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.

Unstructured Meshing Technologies

FASTMath Team Members: M.F. Adams¹, K. Devine², V. Dobrev³, D. Ibanez², K.E. Jansen⁴, M. Knepley⁵, T.V. Kolev⁶, O. Sahni⁶, S. Seo⁶, M.S. Shephard⁵, G.M. Slota⁵, C.W. Smith⁶, LBL, 53NL, 6LNL, 4CU, 5Buffalo, 6RPI

Unstructured Meshing Technology Developments

- Conservative coupling of particle and adaptive mesh FEM discretizations in Petsc
- New DM/Parma manager to 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
- Efficient particle-to-mesh and mesh-to-particle operations
- Mesh-based XGC edge plasma code up to delta-f ion and electron push operational, performance optimization initiated
- Mesh-based GTR impurity transport in initial stage of testing using mesh and particle structures designed for GPUs

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

Mesh and data analytics

- In Situ Vis and Data Analytics – Tools to gain insight as simulations execute
- Tools to support PIC on unstructured meshes
- Bringing unstructured mesh adaptation to UQ
- Applications include nuclear reactors, multiphase flows
- 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

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 processes with GPUs and PGAs
- Relevant Software tools
- PULP and XtraPULP - github.com/HPCGraphAnalysis/PULP/
- EndGame - student.github.io/EndGame/
- Operations supported by these tools include
  - Load balance meshes in terms of element, vertices, or multiple mesh entity types
  - Assign independent 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

Unstructured Mesh for PIC

- Particle-grid interaction: Electron beam thermalizing with ions
- Electrostatic potential fluctuation at four toroidal angles for mesh-based XGC

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 data analytics
- 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.

Unstructured Mesh Applications

- SciDAC Application Partnership Interactions
  - CTTS: H3D-C1 mesh infrastructure and adaptive meshing (PUMI)
  - RF Fusion: EM and thermofluids solvers (MFEM), RF Fusion: Geometry and meshing (PUMI, Simmetrix)
  - HPS: Parallel mesh version of XGC (PUMI, EnGRID)
  - HPS: Mesh generation tools (PUMI, Simmetrix)
  - PS2: 3D particle tracking for GTR (PUMI)
  - TDS: High-Order FEM for fusion (MFEM)
  - ODHS: Support for portable performance (Kalos)
  - ProSyst: Ice sheet modeling (MMAS Albany)
  - ProSyst: Graph algorithms for icecore/peninsula detection (Zoltan2)
  - Additional DOE Applications
    - E3SM HOME: Task placement in atmospheric modeling (Zoltan2)
    - CMDV and E3SM: Load balancing and task placement in coupled climate components (Zoltan2/Zoltan2)
    - BLAST: High-Order Fluids Element Hydrodynamics (MFEM)
    - LGR: Mesh adaptation in multi-dimensional hydrodynamics (Omega_h)
    - ATOM: Load balancing in engineering mechanics codes (Zoltan2)
    - ASC: Load balancing in engineering mechanics codes (Zoltan2)

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