Unstructured Meshing Technologies

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Unstructured meshes can yield required levels of accuracy using many fewer unknowns at the cost of more complex data structures and algorithms. FASTMath is providing the parallel unstructured mesh structures and services needed by applications targeted for exascale computers

FASTMath Unstructured Mesh Developments

Technology development driven by needs of a broad set of DOE applications

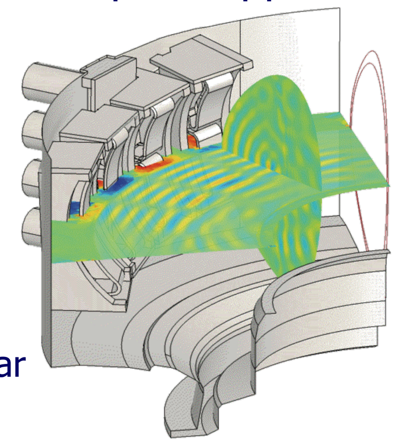
Technology development areas:

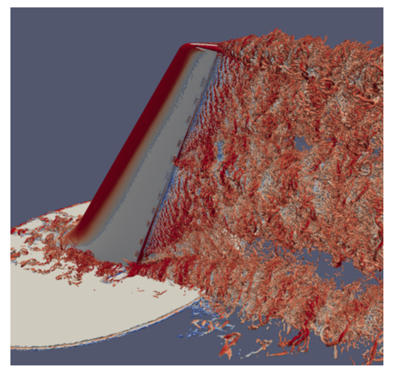
- Unstructured Mesh Analysis Codes – Support application's PDE solution needs
- Performant Mesh Adaptation – Parallel mesh adaptation to integrate into analysis codes to ensure solution accuracy
- Dynamic Load Balancing and Task Management – Technologies to ensure load balance and effectively execute operations by optimal task placement
- Unstructured Mesh for PIC – Tools to support PIC on unstructured meshes
- Unstructured Mesh for UQ – Bringing unstructured mesh adaptation to UQ
- In Situ Vis and Data Analytics – Tools to gain insight as simulations execute

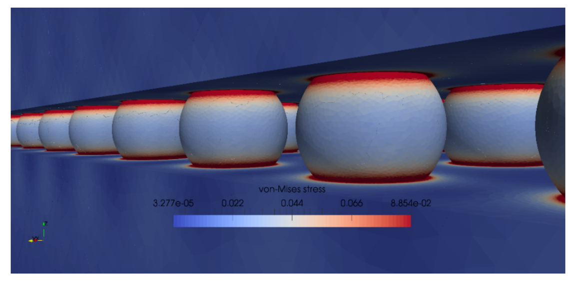
Unstructured Mesh Analysis Codes

Advanced unstructured mesh analysis developed/supported by FASTMath

- MFEM – High-order F.E. framework
  - Arbitrary order curvilinear elements
  - Applications include shock hydrodynamics, Electromagnetic fields in fusion reactors
- ALBANY – Generic F.E. framework
  - Builds on Trilinos components
  - Applications include ice modeling, non-linear solid mechanics, quantum device modeling
- PHASTA – Navier Stokes Flow Solver
  - Highly scalable code including turbulence models
  - Applications include nuclear reactors, multiphase flows
- Landau Collision Integral Solver
  - Addressing key set of PDE's from plasma physics

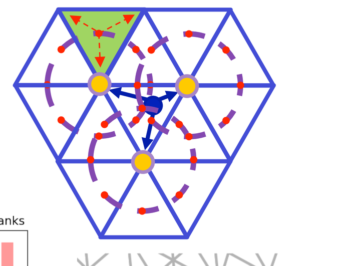


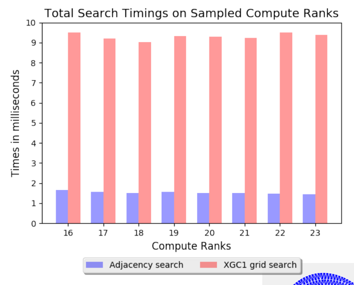


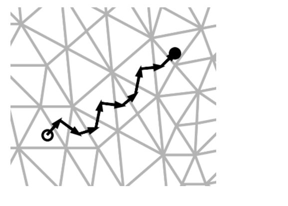


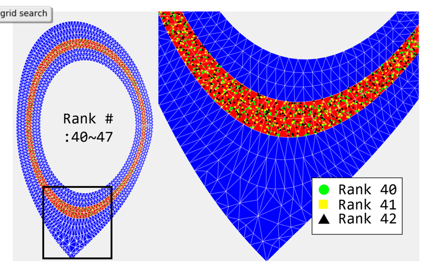
Unstructured Mesh for PIC

- A set of services to support distributed mesh particle-in-cell simulations is under development (PUMIpic)
- Services needed for PIC
  - PIC code specific optimal mesh distribution with large overlaps to avoid communications during a push operation
  - Particles migration and dynamic load balancing
  - Fast adjacency searches and wall intersections
  - Efficient particle-to-mesh field operations (can involve non-trivial neighborhoods)
  - Efficient mesh-to-particle field operations
  - Support for PDE field solves
- Status
  - Components defined and implemented (not fully optimized)
  - Integrated into in new version of XGC (basic physics only)
  - Procedures to support GITR under design and development



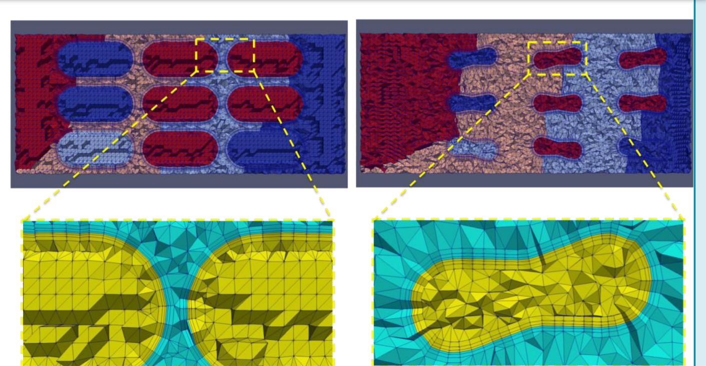




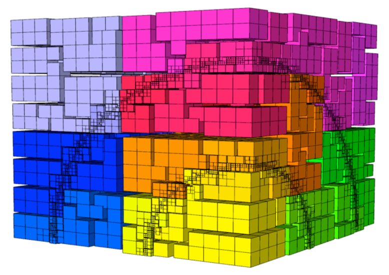


Performant Mesh Adaptation

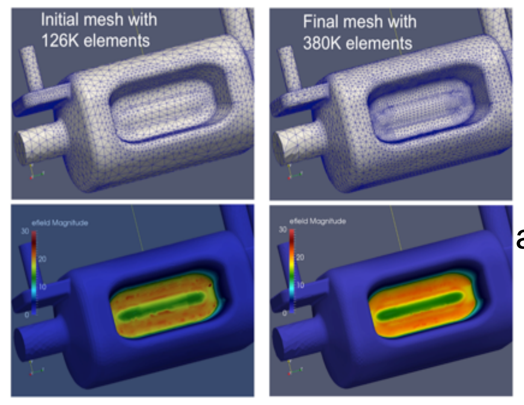
- Parallel Mesh Adaptation Capabilities
  - Generalized conforming anisotropic simplex mesh adaptation including mixed boundary layers
  - Maintain linkage to high-level domain definition
  - Non-conforming adaptation through sub-division
  - Full account for curved element adaptation including optimized curved mesh modification operations
  - Evolving geometry including mesh motion and adaptivity
  - Field transfer tools for adaptively evolving meshes
- Performant Adaptation Developments
  - GPU based conforming mesh adaptation – substantial speed-up over CPU version, coupling MPI and CUDA for mesh adaptation
  - Supporting unstructured mesh operations using Kokkos performance portable framework
  - Support alternative methods of ordering dof
  - Generalization of assembly operations for constructing global matrices
  - Improvements for multicore systems and consideration of pipelined parallelism for FPGAs



Combined mesh motion and adaptation to account for evolving geometry



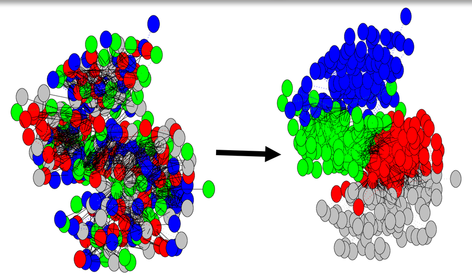
Parallel non-conforming mesh adaptation



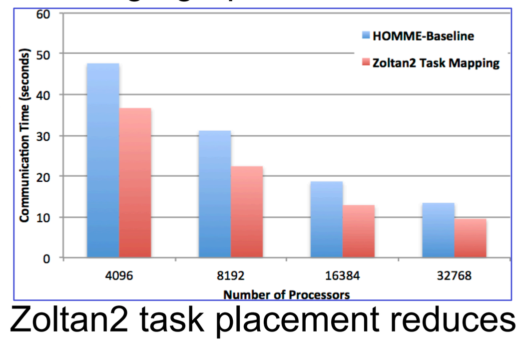
Parallel curved mesh adaptation

Dynamic Load Balancing and Task Management

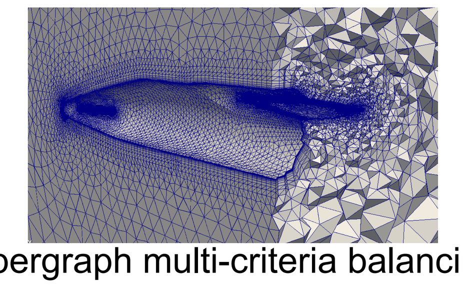
- Development Activities
  - Massively parallel graph algorithms – parallel tools to determine the distribution of computational operations to attain load balance with min. communication
  - Architecture-aware load balancing and task mapping – Reduce application communication time by increasing data locality within nodes and across networks
  - Multi-criteria dynamic partition improvement - accelerating diffusive procedures with GPUs and FPGAs
- Relevant Software tools
  - PuLP and XtraPuLP - github.com/HPCGraphAnalysis/PuLP/
  - Zoltan and Zoltan2 - www.cs.sandia.gov/zoltan/
  - EnGPar – scorec.github.io/EnGPar/
- Operations supported by these tools include
  - Load balance meshes in terms of element, vertices, or multiple mesh entity types
  - Assign interdependent tasks to "nearby" cores in computer network
  - Load balance rows and columns for equation solvers
  - Restore load balance after mesh adaptation
  - Balance particle push operation in PIC codes without explicitly representing particles



The XtraPuLP graph partitioner can partition irregular trillion-edge graphs in minutes



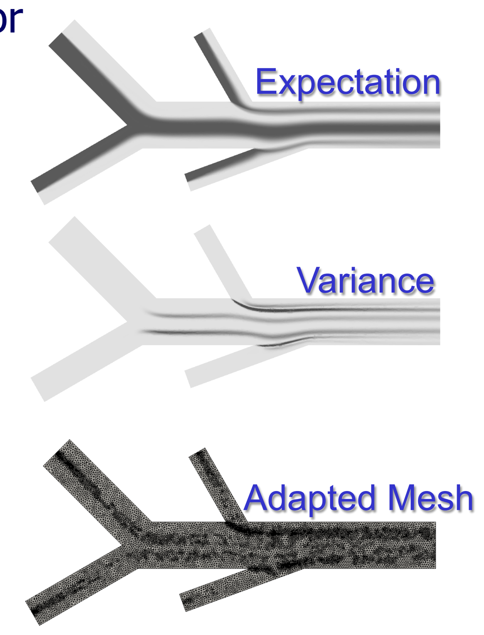
Zoltan2 task placement reduces E3SM HOMME communication time up to 31%



Hypergraph multi-criteria balancing for boundary layer meshes

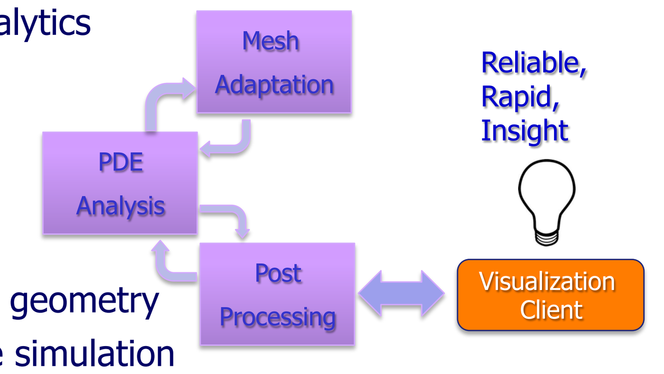
Unstructured Mesh for UQ

- Adaptive control of discretization a prerequisite for the effective application of UQ operations
- Substantial potential for joint adaptivity in the physical and stochastic domains
  - Preliminary study mesh adaptivity in the physical space with spectral/p-adaptivity in the stochastic space
  - Target of consideration of geometric uncertainty where unstructured meshes will be critical
- Developments
  - Stochastic space error estimators
  - Basis and sample reduction strategies
  - UQ driven load balancing



In Situ Vis and Data Analytics

- Solvers scaled to 3M processes producing 10TB/s need in situ tools to gain insight to avoid to 4x cost involved with saving data
  - Substantial progress made to date in live, reconfigurable, in situ visualization
  - Effort now focused on user steering and data analytics
- Target in situ operations
  - Live, reconfigurable in situ data analytics
  - Live, analyst-guided grid adaptation
  - Scalable data reduction techniques
  - Live, reconfigurable problem definition, including geometry
  - Live, parameter sensitivity analysis for immersive simulation



Unstructured Mesh Applications

SciDAC Application Centers

- CTTS: M3D-C1 mesh infrastructure and adaptive meshing (PUMI)
- RF Fusion: EM and thermofluids solvers (MFEM),
- RF Fusion: Geometry and meshing (PUMI, Simmetrix)
- HPBS: Parallel mesh version of XGC (PUMIpic, EnGPAR)
- HPBS: Mesh generation tools (PUMI, Simmetrix)
- Plasma Surface Interactions: 3D particle tracking for CITR (PUMIpic)
- ProSPect: Ice sheet modeling (MPAS Albany
- ProSPect: Graph algorithms for iceberg/peninsula detection (Zoltan2)
- DEMSI: Support for portable performance (Kokkos)

Other DOE Applications

- E3SM HOMME: Task placement in atmospheric modeling (Zoltan2)
- CMDV and E3SM: Task placement in coupled climate components (Zoltan2)
- BLAST: High-Order Finite Element Hydrodynamics (MFEM)
- Alexa: Mesh adaptation in multi-material hydrodynamics (Omega_h)

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

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