupled strategies to enable adaptive scale resolution in coupled physics simulations.
- ★ SHARP: Multiphysics reactor simulations



MOAB – PETSc interactions

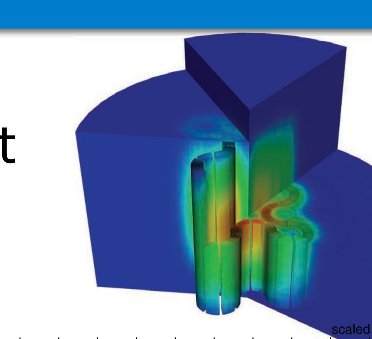
Goal: Ease creation of computational solvers with portable abstractions for traversal over unstructured meshes

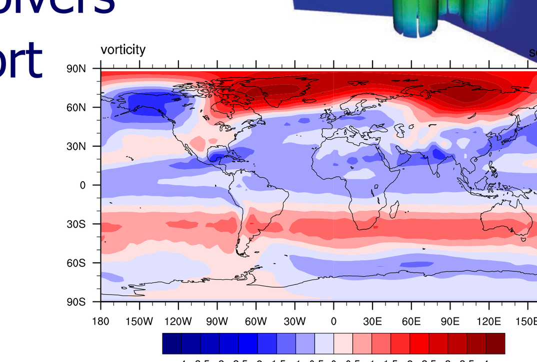
- ➢ Flexible memory sharing between libraries
- ➢ Multi-component strided/interleaved component field access
- ➢ Analyze efficient unstructured mesh traversal, FD/FEM-type operator assembly for relevant problems in multi-dimensions.
- ➢ Capabilities to define field components, manage degrees-of-freedom, local-to-global transformations.



Application Impact

- ★ CMB: Computational Model Builder
- ★ MBCSLAM: Conservative multi-tracer transport
- ★ Diablo: Mortar element Structural Mechanics
- ★ SpaFEDTe: Discontinuous Galerkin solvers
- ★ PROTEUS: FE-based neutron transport
- ★ DAG-MCNP: Monte Carlo transport
- ★ MoFEM: *h-p* adaptive FEA code
- ★ Nek5000: SEM-based CFD
- ★ Par-NCL: Climate data analysis





Ongoing and future efforts

- ★ Thread-safe geometry and mesh query implementations,
- ★ Array-based parallel adaptive mesh refinement (AMR),
- ★ Improved point location schemes and computational geometry-based intersections for conservative solution transfer,
- ★ Multi-physics algorithmic explorations with MOAB and CouPE,
- ★ Integration of MOAB with MCT to be used with CESM/ESMF,
- ★ Extend language-agnostic application support while also utilizing the DMMoab infrastructure for new computational solvers.

More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130

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