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 computations.

FASTMath Unstructured Mesh Developments

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

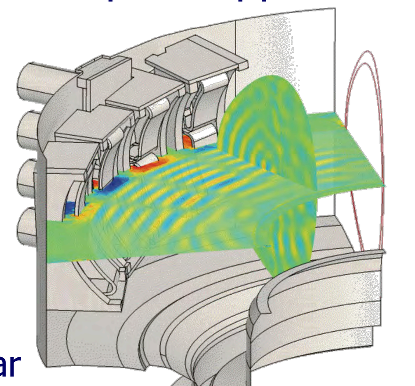
Technology development areas:

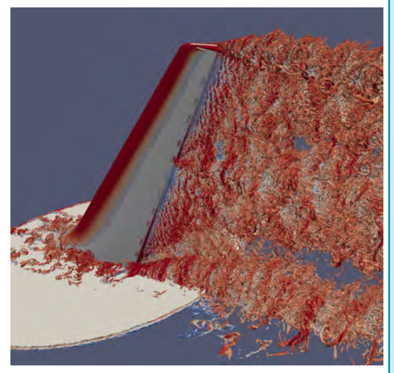
- Unstructured Mesh Analysis Codes – Support application's PDE solution needs
- Performant Mesh Adaptation – Parallel mesh adaptation integrated into analysis codes to ensure solution accuracy
- Dynamic Load Balancing and Task Management – Technologies to ensure load balance and effectively execute operations 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

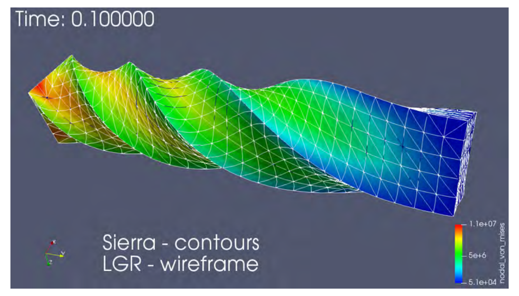
Unstructured Mesh Analysis Codes

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/LGR – 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 with implicit and explicit tracking
- Landau Collision Integral Solver
  - Addressing key set of PDEs from plasma physics

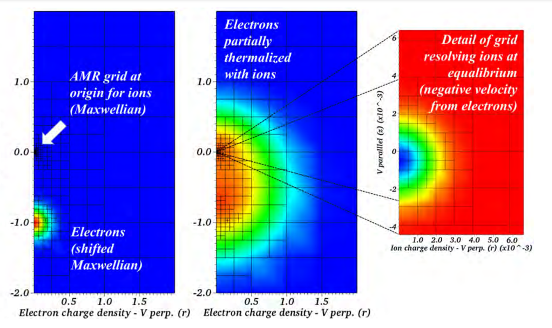




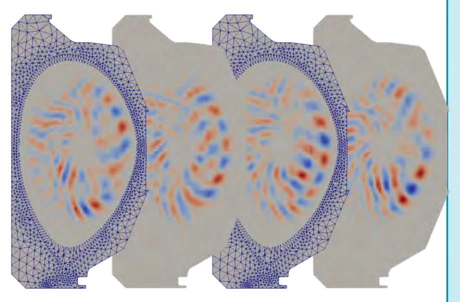


Unstructured Mesh for PIC

- Conservative coupling of particle and adaptive mesh FEM discretizations in PETSc
  - New DMSwarm manages parallel particle fields in PETSc
  - Particles migration and dynamic load balancing
  - Symplectic integrators of order 1 to 4 implemented
- Distributed mesh particle-in-cell infrastructure
  - PIC code specific 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 and mesh-to-particle operations
  - Mesh-based XCG edge plasma code up to delta-f ion and election push operational, performance optimization initiated
  - Mesh-based GITR impurity transport in initial stage of testing using mesh and particle structures designed for GPUs



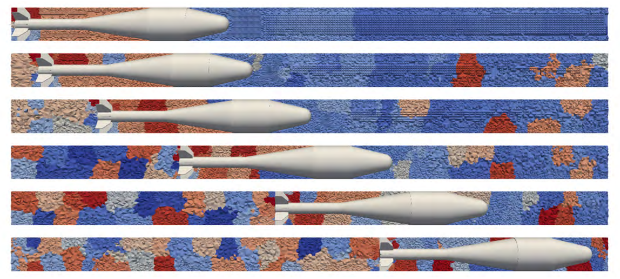
Particle-grid interaction: Electron beam thermalizing with ions



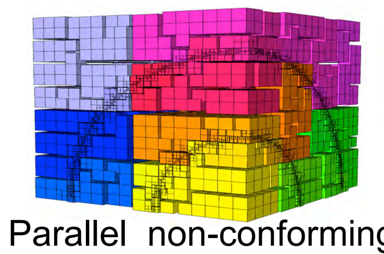
Electrostatic potential fluctuation at four toroidal angles for mesh-based XGC

Mesh Adaptation

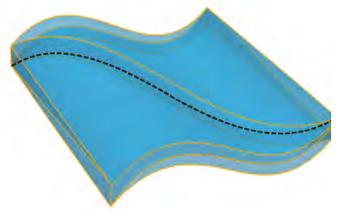
- Generalized conforming anisotropic simplex mesh adaptation including mixed boundary layers
- Maintain linkage to high-level domain definition
- Non-conforming adaptation through sub-division
- Fully account for curved element adaptation including optimized curved mesh modification operations
- Evolving geometry including mesh motion and adaptivity



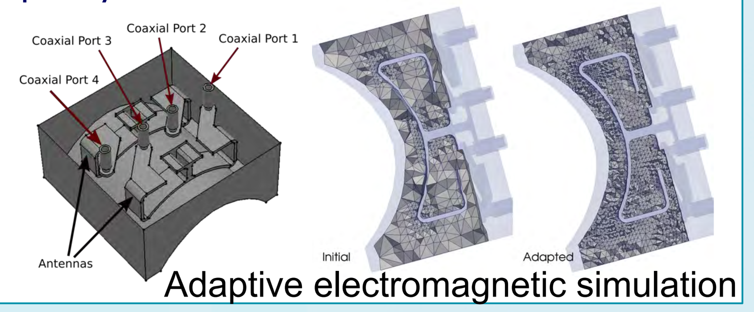
Combined mesh motion and adaptation to account for evolving geometry



Parallel non-conforming mesh adaptation



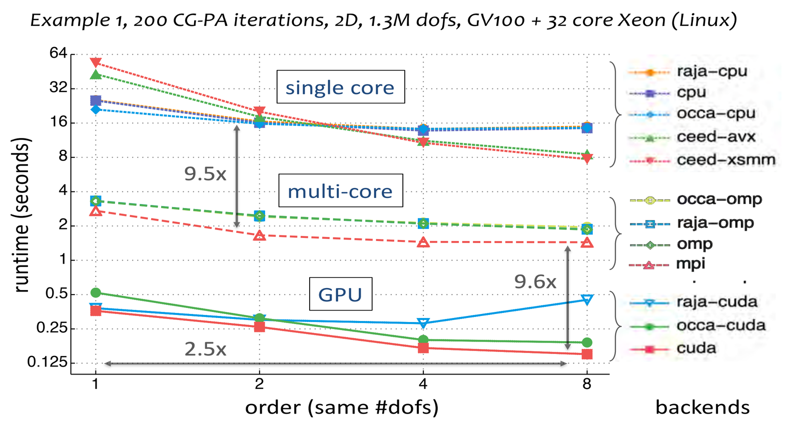
High order mesh curving



Adaptive electromagnetic simulation

Pefromant Unstructured MeshTechnologies

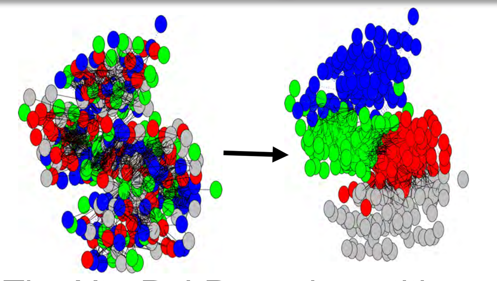
- GPU accelerated unstructured analysis codes
- GPU based mesh adaptation
- Supporting unstructured mesh operations using Kokkos performance portable framework
- Support alternative methods of ordering DOFs
- Otimized data structures and algorithms for execution on GPUs
- Improvements for multicore systems and consideration of pipelined parallelism for FPGAs



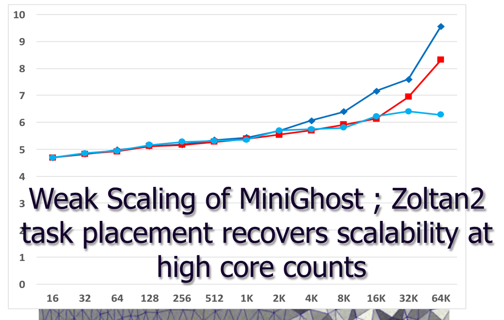
Initial MFEM v4.0 results

Dynamic Load Balancing and Task Management

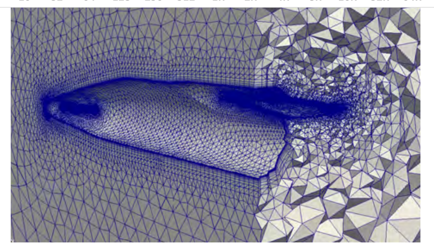
- Massively parallel graph algorithms – parallel tools to determine the distribution of computational operations to attain load balance with min. communication
- Architecture-aware load balancing and task mapping – reduce application communication time by increasing data locality within nodes and across 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



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



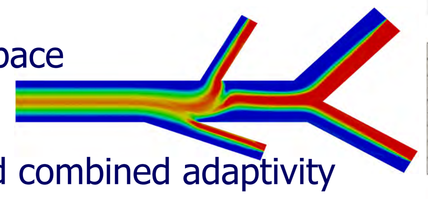
Weak Scaling of MiniGhost ; Zoltan2 task placement recovers scalability at high core counts

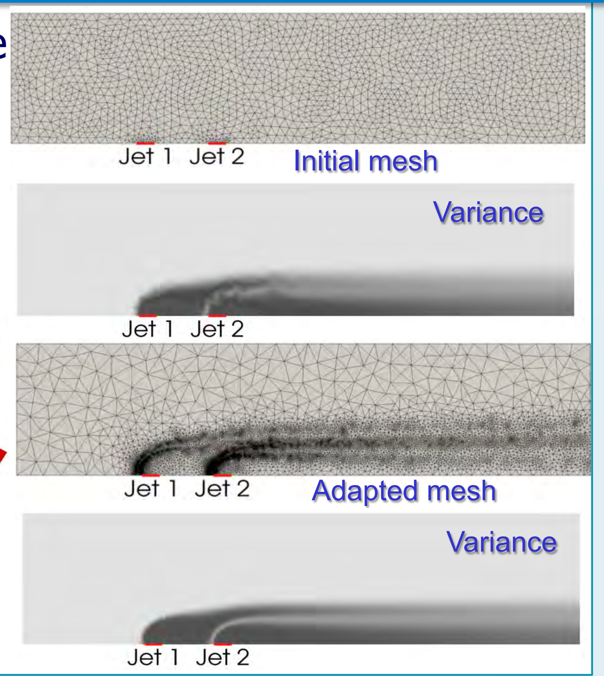


Hypergraph multi-criteria balancing for boundary layer meshes

Unstructured Mesh for UQ

- Adaptive control of discretization is a prerequisite for the effective application of UQ operations
  - Mesh adaptivity in the physical space and spectral/p-adaptivity in the stochastic space
  - Non-uniform/spatially varying stochastic fields
  - Anisotropic adaptive control
  - Multi-fidelity modeling in UQ space
- Developments
  - Stochastic error estimators and combined adaptivity
  - Basis and sample reduction strategies
  - Multi-resolution error control strategy
  - Application for problems with general geometries





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
  - Live, reconfigurable, in situ visualization
  - Focus on user steering & data analytics
- Target in situ operations
  - Live, reconfigurable in situ data analytics
  - Live, analyst-guided grid adaptation
  - Scalable data reduction techniques
  - Reconfigurable problem geometry
  - Parameter sensitivity for immersive sim.

# elements in the mesh	Flow solve w/o filter	Filter	Size of data extract	Total Blocking Time (Filtering + aggregation + transfer time)	
				Current	
3.32 B	14.3 s	Slice	240 MB	0.200 s	1.4 %
		Contour	3796 MB	0.586 s	4.1 %
416 M	1.84 s	Slice	64.8 MB	0.175 s	9.5 %
		Contour	1006 MB	0.269 s	14.6 %
52 M	0.474 s	Slice	18.5 MB	0.158 s	33.3 %
		Contour	276 MB	0.215 s	45.4 %

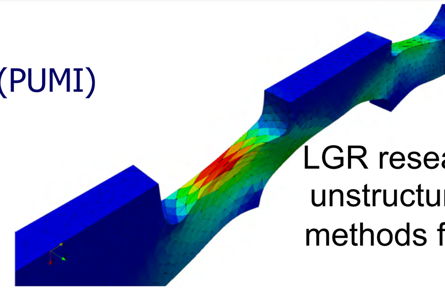
Unstructured Mesh Applications

SciDAC Application Partnership Interactions

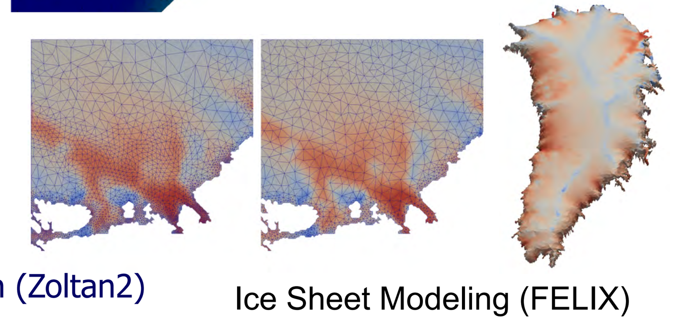
- CTTS: M3D-C1 mesh infrastructure and adaptive meshing (PUMI)
- RF Fusion: EM and thermofluids solvers (MFEM),
- RF Fusion: Geometry and meshing (PUMI, Simmetrix)
- HPBS: Parallel mesh version of XGC (PUMIpic, EnGPAR)
- HPBS: Mesh generation tools (PUMI, Simmetrix)
- PSI2: 3D particle tracking for GITR (PUMIpic)
- TDS: High-Order FEM for fussion (MFEM)
- DEMSI: Support for portable performance (Kokkos)
- ProSPect: Ice sheet modeling (MPAS Albany)
- ProSPect: Graph algorithms for iceberg/peninsula detection (Zoltan2)

Additional DOE Applications

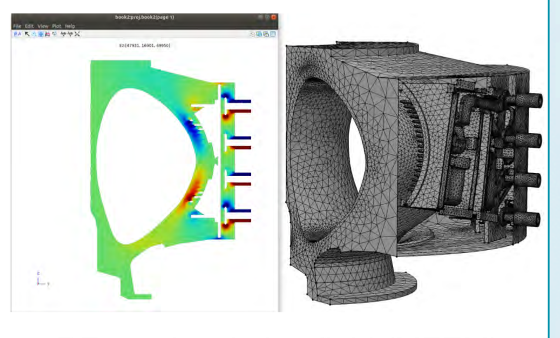
- E3SM HOMME: Task placement in atmospheric modeling (Zoltan2)
- CMDV and E3SM: Load balancing and task placement in coupled climate components (Zoltan/Zoltan2)
- BLAST: High-Order Finite Element Hydrodynamics (MFEM)
- LGR: Mesh adaptation in multi-material hydrodynamics (Omega_h)
- ATDM: Redistribution in multigrid solvers (Zoltan2)
- ASC: Load balancing in engineering mechanics codes (Zoltan2)



LGR research into stable unstructured tetrahedral methods for plastic solids



Ice Sheet Modeling (FELIX)



RF result solution field (MFEM)

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

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