FASTMATH

Unstructured Mesh Technologies for Fusion Simulation Codes

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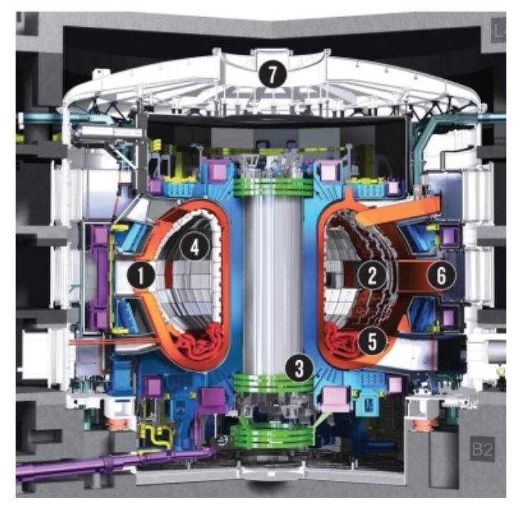
Unstructured meshes are well suited to modeling the complex physics and geometries of fusion reactors. FASTMath and the fusion SciDACs are supporting the development of unstructured mesh technologies needed by the fusion SciDAC Partnerships for their near-exascale simulations.

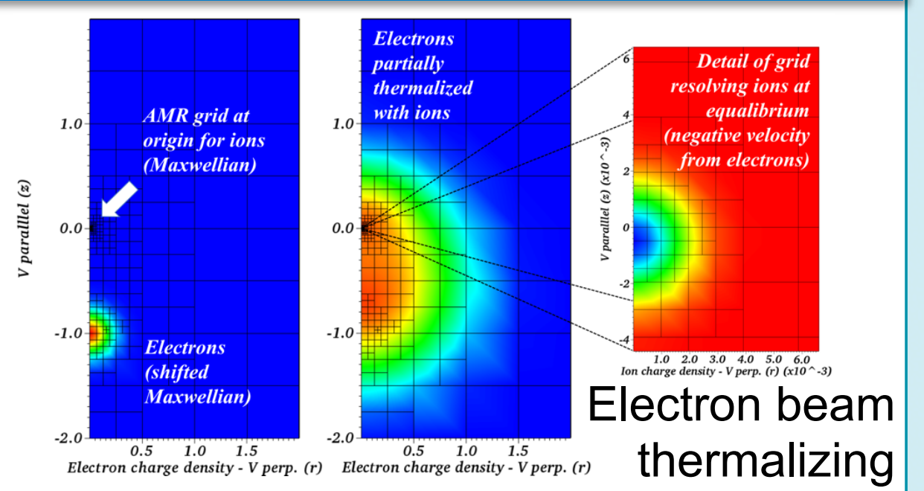
Areas of Development



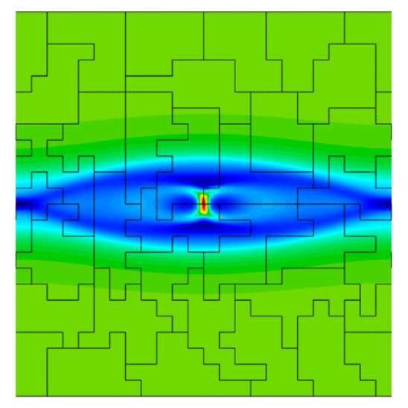
- Finite Element solvers for runaway electron kinetics and MHD
- Mesh generation/adaptation advances for fusion SciDACs
- Support of M3D-C1 extended MHD code for core plasma
- Adaptive RF simulation workflow
- Infrastructure for unstructured mesh PIC simulations
- XGCm – mesh-based version of the XGC edge plasma code
- GITRm – mesh-based version of the GITR impurity transport code

Solver for Runaway Electron Kinetics

- Conservative solver for runaway electron kinetics
  - Discretization of the Landau collision integral
  - Conserve mass, momentum and energy, more if desired
  - DMSwarm manages parallel particle fields in PETSc
  - Symplectic integrators of order 1 to 4 implemented
  - Non-conforming mesh adaptation
- Scalable MHD solver
  - Builds on MFEM high-order finite element solver
  - Non-conforming mesh adaptation
  - Dynamic mesh adaptation applied to the island coalescence problem



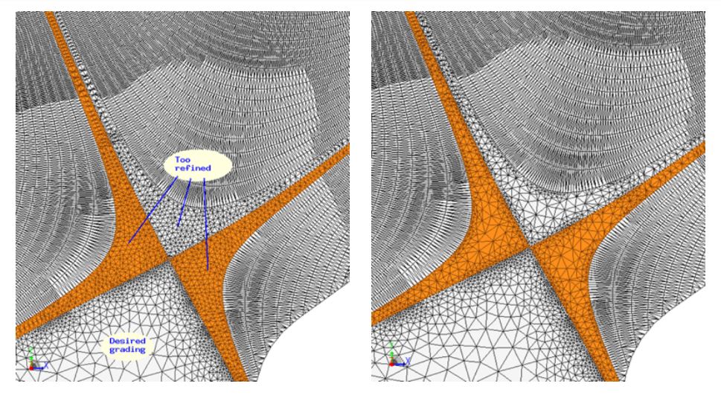
Electron beam thermalizing with ions



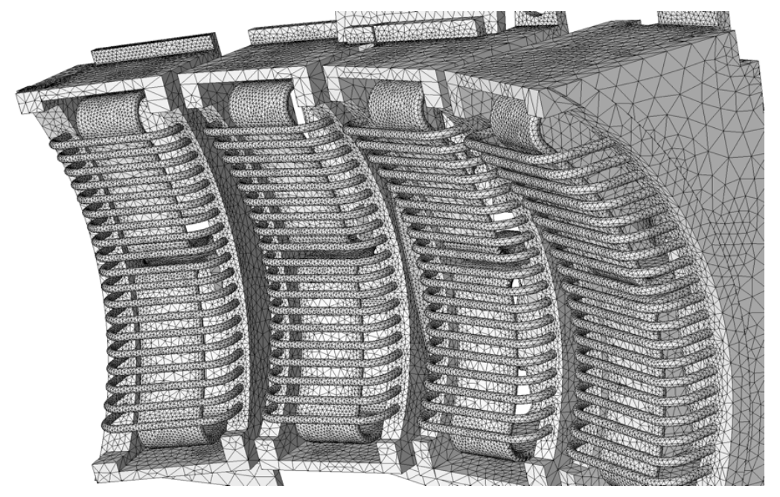
Island coalescence simulation

Mesh Generation/Adaptation

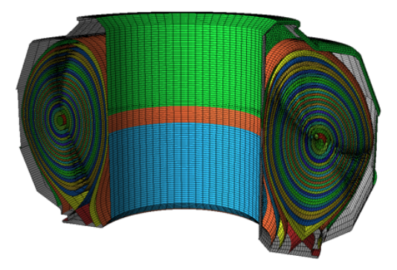
- Tokamak geometry and meshing
  - Reordering mesh for better memory access
  - ITER, DIII-D, Alcator C-MOD, NSTX, KSTAR, etc.
  - EFIT physics geometry
  - Improved mesh quality
- Higher order curved mesh generation
- Higher order curved mesh adaptation
- Special meshing tool for hPIC



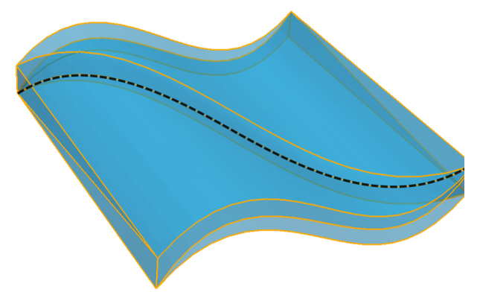
Improved XGC mesh control



Curved mesh for complex geometry

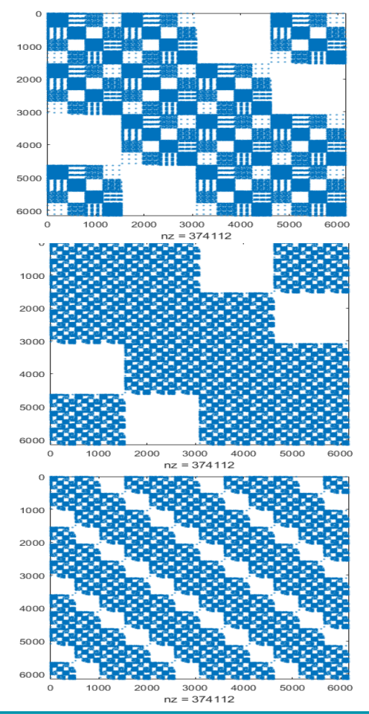


3D mesh for GITRm



High order mesh curving

Support for M3D-C1



- Support of alternative ordering of unknowns
  - By-component DOF ordering
  - Implementation supports ordering at process, poloidal plan or globally
- Support of M3D-C1 mesh infrastructure and software
- Initial support of the addition of PIC to M3D-C1
  - Plan to integrate our developing GPU mesh/particle structures in future

Adaptive RF Simulation Workflow

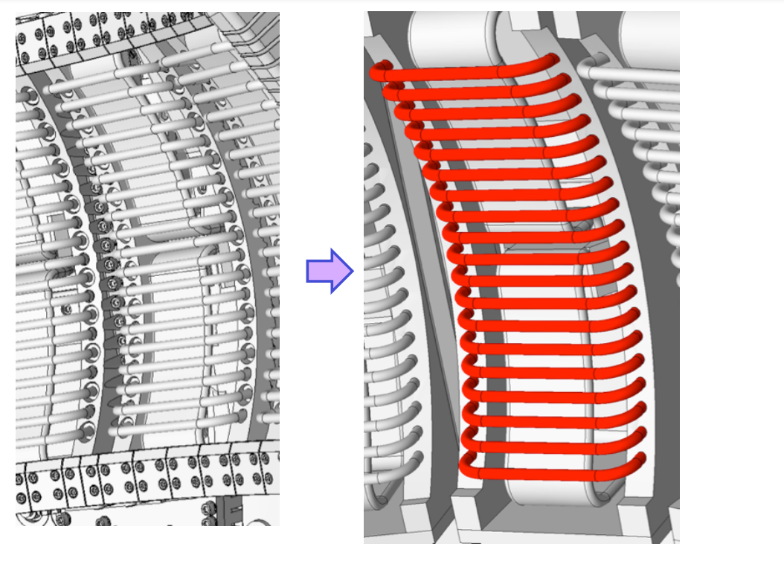
Workflow steps

1. Obtain and clean-up antenna CAD models
2. Combine antenna, reactor and physics geometries
3. Associate analysis attributes
4. Automatic mesh generation
5. MFEM finite element analysis
6. Estimate errors. If below tolerance terminate
7. Adapt mesh and return to step 5

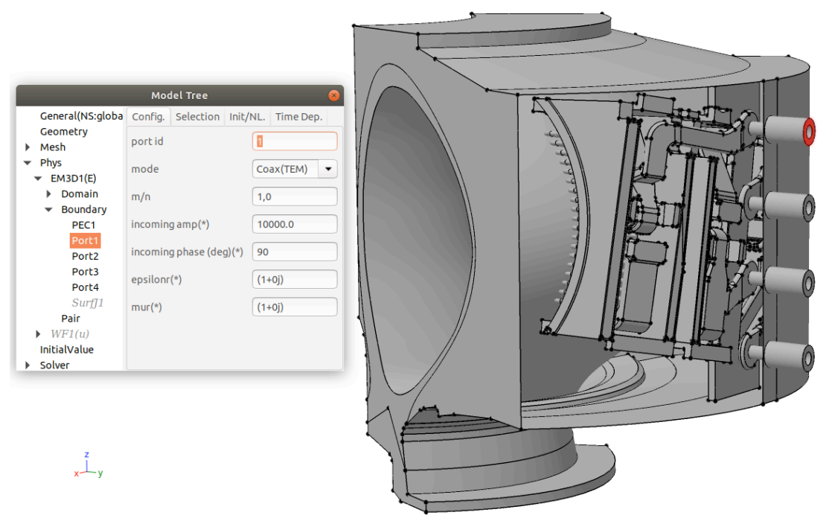
- Steps 1-3 are carried out interactively
- Steps 4-7 are automated and execute in parallel

Tools used

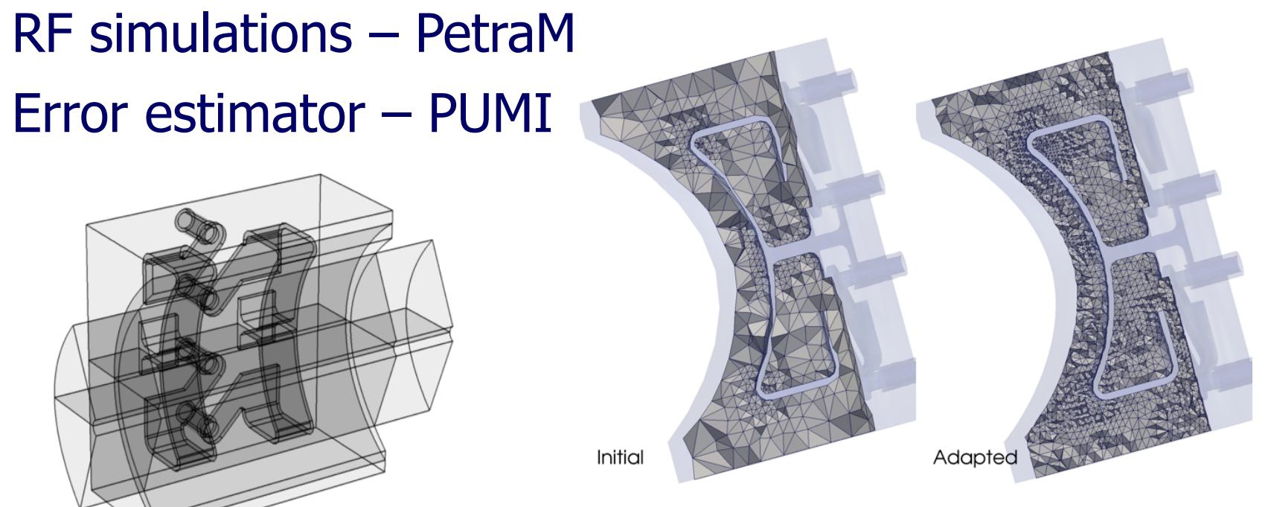
- Geometry – Simmetrix SimModeler, CAD systems, EFIT
- Mesh generation – Simmetrix MeshSim
- Mesh services and curved mesh adaptation – PUMI
- High-order finite element analysis – MFEM
- RF simulations – PetraM
- Error estimator – PUMI



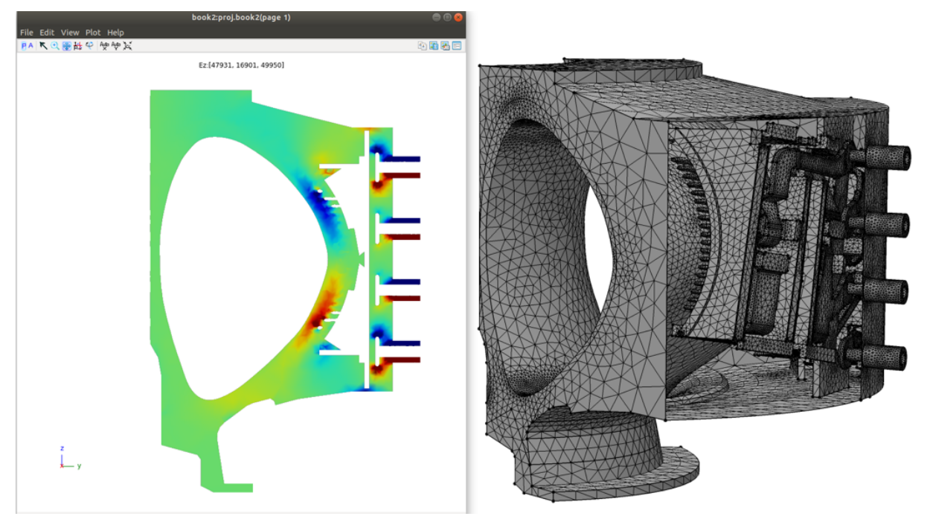
CAD model clean-up



Combined geometry



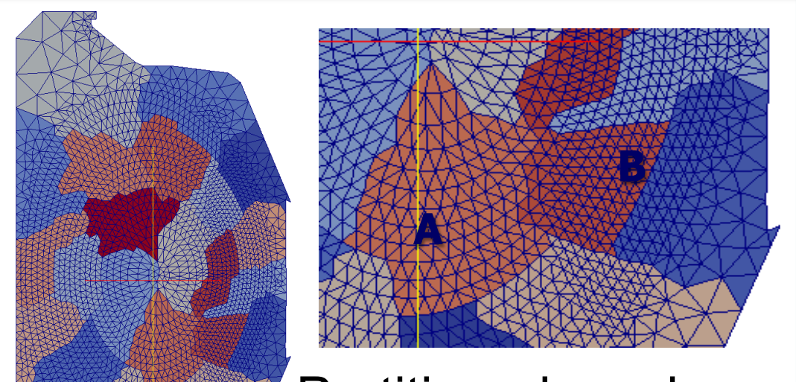
Example adaptive mesh



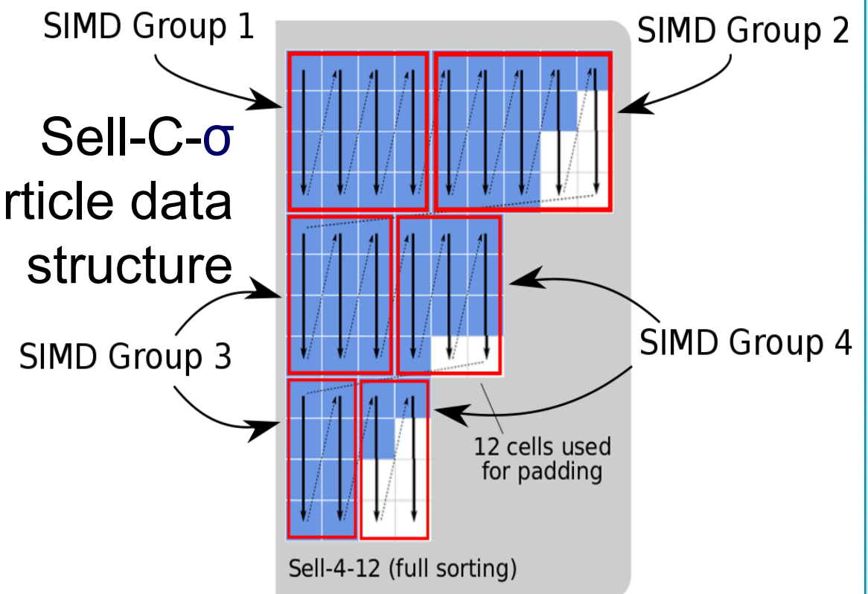
MFEM Analysis

Infrastructure for Unstructured Mesh PIC

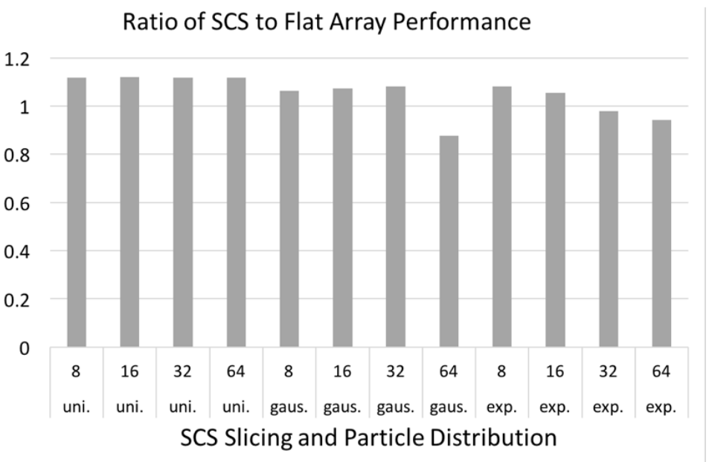
- Mesh-based particle-in-cell infrastructure
  - PIC code specific optimal mesh distribution
  - Particles migration and dynamic load balancing
  - Fast adjacency searches and wall intersections
  - Efficient particle-to-mesh and mesh-to-particle operations
- PICpart definition (in more data efficient version)
  - PICpart with be a "part" of partitioned mesh
  - Plus neighboring and close parts up to the full mesh
  - Memory requirements reduced from original approach
- Mesh data structure
  - Omega - GPU enabled mesh topology data structure
  - BFS-like algorithms for effective local performance
  - On-node OpenMP or CUDA parallelism using Kokkos
- Particles structures critical for GPU performance
  - Particles related to elements
  - Sell-C-σ defined for particles/element – needed to be more advanced than flat arrays due variable # particles/element
  - Coordinating with the COPA ECP particle co-design center



Partitioned mesh – PICpart is collection of partition parts



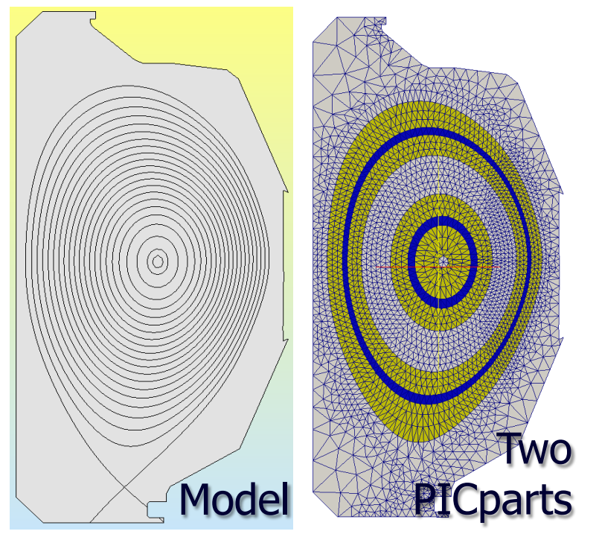
Sell-C-σ particle data structure

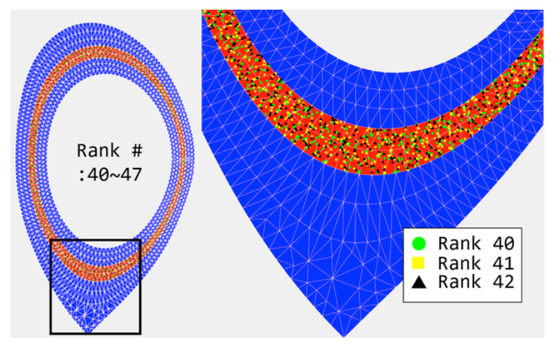


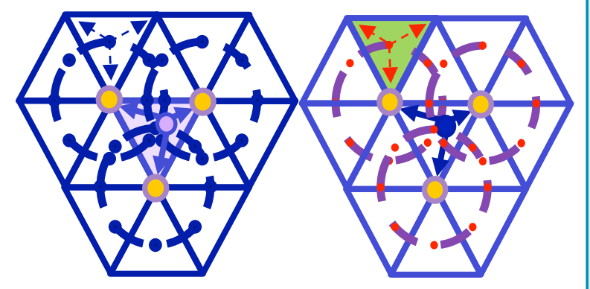
SCS is within 20% of flat array performance, faster in many of the non-uniform distributions

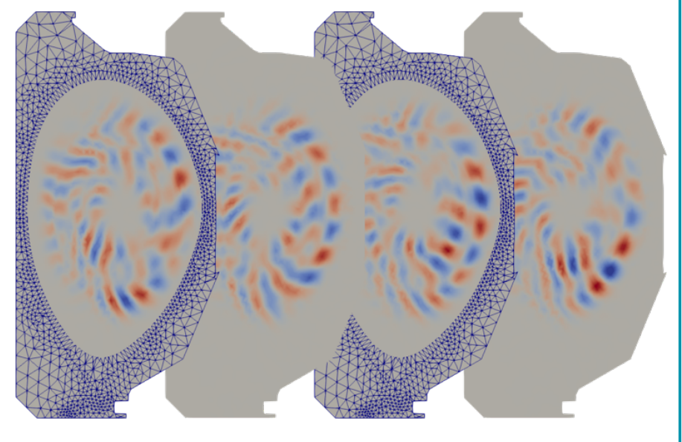
Mesh-Based Edge Plasma PIC Code

- Implementing XGC physics and numerics
  - Since data structures are changed code being rewritten in C++
- Status
  - Based on original PUMI structures – GPU focused structures will be integrated later – will only influence mesh/particle operations
  - Mesh/particle interaction operations
  - Mesh solve in place (needs optimization)
  - Ion and electron push (including subcycling)
  - Initial δf simulations
  - Performance evaluation and improvement underway
- Small δf test case – 6.2K elements, 8 poloidal planes
  - 300k particles/rank, 64-512 ranks, 1-8 Cori KNL nodes
  - Total timings (minus FE solve) equivalent to XGC1
- Medium δf test case – 127k elements, 8 poloidal planes
  - 300k particles/rank, 256-1024 ranks, 4-16 Cori KNL nodes
  - Push operation 25% faster than XGC (key and encouraging)
  - Total time double XGC – need new structure to optimize
  - Buffer zone has substantial influence on timings





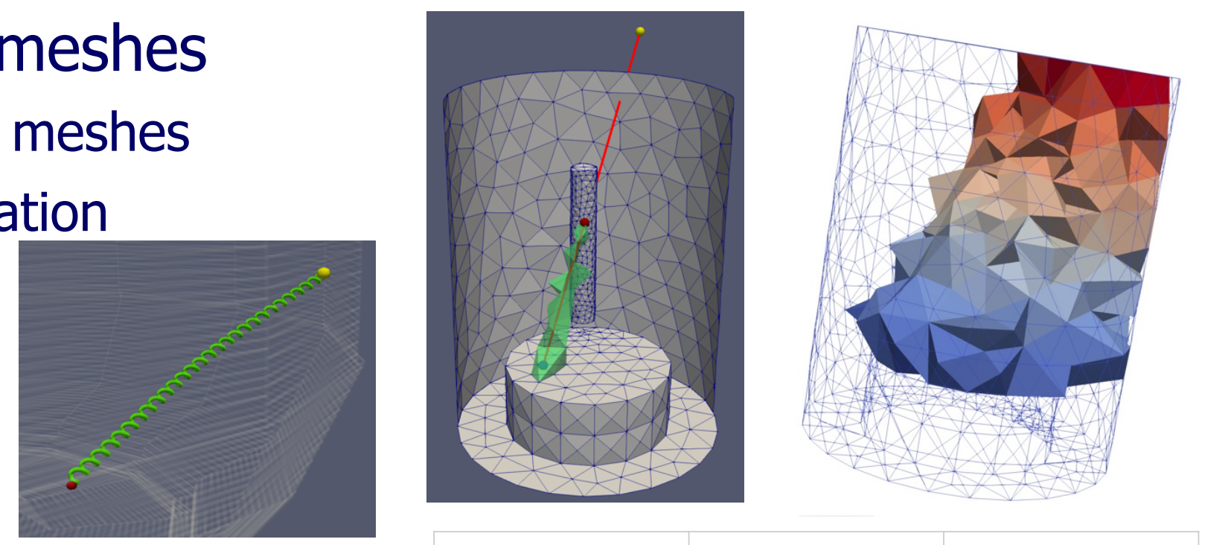


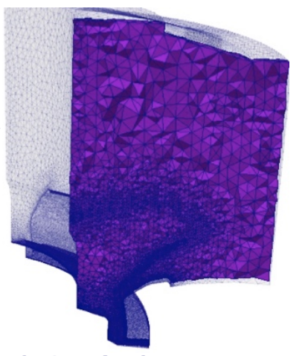


Electrostatic potential fluctuation at four toroidal angles for mesh-based XGC

Mesh-Based Impurity Transport Code

- Operates in 3D unstructured graded meshes
  - 3D adjacency search - effective on graded meshes
  - Mesh entity classification for efficient operation
  - Wall intersection implemented
  - Elements where distance tracking preprocessed to know when needed
  - Boris move implemented
  - Omega mesh and new particle data structures
  - Initial tests, including GPU execution, underway
  - Working with U. Tenn and ORNL to define appropriate verification tests
- Executed 20 push, search, rebuild iterations on PISCES mesh (~6k tets) on a GPU
  - Results comparable to those executed on background grids





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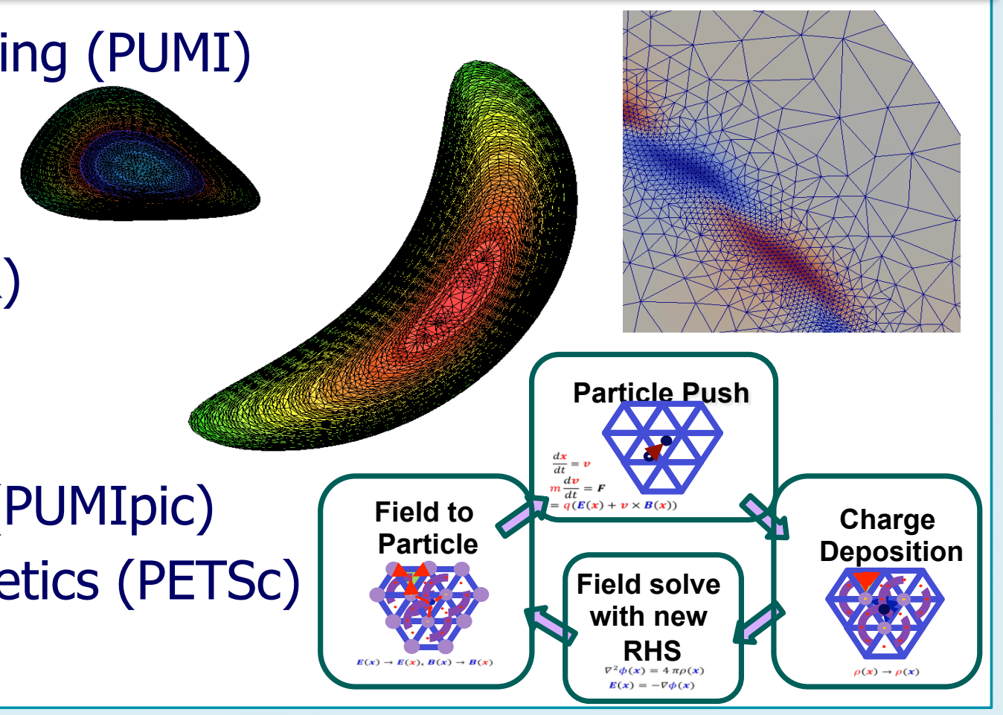
Fusion Partnership Interactions

- 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: Parallel mesh version of GITR (PUMIpic)
- PSI2: Block structured mesh for specific hPIC version (PUMIpic)
- SCREAM: Conservative solver for runaway electron kinetics (PETSc)
- TDS: Scalable MHD solver (MFEM)



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