Unstructured Meshing Techniques

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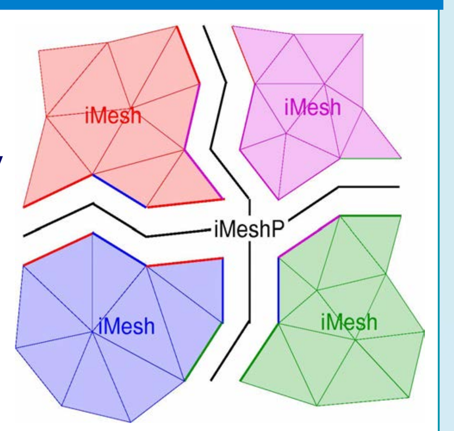
Unstructured meshes, often adaptively defined, can yield required levels of accuracy using many fewer degrees of freedom at the cost of more complex parallel data structures and algorithms. FASTMath is providing the parallel unstructured mesh data structures and services needed by developers of PDE solution procedures targeted for exascale computers

Parallel Meshes for Exascale (iMeshP)

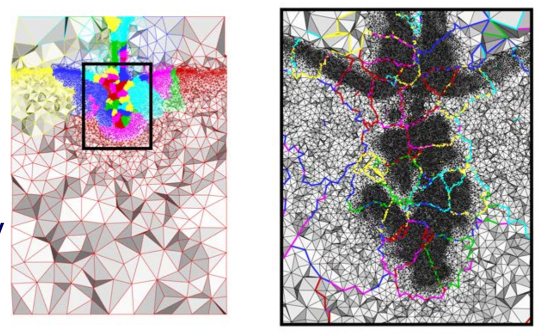
iMeshP: Interface for distributed unstructured meshes to manage/query/modify the meshes in parallel

- Multiple parts – treats each part as serial mesh with part boundary
- Partition model – coordinates communication between parts
- Owner rules – supports coordination of parallel mesh modification on part boundary
- Features – migration (entity, set, tags), ghosting, partitioning



Currently two iMeshP implementations

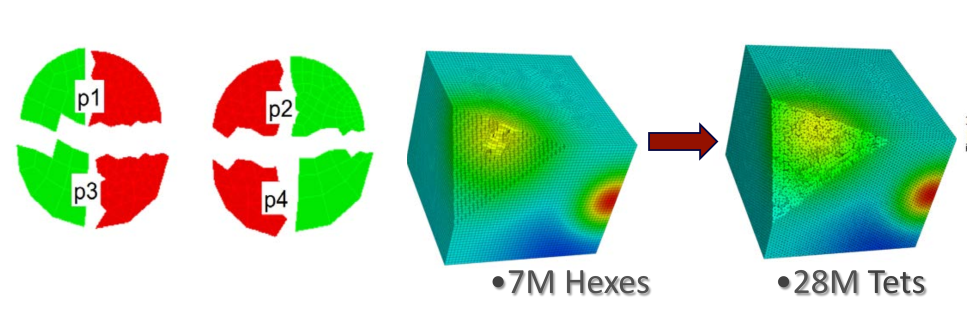
- MOAB/iMeshP
  - Compact representation that takes full advantage of mesh sets
  - iMeshP query functionality on single-part-per-process (native MOAB parallel model also accessible, through iMesh)
  - Tested on up to 16k cores
- FMDB/iMeshP
  - Representation designed for evolving (adapted) meshes
  - Multiple parts per process operational
  - Developing architecture aware partitioning methodology
  - Tested to 128K cores

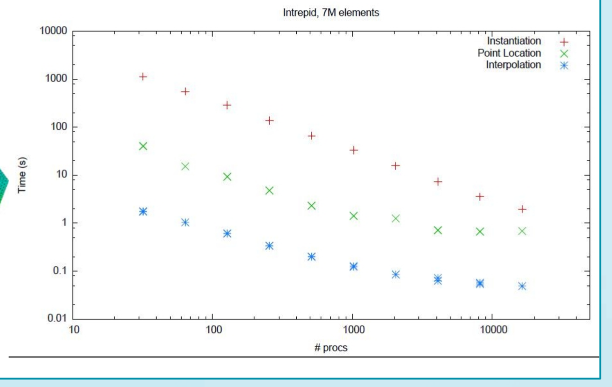


Mesh-to-Mesh Solution Coupling (MBCoupler)

Goal: Coupling existing codes for multi-physics

- MBCoupler: provides parallel point location, solution interpolation, and various constraint enforcement schemes (e.g. global conservation) for a variety of discretization (FE, SE) and element types (tet, hex)
- Coupe: driver for various loose and tight coupling schemes, coordinating calls to physics modules, solution transfer, and convergence/time stepping





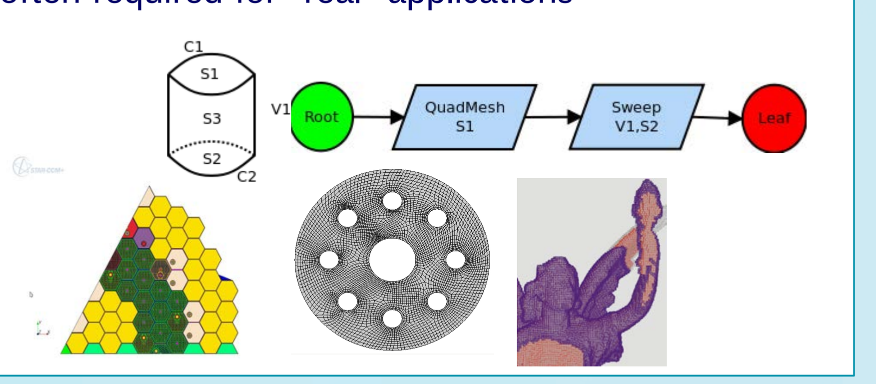
Meshing Coordination Library (MeshKit)

Mesh generation algorithm implementations scattered across multiple libraries/ codes, with limited CAD suupport

- Difficult to mix 'n match, but that's often required for "real" applications

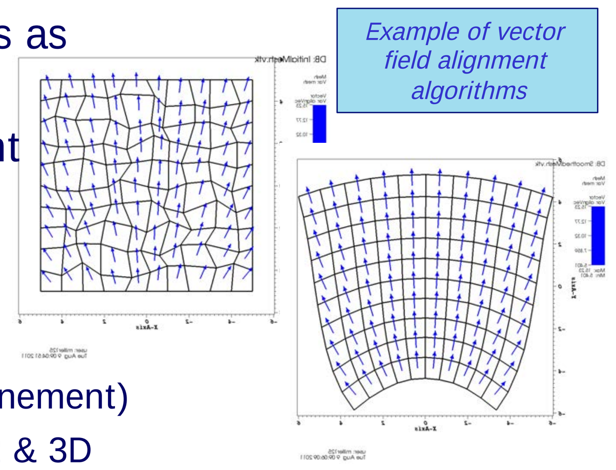
MeshKit provides a graph-based view of the meshing process

- Algorithms for tri/tet, quad/hex
- copy/move
- smooth, etc.

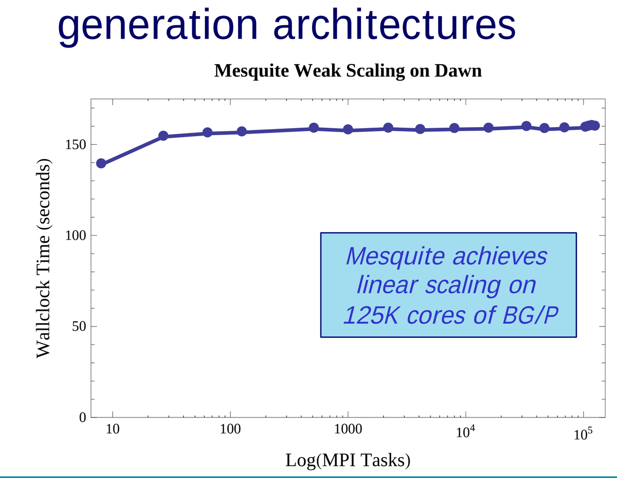


Mesh Optimization (Mesquite)

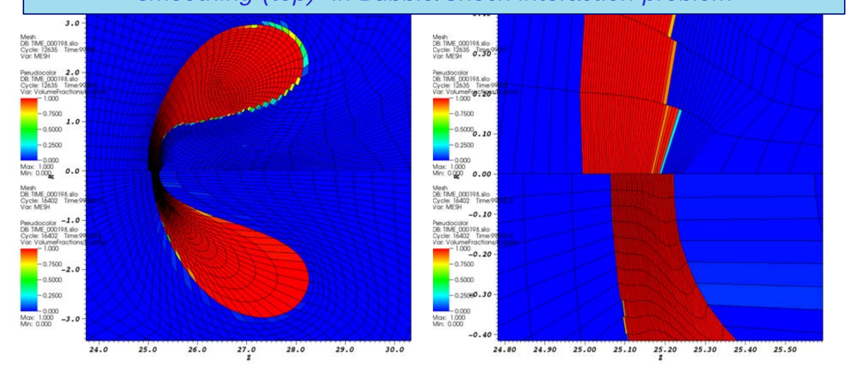
- Mesh quality remains important for applications as systems increase in size and complexity
- Mesquite poses the mesh quality improvement problem as an optimization problem
  - Element quality as a function of vertex locations
  - Target matrix paradigm to represent problem dependent element characteristics (e.g. vector field alignment, boundary meshes, anisotropies, refinement)
  - Useful for structured, unstructured, hybrid grids in 2 & 3D



- Parallel solution algorithms in Mesquite scale well on to 125,000 cores on BG/P
- New parallel interface smoothing capabilities are effective on difficult bubble/ shock interaction problem in ALE simulation
- Currently working on mixed programming model approaches for next generation architectures



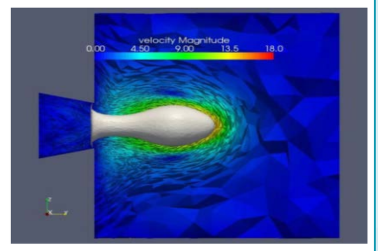
Side-by-side comparison of Mesquite (bottom) with equipotential smoothing (top) in Bubble/Shock interaction problem



Mesh Adaptation (MeshAdapt)

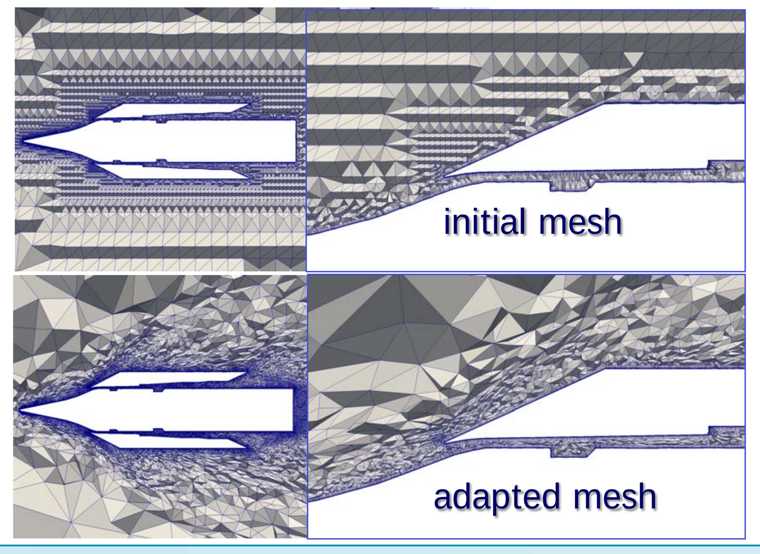
A general parallel mesh adaptation tool (run to 64K cores so far)

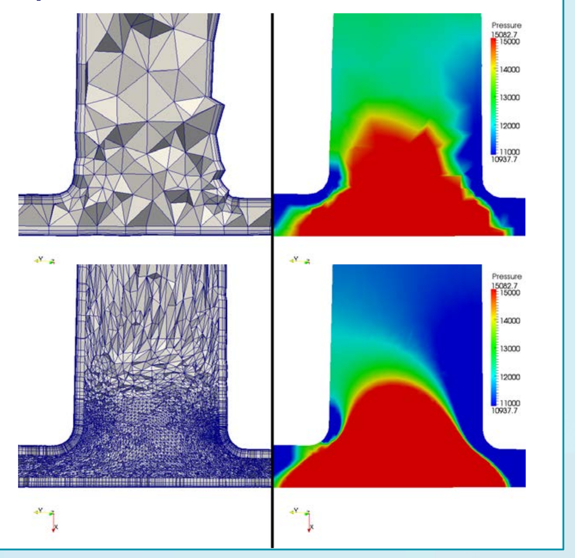
- Accepts a mesh metric field defined on the current mesh as input
- Uses local mesh modification (and solution transfer) to adapt mesh to match the requested mesh sizes and shapes
- Runs in parallel and linked with dynamic load balancing



Recent additions

- Adapts boundary layers meshes with mixed element types
- Adapts curved meshes (quadratic element shapes) with curved shape control
- Boundary layer thickness adaptation being developed
- Boundary layer and curved element adaptation in parallel

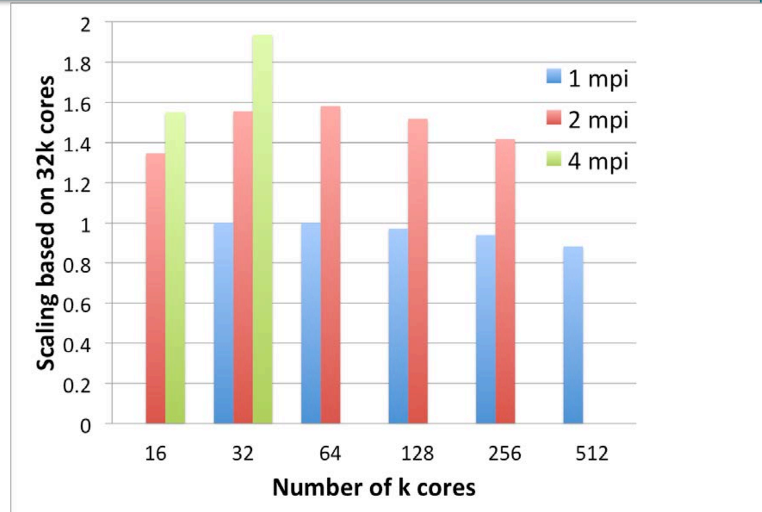




Massively Parallel PDE Solver (PHASTA)

Implicit, Adaptive Grid CFD

- Strong scaling on Mira
- Variable MPI processes/core
- 1/core 88% scaling 32k->512k
- 2/core 135-158% scaling
- 4/core 150-193% scaling

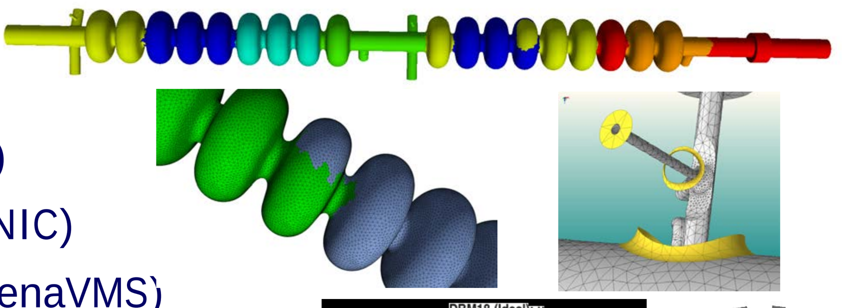


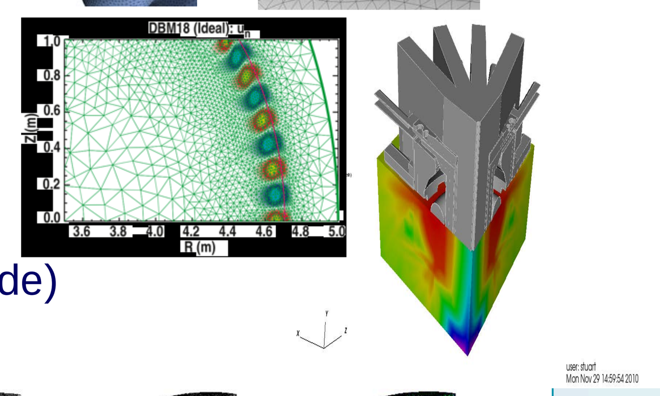
Partitioning pipeline

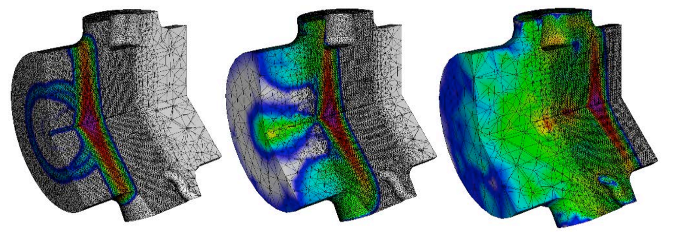
- Zoltan ParMetis of 52M elements to 16k parts (global)
- Refinement to 3.3B then Zoltan HyperGraph up to 1536k parts

Application List

- Accelerator Modeling (ACE3P)
- Climate data analysis (Par-NCL)
- FE-based neutron transport (UNIC)
- Fluid/Structure interaction (AthenaVMS)
- Fusion Edge Physics (XGCI)
- Fusion first wall chemistry & dynamics (XLOTL)
- Fusion Plasmas (M3DC1)
- High-speed viscous flows (FUN3D – A NASA code)
- Monte Carlo neutron transport (DAG-MCNP)
- Multiphase reactor flows (PHASTA)
- SEM-based CFD (Nek5000)
- Solid Mechanics (Albany)







Future Plans

Continue to provide unstructured mesh data structures and services to SciDAC and other DOE applications

Focus of technical developments on

- Algorithms needed to operate on exascale systems
- Effective implementation on exascale systems
- Extend and expand services to meet the needs of applications
  - On exascale systems (parallel meshes, partitioners, etc.)
  - To provide new functions (solution transfer, boundary layer adapt., etc.)

More Information: http://www.fastmath-scidac.org or contact Mark Shephard, shephard@rpi.edu, 518-276-8044

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