Unstructured Mesh Solver Interactions

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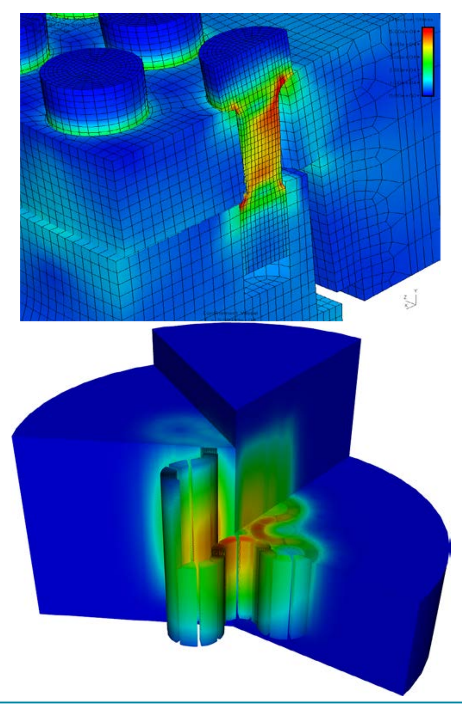
Unstructured mesh usage is fundamental to several real world simulation applications and efficient solver interactions are critical to enable scientists to concentrate on scientific discoveries better. The FASTMath team is developing several strong mesh-solver interface components that implement efficient parallel mesh handling/traversal capabilities into analysis codes with reduced memory and communication overheads.

Unstructured Mesh and Solvers Interactions

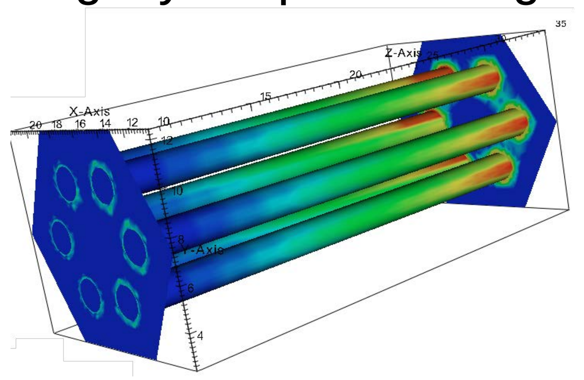
- Several SciDAC and DOE applications dominated by complex geometry and/or highly varying spatial anisotropy, utilize FASTMath mesh tools.
- Interoperable interfaces between the mesh and solver infrastructures reduce computational complexity and improve software productivity.
- A list of applications exist that directly leverage the mesh-solver interactions in FASTMath technologies:
  - Multiphysics component-based simulation (SHARP)
  - Multiphase reactor flows (PHASTA)
  - Fusion first wall chemistry & dynamics (XOLOTL)
  - Conservative multi-tracer transport (MBCSLAM)
  - FE-based neutron transport solver (PROTEUS)
  - SEM-based CFD solver (Nek5000)
  - Fluid/Structure interaction (AthenaVMS)
  - Complex Flow problems/Solid Mechanics (Albany)

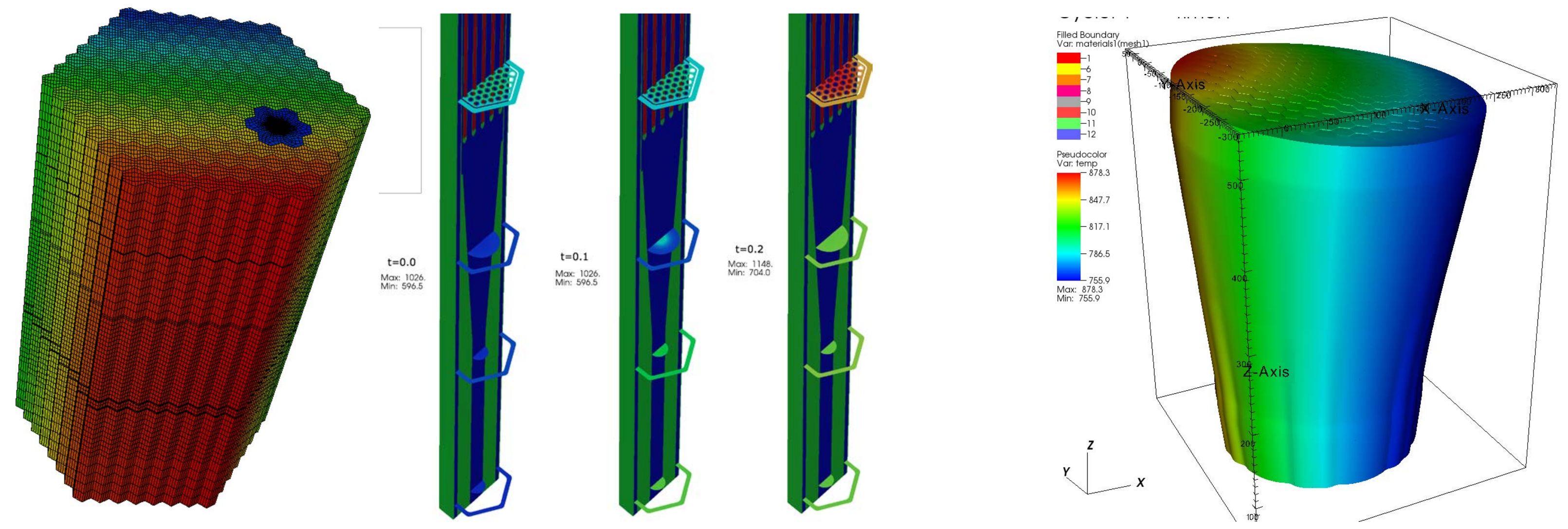


Parallel MultiPhysics Reactor Simulation

- A flexible multiphysics framework, CouPE, based on MOAB and PETSc, has been developed to solve tightly coupled problems with loosely coupled software interfaces.
- Plug-and-play with existing physics modules enabled through conservative solution transfer between disparate meshes.
- Provide several different Operator-Split and tightly coupled strategies to enable adaptive resolution of scales in nuclear reactor simulations.

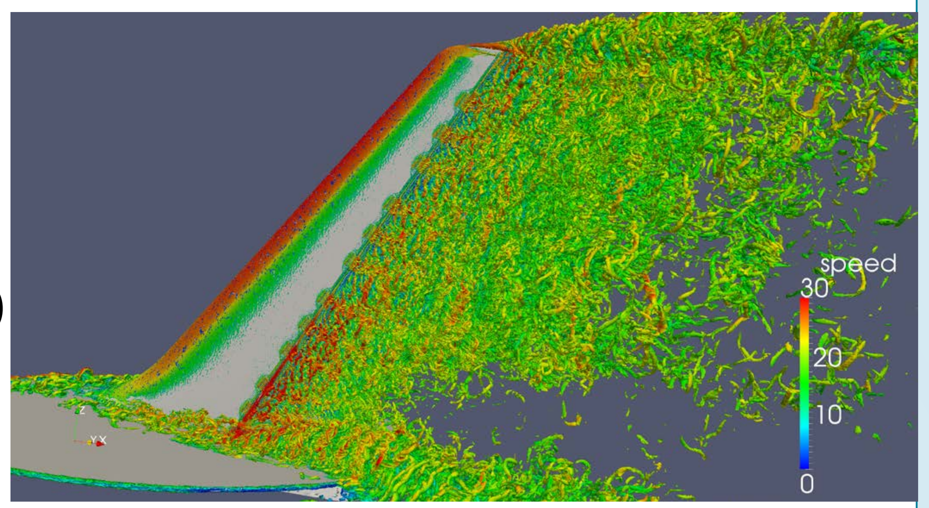
SHARP toolkit couples 3 large physics codes; Several successful demonstrations on petascale computers.



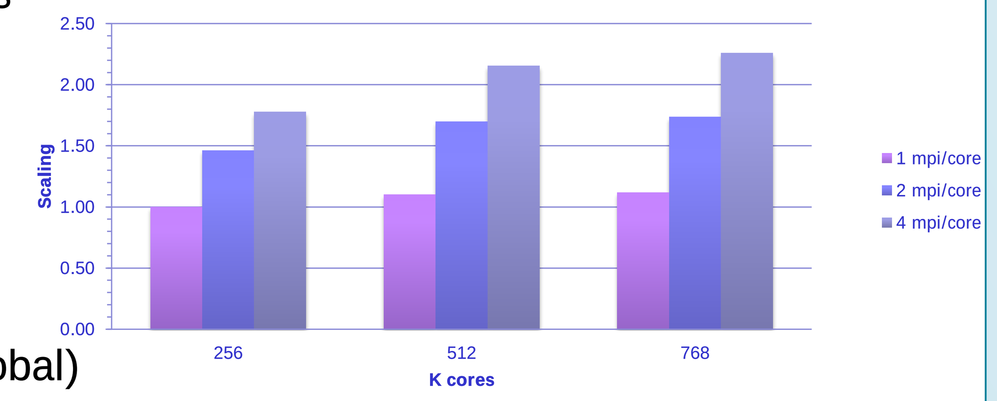


Massively Parallel PDE Solver (PHASTA)

- Implicit, Adaptive Grid CFD
- Extreme Scale Applications:
  - Aerodynamics flow control
  - Multiphase flow
- Early Science Project (MIRA)
- Full Machine Strong scaling
  - Variable MPI processes/core
  - 92 Billion Tetrahedra
  - 262144 to 3,145,728 parts
  - 1/core 100% scaling
  - 2/core 146-155% scaling
  - 4/core 178-226% scaling
- Partitioning pipeline
  - Zoltan ParMetis of 180M elements to 16k parts (global)
  - Refinement to 92B then Zoltan HyperGraph up to 3072k parts



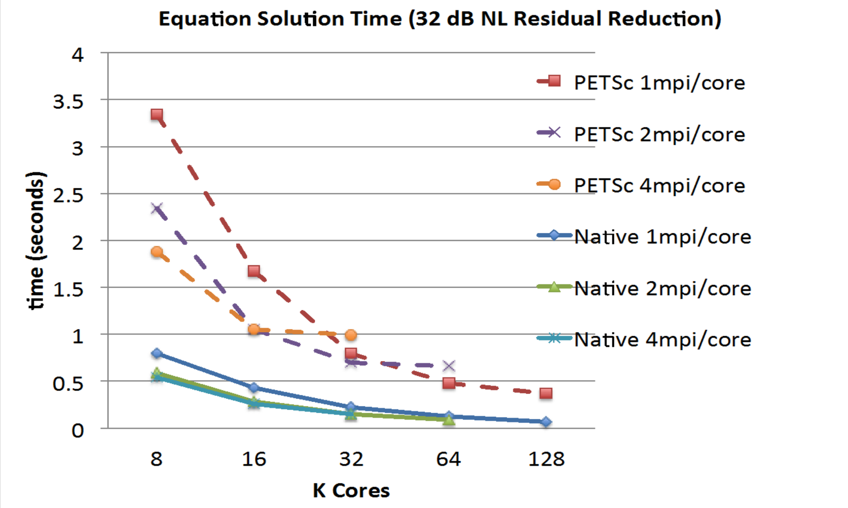
92 billion tetrehedra

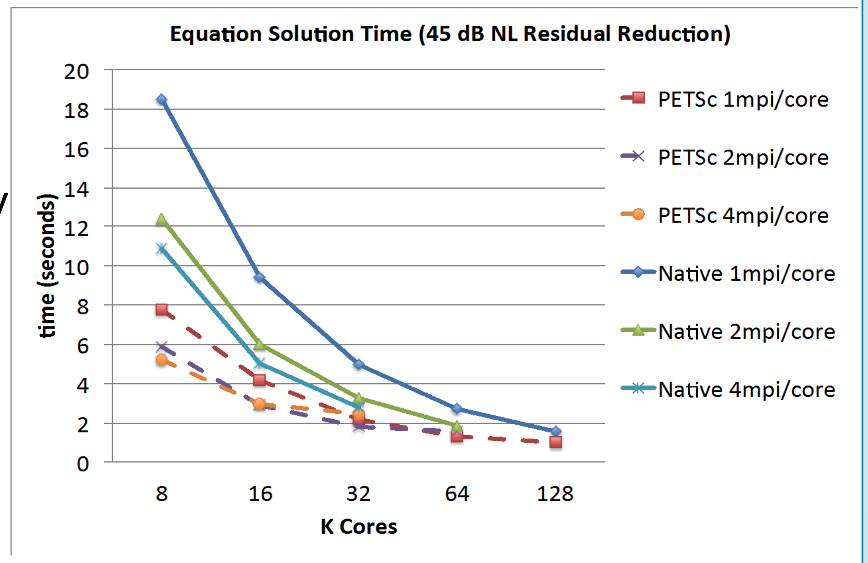


PHASTA – PETSc Coupling

PETSc linked to PHASTA to provide an alternative solver

- Element level equation formation remains native:
- PETSc functions assemble LHS and RHS
- PETSc MatAssembly performs additional step of building globally complete matrix (not done in native solver)
- Relative efficiency depends on tolerance of the solve- tighter tolerance more efficient with PETSc
- Multiple processes per core currently benefit native solver more than PETSc
- MatAssembly times (not shown) were identified as a scaling bottleneck (currently working with PETSc team to resolve)



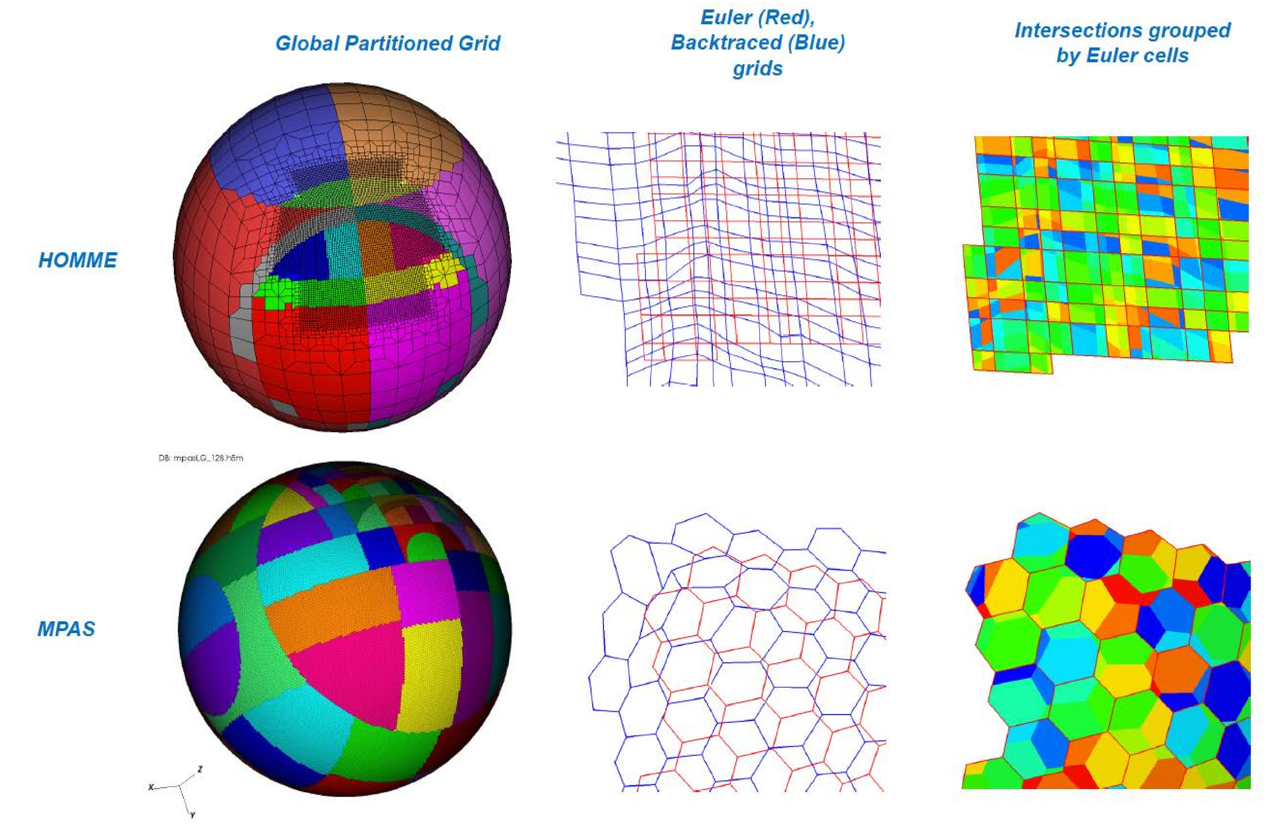


MOAB – PETSc Coupling

- Native MOAB implementation to expose the underlying array-based mesh data structures through the DM (Discretization Manager) object in PETSc. This is the DMMoab object (Petsc-3.5).
- Some features of DMMoab:
  - Design resembles structured (DMDA) and unstructured (DMPlex) interfaces.
  - Provides ability to discretize physics with FEM based on a native MOAB mesh while leveraging the scalability of PETSc solvers and preconditioners.
  - Support both strided and interleaved access of field components; Opens up better preconditioning strategies.
  - Analyze efficient unstructured mesh traversal, FD/FEM-type operator assembly for relevant problems in multi-dimensions.
  - Provide optimized computation of the physics residuals using PETSc Vec that reuses the contiguous memory provided by MOAB tags.
  - Capabilities to define field components, manage degrees-of-freedom, local-to-global transformations are available as part of DMMoab.
- Quantify total memory savings by sharing vector spaces; Use reduced block filling of coupled component terms.
- Several examples available in PETSc; Primary motivation to enable scalable, unstructured ADR solvers in XOLOTL (PSI).

Tracer Transport for Atmospheric Modeling

Conservative Semi-Lagrangian (CSLAM) tracer transport on arbitrary parallel meshes for CAM (SE, FV, MPAS, ...) based on MOAB.



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

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