Unstructured Mesh Technologies for Fusion Simulation Codes

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Simmetrix Inc.

Outline:

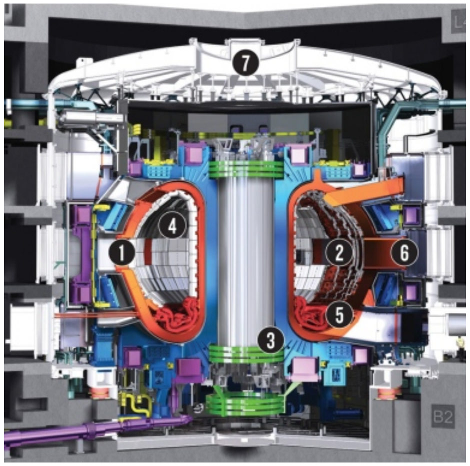
- Geometry and Meshing
- Supporting continuum analysis codes
- Distributed unstructured mesh based PIC

Simmetrix Inc.   FASTMATH   SCOREC

Background

Why unstructured meshes for fusion simulations?

- High fidelity simulations must accurately represent fusion device geometry
- Codes have specific meshing requirements
- Unstructured meshes deal with any geometry, can meet many meshing requirements



RPI's Scientific Computation Research Center (SCOREC)

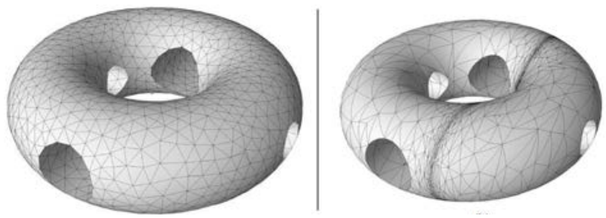
- Developing parallel unstructured meshing technologies starting in SciDAC 1
- Efforts for fusion SciDAC centers has grown

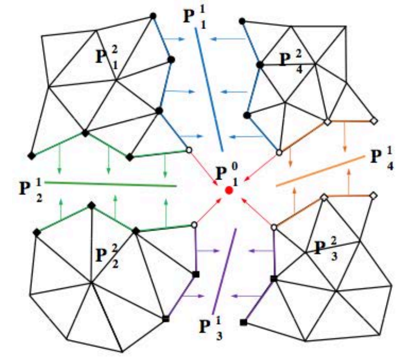
Simmetrix Inc.

- Produces interoperable geometry and meshing components used by CAE software companies
- SCOREC takes advantage Simmetrix technologies in tools developed for fusion SciDACs

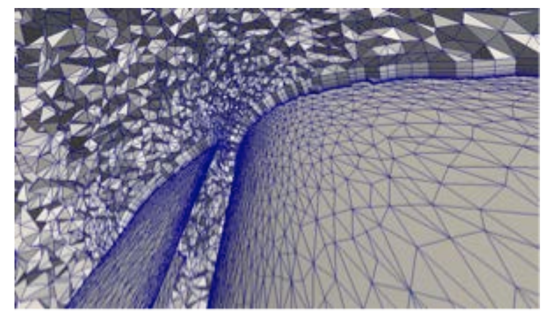
FASTMath Unstructured Mesh Technologies

- Parallel Unstructured Mesh Infrastructure (PUMI) (RPI)
  - Complete mesh topology (O(1) adjacencies)
  - Mesh level interprocess communications
  - Partition modification
  - Read only copies
  - Mesh level fields

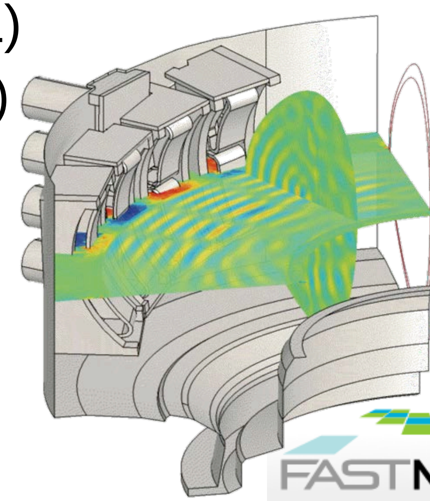




- Parallel mesh adaptation (MeshAdapt) (RPI)
  - Geometry consistent, anisotropic, conforming
  - In-memory integration with several codes



- Dynamic load balancing
  - Zoltan - graph and geometric load balancing (SNL)
  - EnGPar – multicriteria partition improvement (RPI)
- Unstructured mesh analysis codes
  - MFEM – high order FE framework (LLNL)
  - Albany – generic FE framework (SNL)
  - Phasta – NS flow solver (Colorado, RPI)

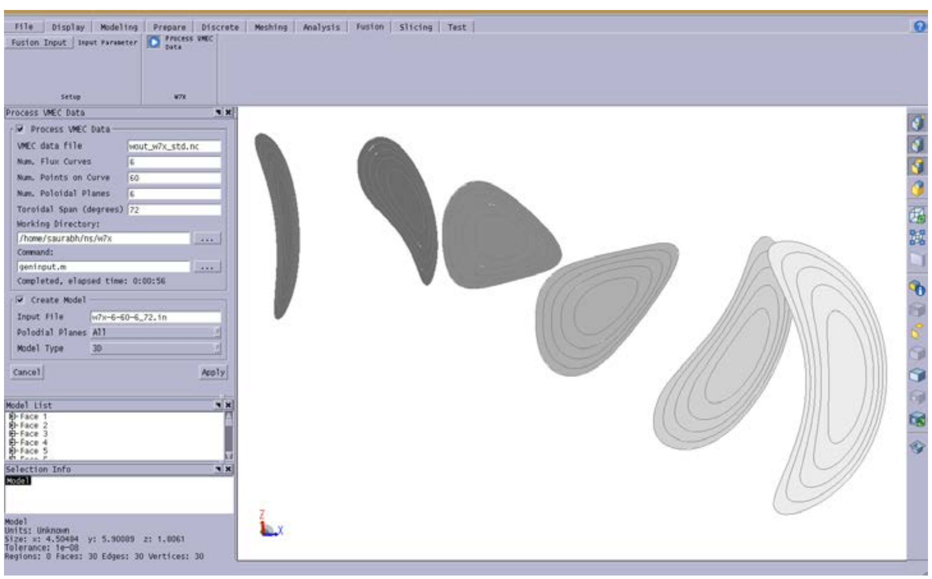


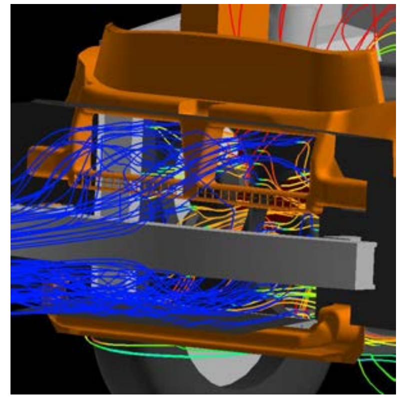
FASTMATH

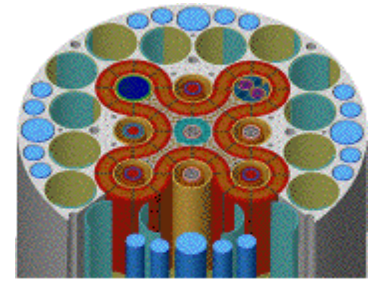
Simmetrix Geometry and Meshing

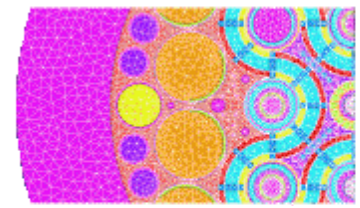
Component software for simulation-based engineering

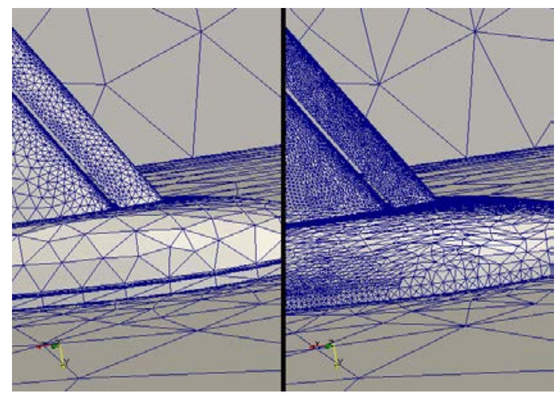
- Direct links to CAD, geometry simplification and combination
- Fully automatic parallel meshing with flexible mesh control
- Mesh-based field manipulation
- Customizable user interface

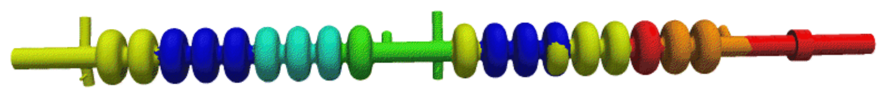


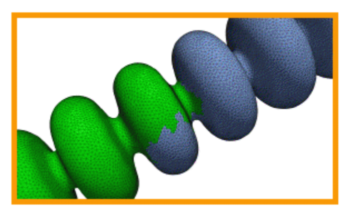


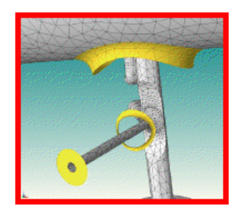












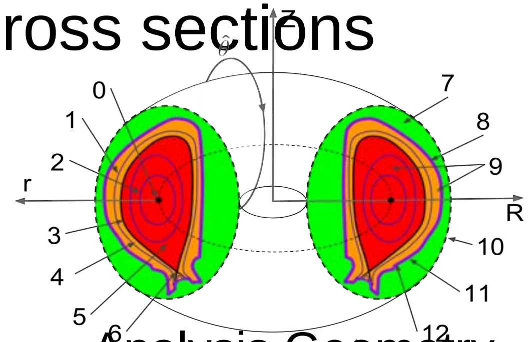
Technologies Being Developed for Fusion SciDACs

- Tokamak cross section geometry and meshing
  - Includes “physics geometry” and specific meshing functions to meet XGC and M3D-C1 requirements.
- 3D geometry cleanup and combination
  - Current focus is for 3D RF simulations
  - Combines CAD, physics geom. & surface meshes into analysis geometry
- Mesh generation including curved elements
  - Specialized tools being considered for stellarator geometry/mesh
- Analysis code support, curved mesh adaptation for high order methods and support for field transfer
  - M3D-C1 builds directly on PUMI mesh infrastructure
  - To be used in MFEM RF simulations and GITR Impurity Transport
- Parallel mesh infrastructure for PIC calculations
  - Version for XGC being tested
  - Version for GITR being designed

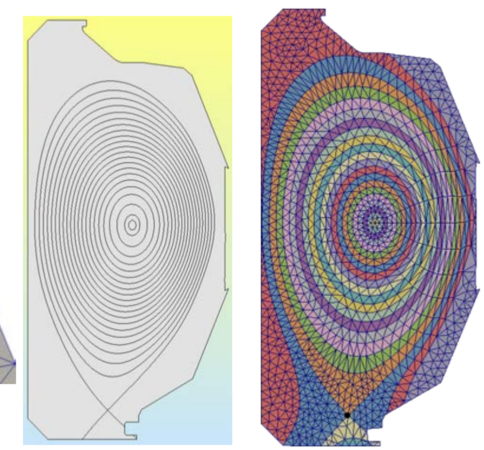
Tokamak Geometry and Meshing

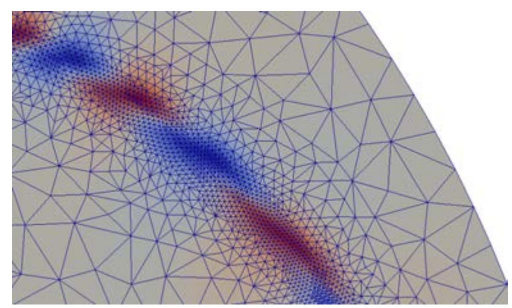
Geometry/meshing tool developed for tokamak cross sections

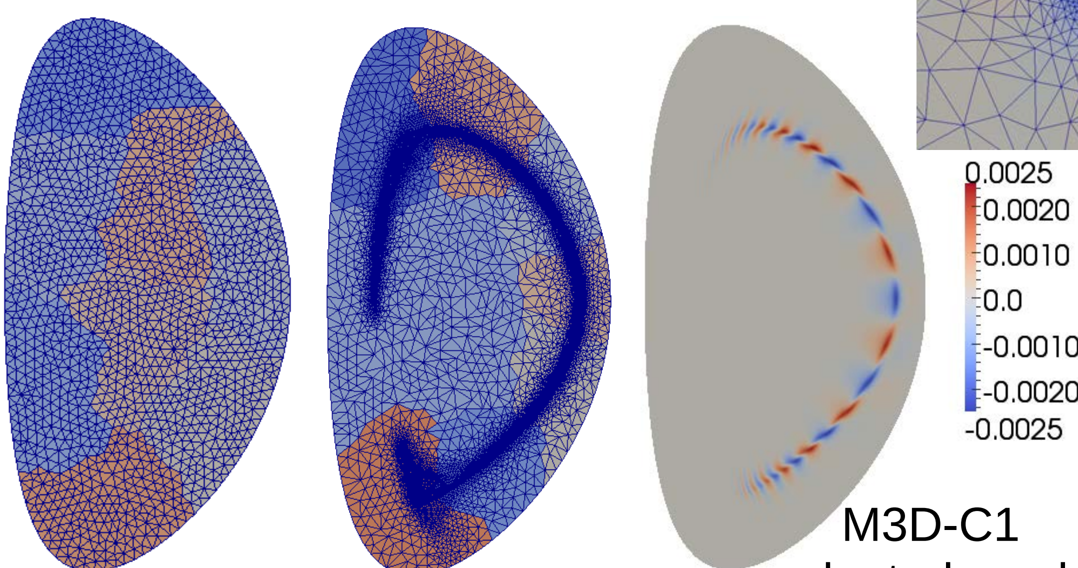
- “Field following” XGC meshes
- 2D to 3D and mesh adaptivity for M3D-C1
- Tokamak cross-section geometry
  - Analytic, spline or discrete physical components – ITER, DIII-D, Alcator C-MOD, NSTX, KSTAR,etc.
  - EFIT defined physics geometry
- Graphical user interface



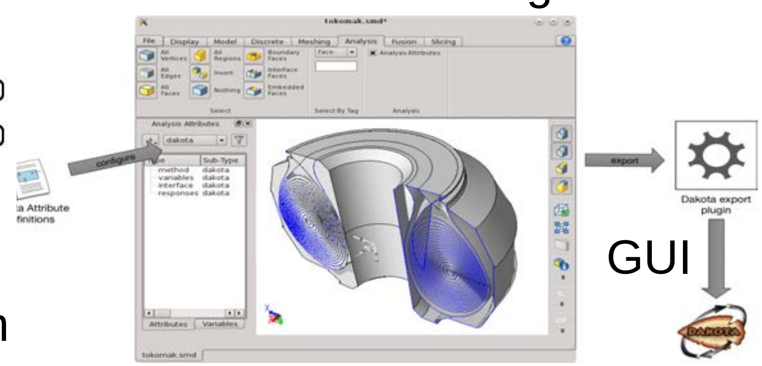
Analysis Geometry


Field following XGC mesh





M3D-C1 adapted mesh



GUI

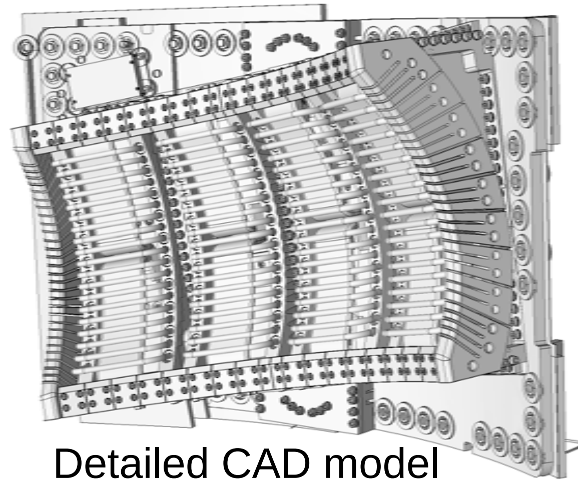
Geometry and Meshing for RF Simulations

Accurate RF simulations require

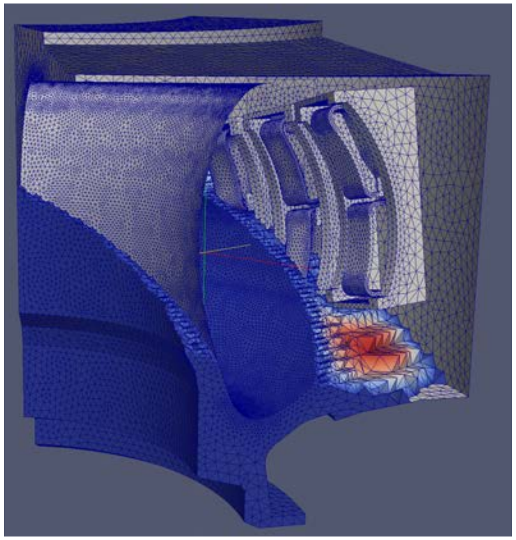
- Detailed antenna CAD geometry
- Extracted physics curves from EFIT
- Faceted surfaces from coupled meshes
- Analysis geometry combining CAD, physics geometry and faceted interfaces
- Well controlled 3D meshes for accurate FE calculations in MFEM
- Integration with up-stream and down-stream simulation codes

Developments underway

- Tools for combining and interacting with geometry from multiple sources
- Integration with curved mesh generation
- Parallel curved mesh adaptation integrated into MFEM
- Integration into the RF simulation workflow



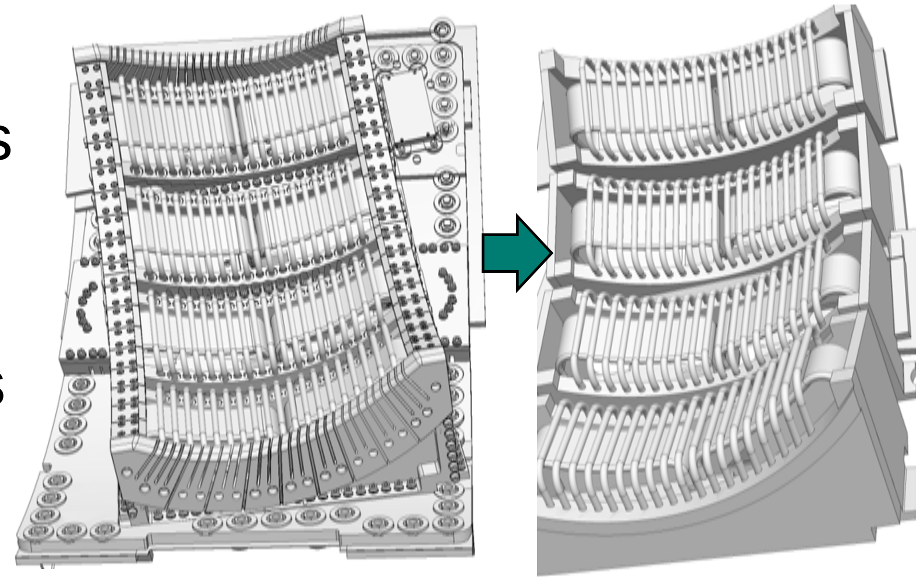
Detailed CAD model of antenna array



Simplified antenna array and plasma surface merged into reactor geometry and meshed

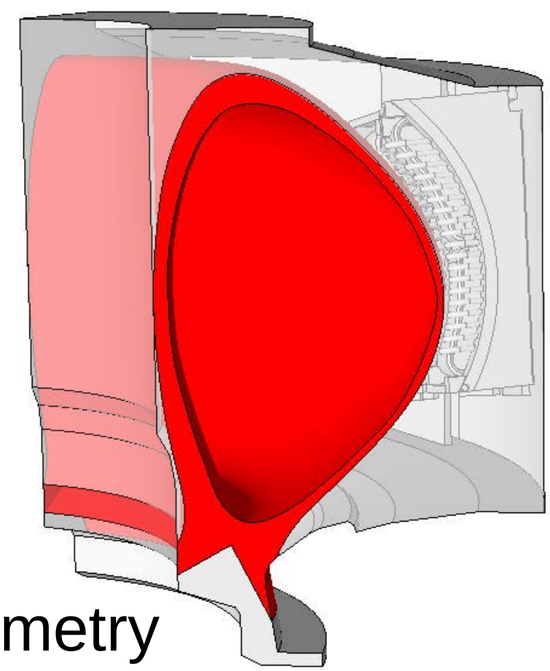
RF Analysis Geometry

De-featuring Antenna CAD:



- Models have unneeded details
- SimModeler provides tools to “de-feature” CAD models
- Bolts, mounts & capping holes removed, closed non-manifold models constructed

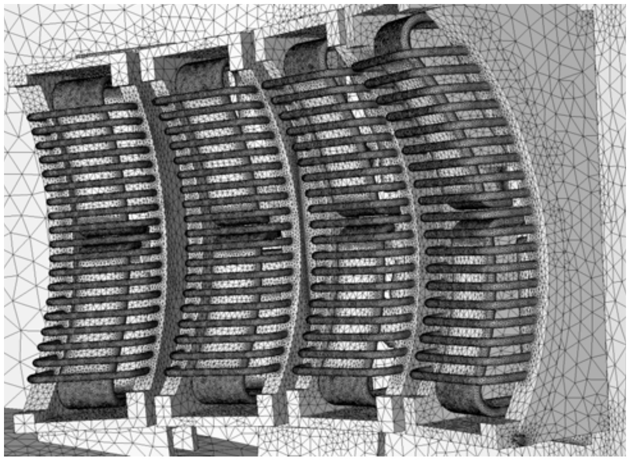
Combining Geometry:



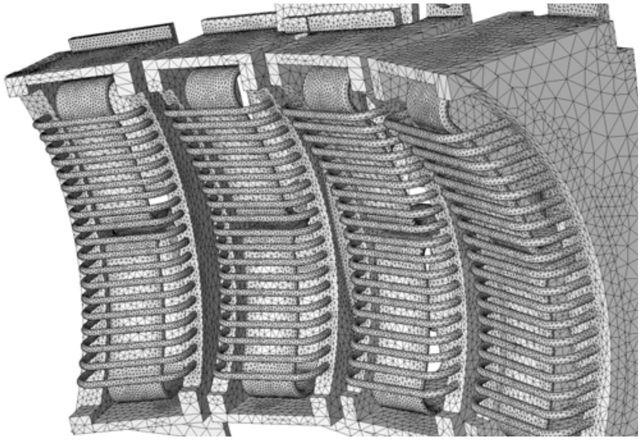
- Import components:
  - De-featured CAD assemblies
  - EFIT curves for SOL (psi = 1.05)
  - TORIC outer surface mesh
- Create rotated surfaces from cross section curves
- Assemble components into analysis geometry

Generate Curved Mesh for RF Simulations

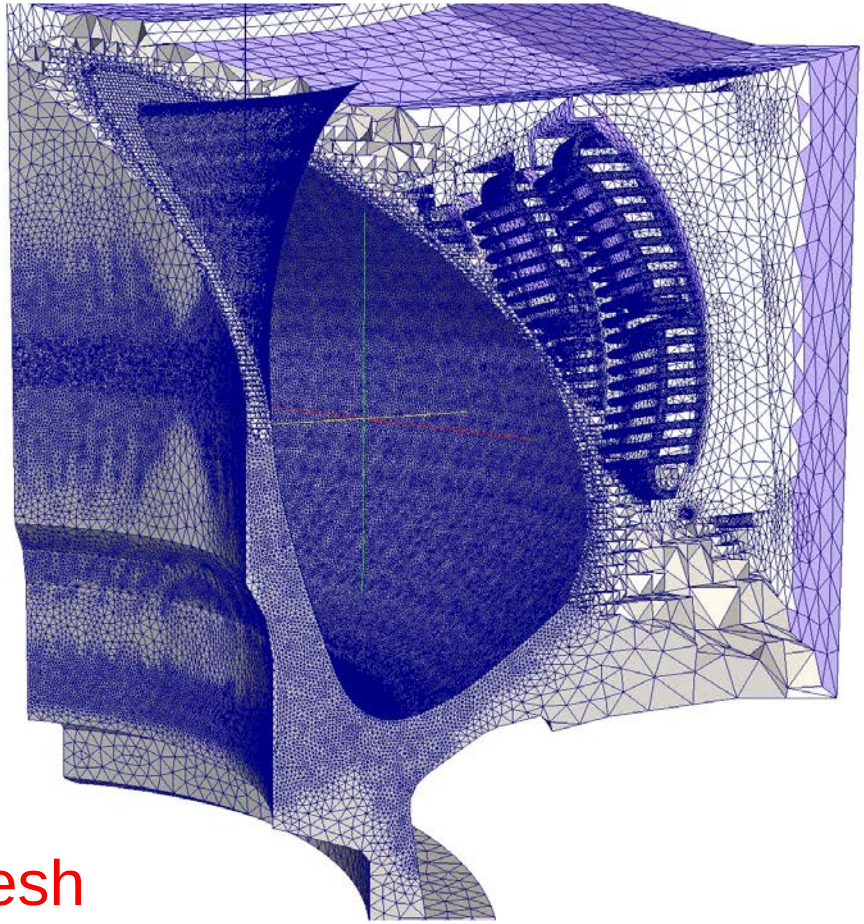
- Mesh controls set on Analysis Geometry
- Mesh generation – linear or or quadratic curved meshed
- Order inflation up to 6th order



Linear mesh
8M elements



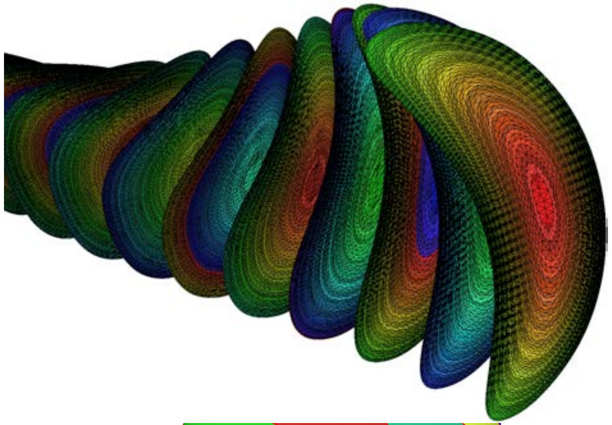
Quadratic mesh
2.5M elements

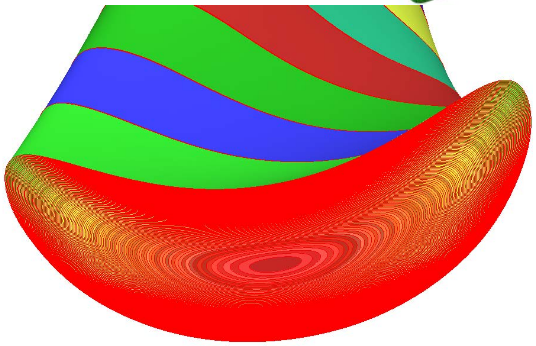


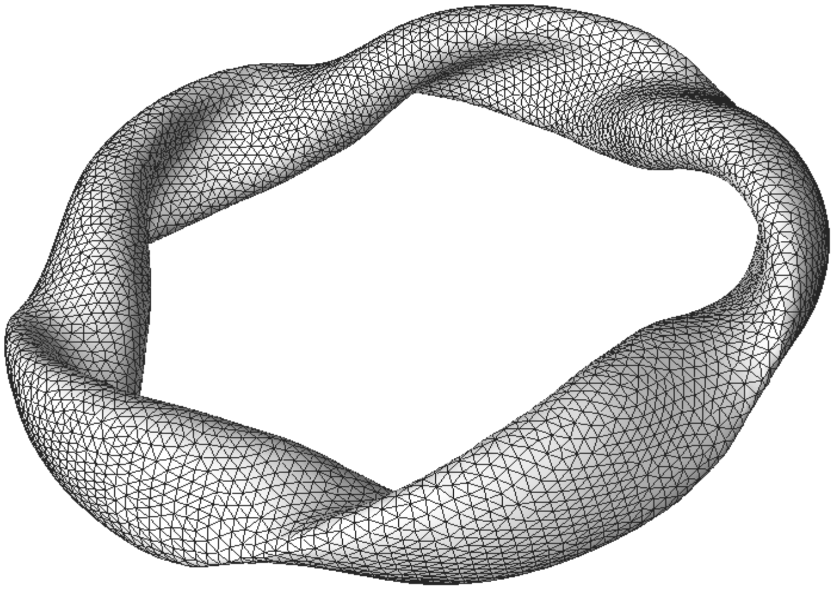
8M elements mesh
with refined SOL

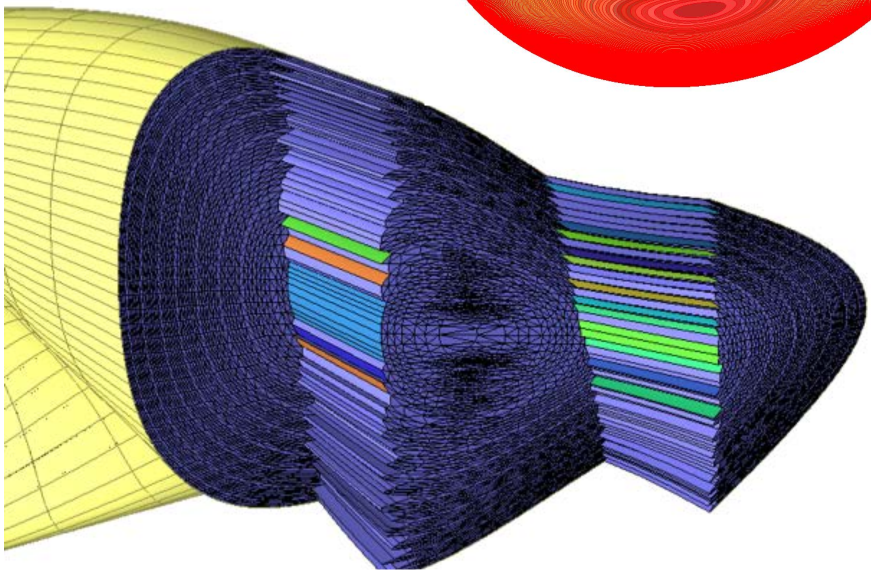
Stellarator Meshing Developments

- Magnetic field data from VMEC used to define poloidal plane slices
- Spline based curves defined on planes
- Lofted spline in the toroidal direction
- Isotropic mesh not ideal
- Working on anisotropic “field following”
- Need to account for remaining geometry









Analysis Code Support and Mesh Adaptation

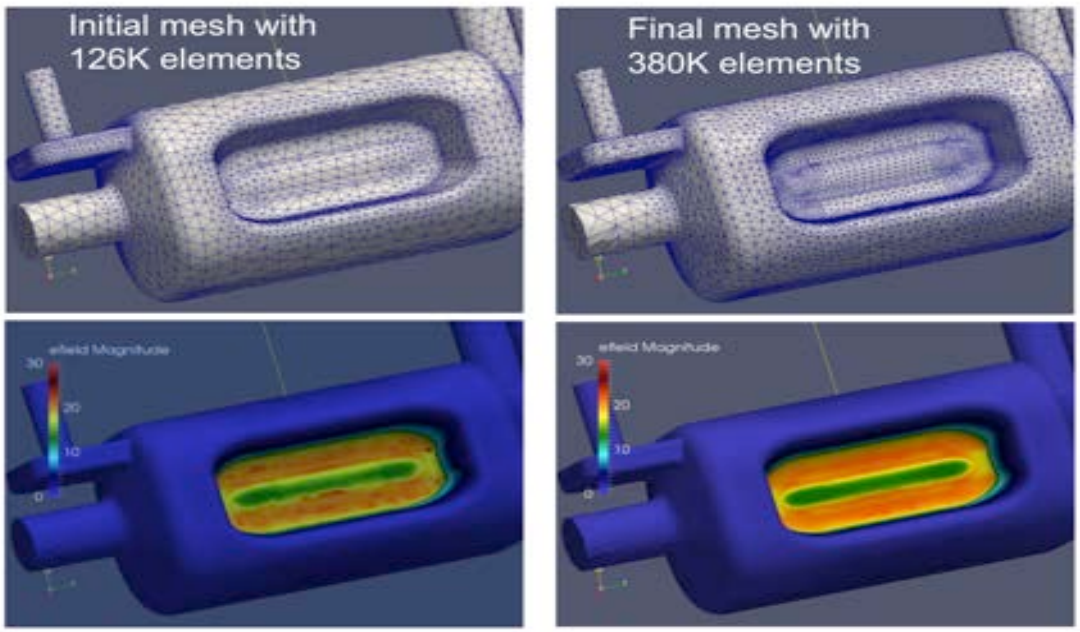
FASTMath parallel mesh adaptation has in-memory integration with nine unstructured mesh analysis codes

For current fusion SciDACs

- M3D-C1 – core MHD
- MFEM – frequency domain EM for RF simulations
- XGC – parallel mesh PIC

EM adaptation example:

- Simulation in Omega3P
- Curved quadratic elements
- Mesh adapted to error indicator defined mesh size field

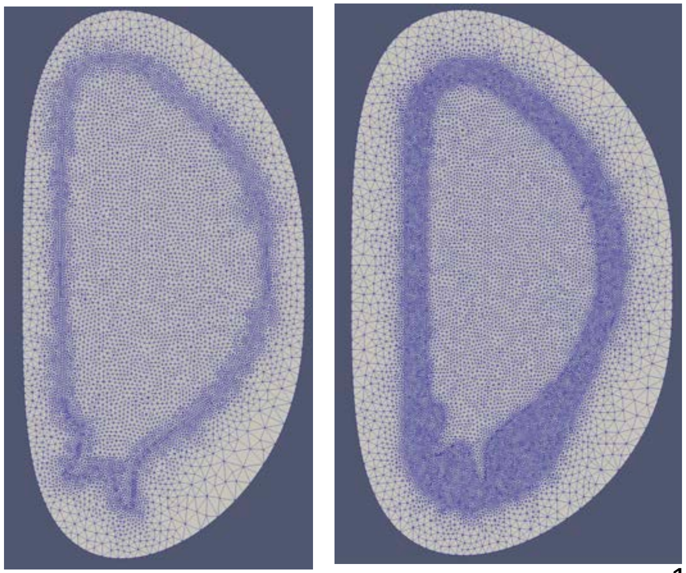


Left shows the initial mesh and first eigenmode electric field.
Right shows adapted mesh and first eigenmode electric field.

Developments for M3D-C1

M3D-C1 built directly on PUMI mesh infrastructure

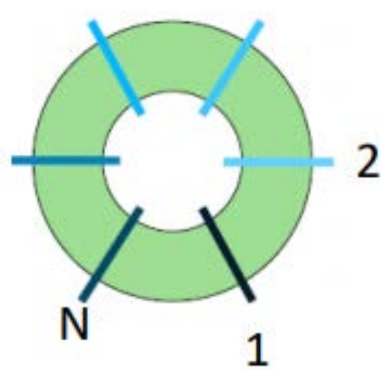
- Support of alternative ordering of unknowns
  - By-node ordering is not ideal for numerical conditioning when the nodal dof list has derivative dof – M3D-C1 has value, 1st and 2nd derivative dof
  - Developing support for by-component ordering – all dof for the value are followed by all dof of the first derivative, etc.
- Improved solver interface toward full thread safe assembly
- Support of PIC capability being added to M3D-C1
  - PUMI based overlap and adjacency based element containment being used in M3D-C1 with PIC
- Extensions to geometry/meshing
  - Flexible options for defining mesh regions used for resistive wall boundary condition

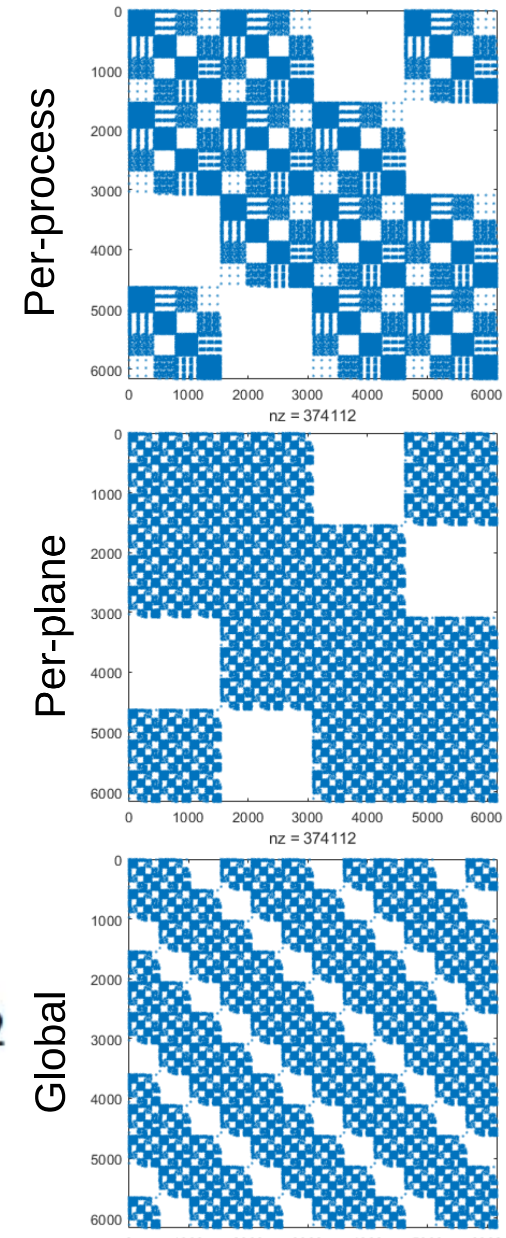


M3D-C1 By Component DOF Ordering

Developing procedure to support the by component dof ordering

- Support ordering for the nodes at the
  - process level,
  - poloidal plan level, or
  - globally
- Alternatives options
  - Yield different matrix sparsity patterns
  - Support different preconditioning options
  - Have very different assembly interprocess communication requirements
  - Likely to yield different solution times
- Implementation is generic - will allow the effective evaluation of the options



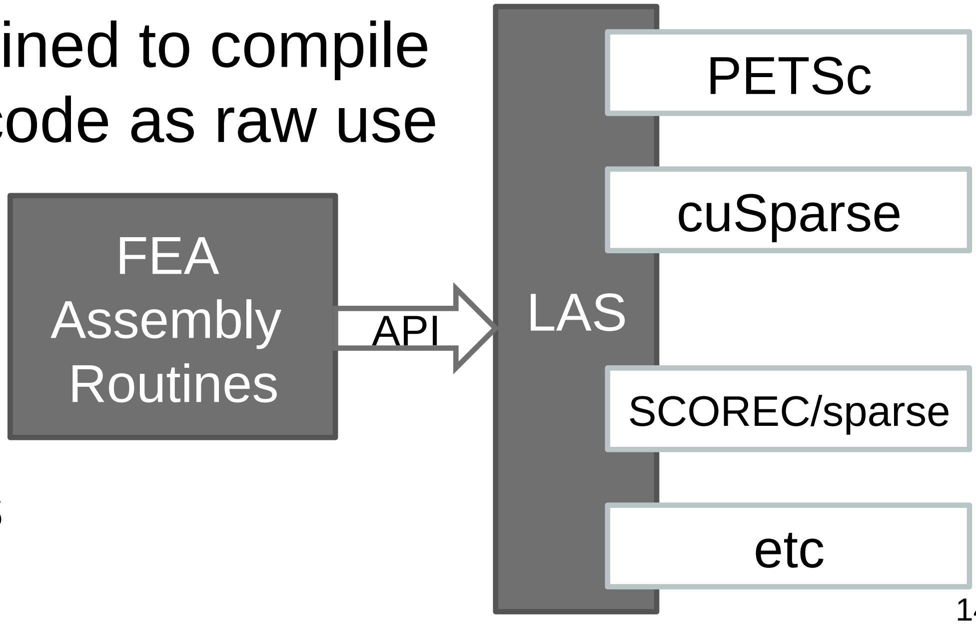


M3D-C1 Linear Solver Interface

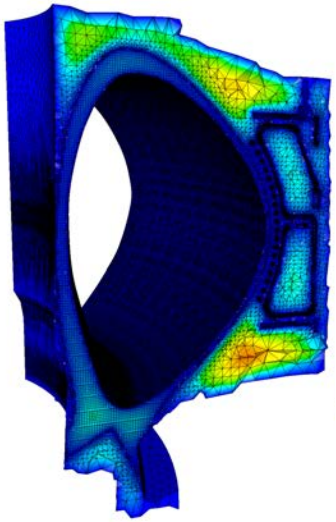
Need more efficient linear system assembly step

As a first step: Implemented a generic linear solver interface (LAS) to wrap multiple supporting linear algebra libraries

- Compile-time decision to target a specific backend library
  - Allows leveraging of best library/implementation for a target machine without touching matrix assembly algorithms
  - Libraries for accelerators (CUDA / PHIs)
  - Libraries for threaded or MPI-only
- LAS API is aggressively in-lined to compile down to identical machine code as raw use of a library backend
- Currently supports
  - cuSparse (CUDA)
  - PETSc
- Planned support for Kokkos



Integration of PUMI/MeshAdapt into MFEM



MFEM ideally suited to address RF simulation needs

- Higher convergence rates of high-order methods can effectively deliver needed level of accuracy
- Well demonstrated scalability
- Frequency domain EM solver developed

Components integrated

- Curve straight sided meshes – includes mesh topology modification – just curving often yields invalid elements)
- Element geometry inflation up to order 6
- PUMI parallel mesh management
- Curved mesh adaptation based on mesh modification
- EngPar for mesh partition improvement

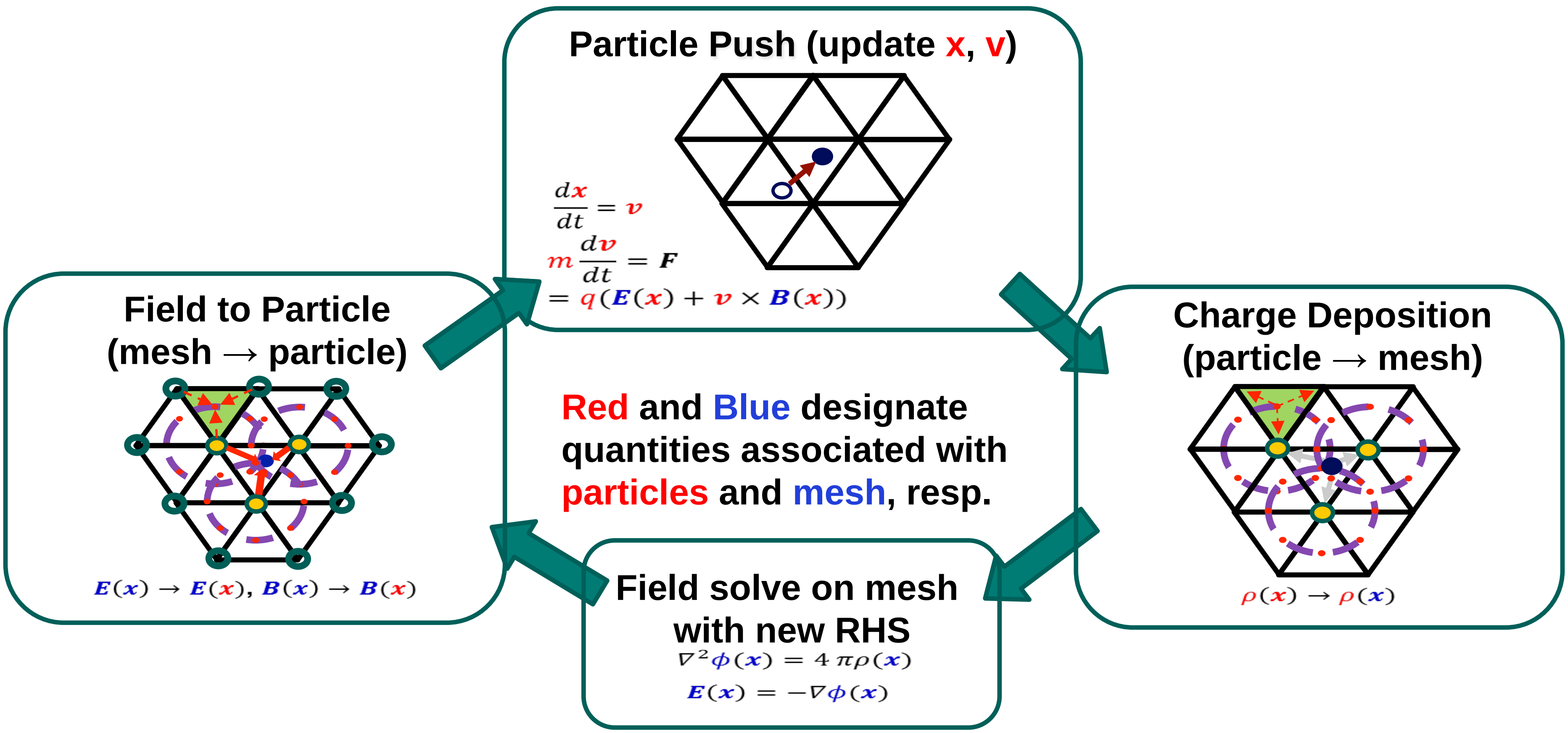
Further integration into PetraM and πScope workflows needed for RF SciDAC

Parallel Unstructured Mesh PIC – PUMIpic

Current approaches have copy of entire mesh on each process

PUMIpic supports a distributed mesh

- Employ large overlaps to avoid communication during push
- All particle information accessed through the mesh

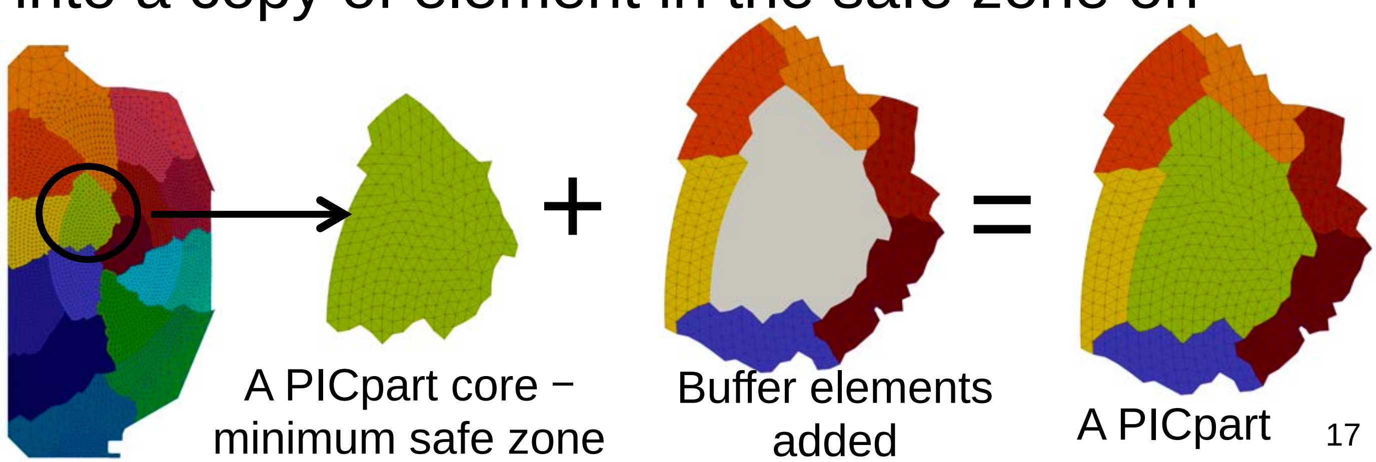


Construction of Distributed Mesh

Steps to construct PICparts:

- Define non-overlaping mesh partition considering the needs of the physics/numerics of the PIC code
- Add overlap to safely ensure particles remain on PICpart during a push
- Evaluate PICpart safe zone: Defined as elements for which particles are "safe" for next push (no communication) – must be at least original core, preferably larger

After a Push particles that move out of a safe zone element must be migrated into a copy of element in the safe zone on another PICpart

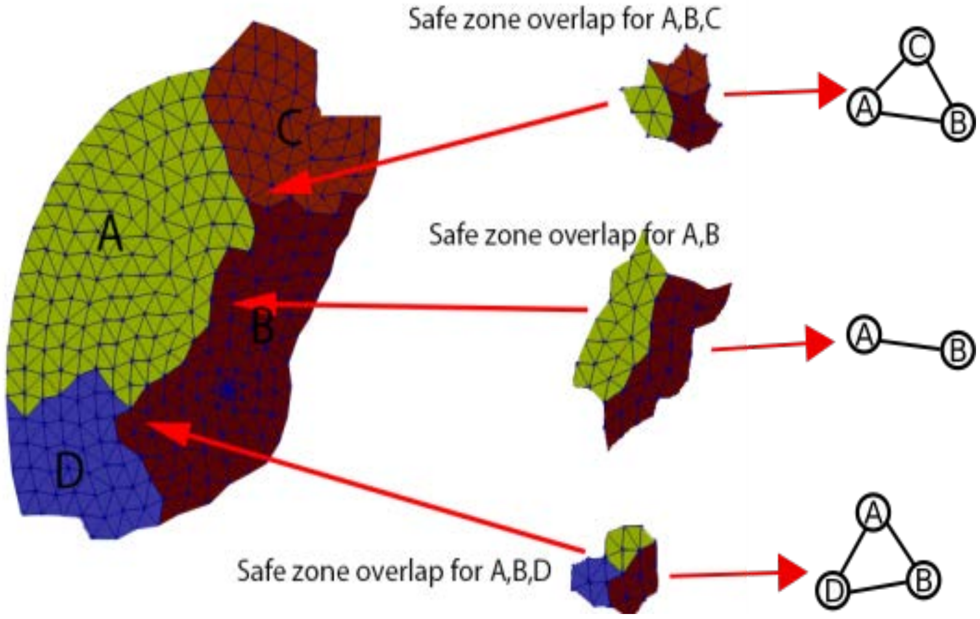


Dynamic Load Balancing

Load balance can be lost as particles migrate

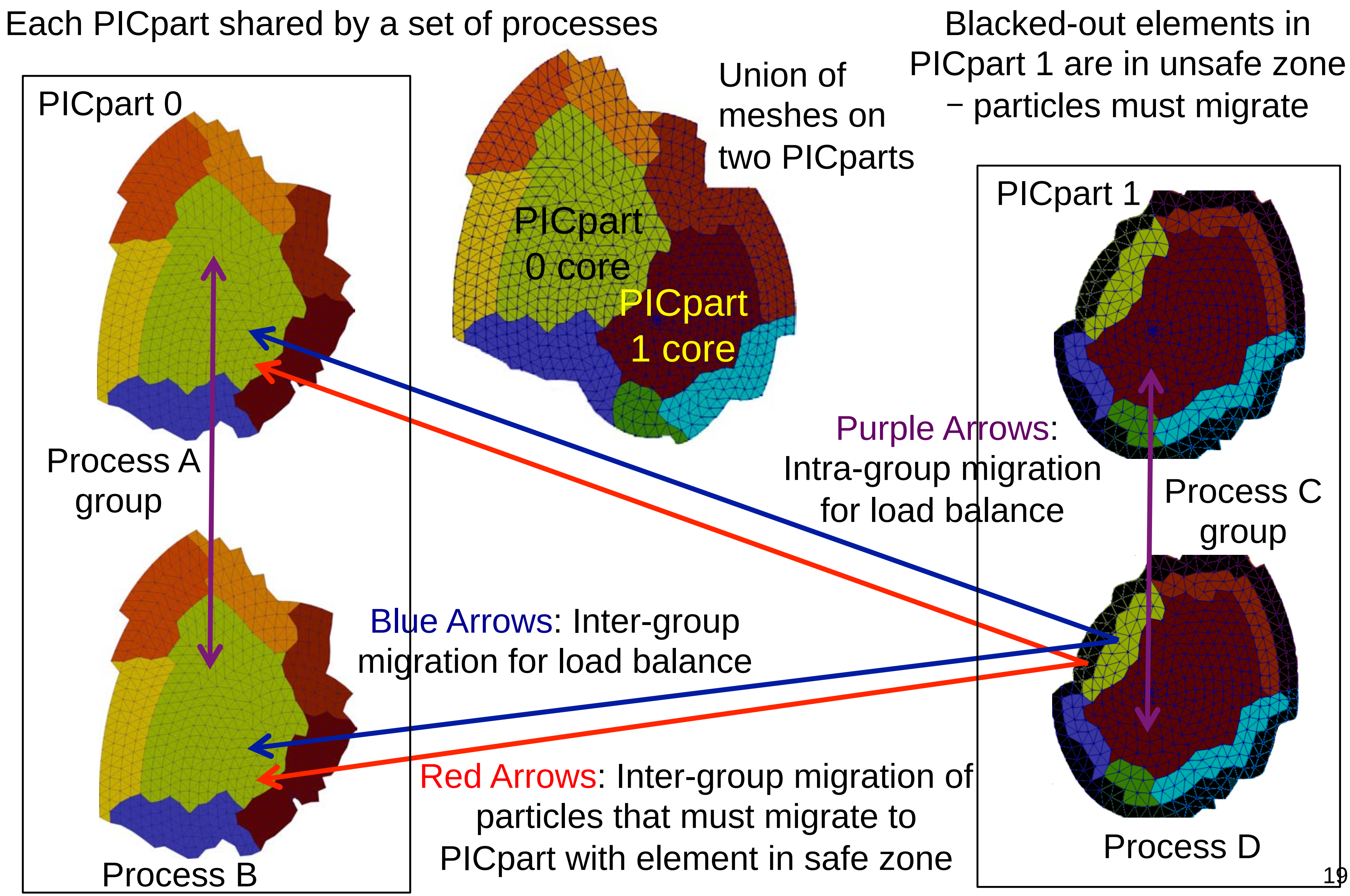
Use EnGPar to repartition the particles for better load balance

- Construct subgraphs connecting processes for each overlapping safe zone
- Set the weights of vertices to be the number of particles in the elements for the overlapping safe zone
- Diffusively migrate weight (# of particles) in each subgraph until processes are balanced



Overlapping safe zones between parts A,B,C, and D near the A-B boundary

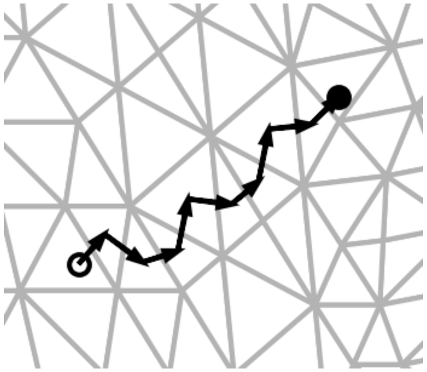
Particle Migration Considerations

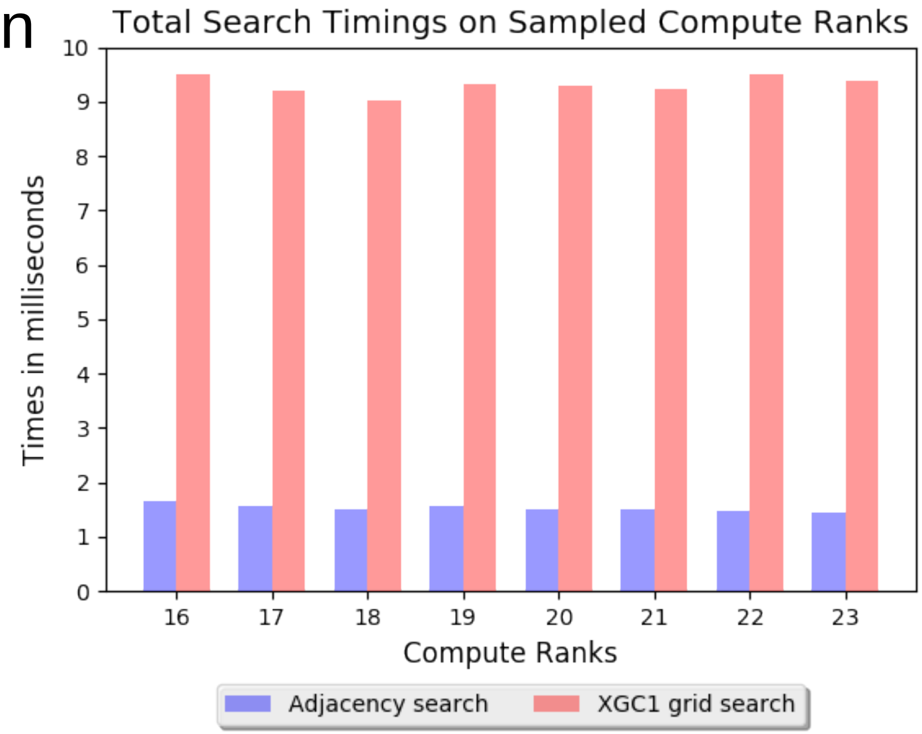


Adjacency-Based Particle Search

Require knowledge of element that particle is in after push

- Particle motion small per time step
- Using mesh adjacencies on distributed mesh (needed information is local due to large overlaps)
- Many particles do not move to new element in a push – optimized parametric inversion for a 2.5 times improvement
- Overall >4 times improvement





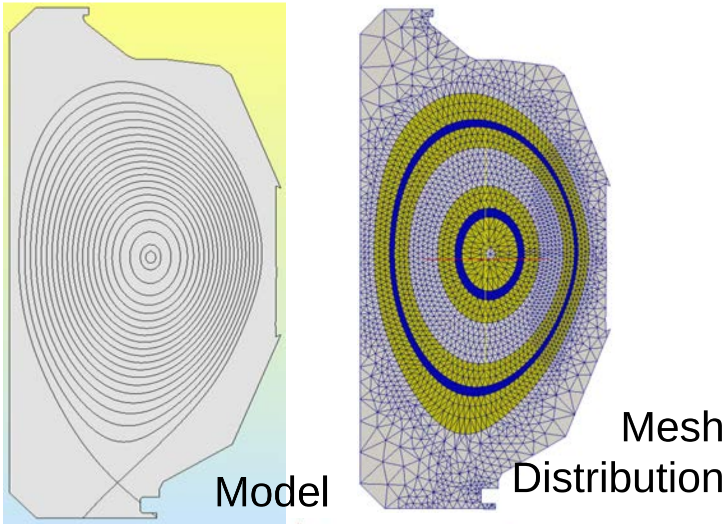
PUMIpic for XGC Gyrokinetic Code

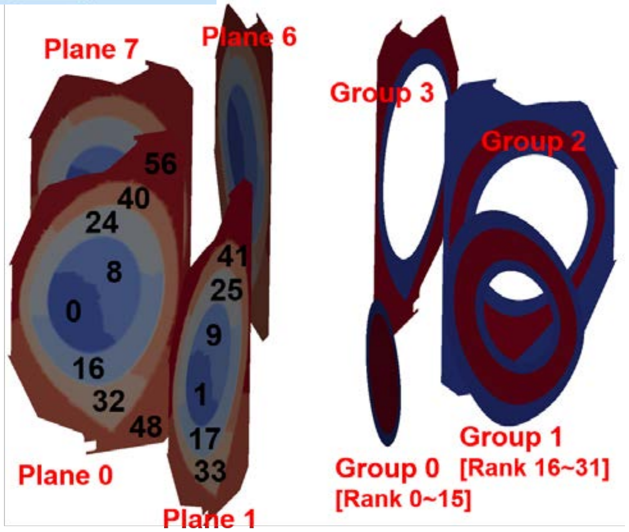
XGC uses a 2D poloidal plane mesh considering particle paths

- Mesh distribution takes advantage of physics defined model/mesh
- Separate parallel field solve on each poloidal plane

Status of development of PUMIpic based version of XGC (XGCM)

- Mesh distribution, adjacency search, particle migration, field transfers and parallel field solve implemented
- Dynamic load balancing approach defined
- Integrated with basic XGC physics operations
- Currently debugging and starting to look at performance

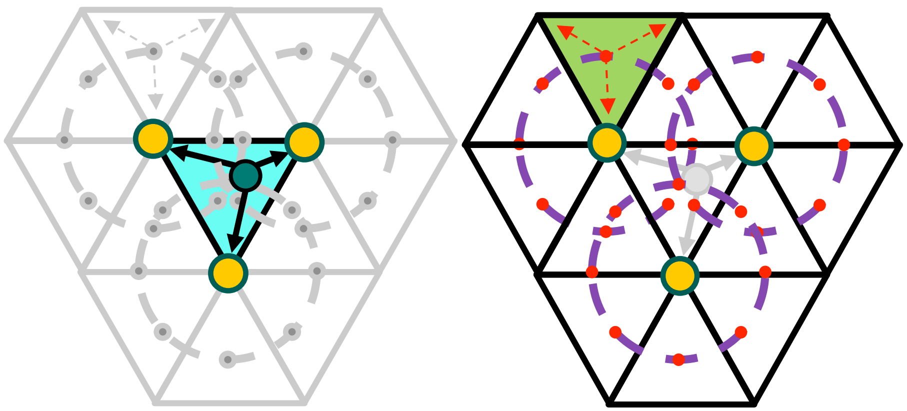




Two-level partition for solver (left) and particle push (right)

XGC field Transfers

- XGC gyro-average scheme for Charge-to-Mesh
  - Pre-computed gyro-ring weight functions
  - Scattering marker particle weights to vertices (left figure) → scattering gyro-ring samples of each “vertex” to vertices of element that the sample is in (right figure)
  - Scattering factors in the latter process pre-calculated once at setup phase with uniform gyro-radius grid
- Must do communication for sums
- Particle values function of fields on bounding poloidal planes
- Mesh level reductions and field association use PUMI
- XGCM Safe zone needed to be set so gyro-ring with max. radius is on process



Charge-to-Mesh

Parallel Field Solve Using PETSc

Solves the gyrokinetic Poisson equation on all poloidal planes simultaneously

- Single copy of XGCM mesh partitioned over N_{ranks}/N_{planes} ranks
  - Avoids having N_{planes} copies of mesh and an increase in memory usage
- Ranks for a given plane form MPI sub-communicators
  - Per-plane solution synchronizations and accumulations within sub-communicators – improved performance due to reduction in collective communication
- Each vertex is owned by multiple MPI ranks
  - Vertex within a single sub-communicator appears to be uniquely owned only by an MPI rank that is a part of that sub-communicator
- Final solution for push is stored as an N_{plane} component PUMI field
  - Each MPI rank stores solution for all planes on every mesh vertex on part
  - Achieved using an intra-plane synchronization of the final solution

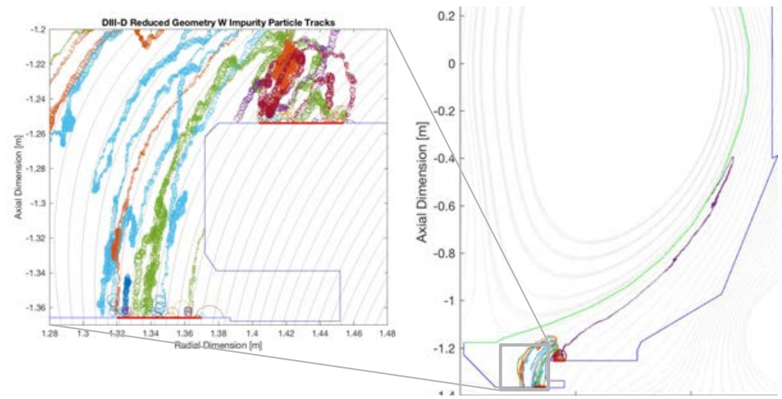
PUMIpic for GITR Impurity Transport Code

PUMIpic capabilities needed for GITR

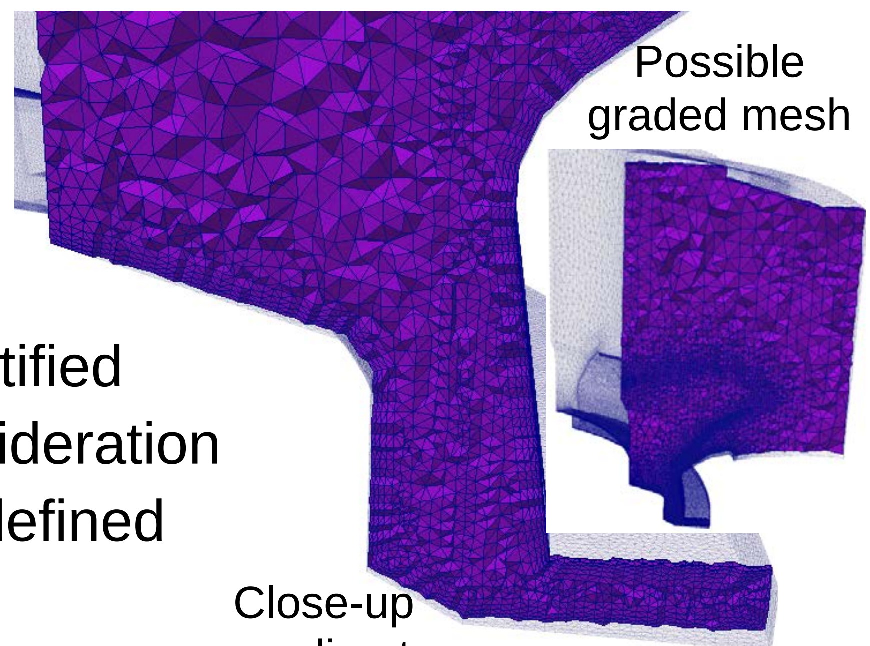
- Fully 3D graded/adapted meshes based on particle distribution
- Wall interactions

Development of distributed 3D mesh version of GITR initiated

- Mesh distribution with large overlap − PUMI
- Adjacency search − 3D extension underway
- Particle migration same as XGCM
- Fast wall intersection − options identified
- Distance to wall options under consideration
- Dynamic load balancing approach defined
- Adaptive mesh control − PUMI



Particle traces



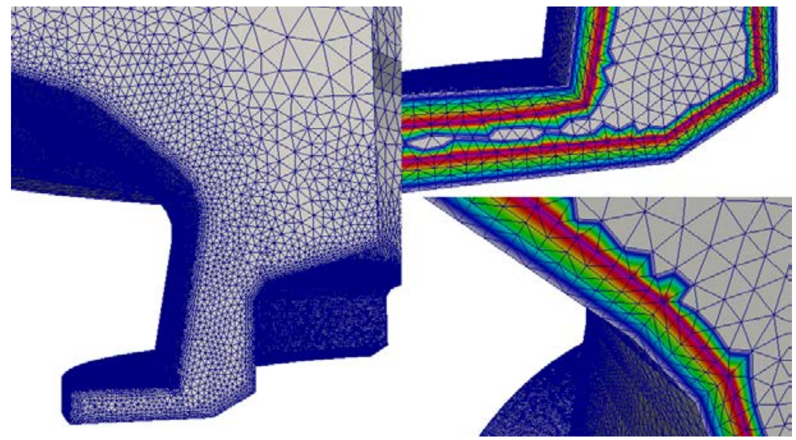
Possible graded mesh

Close-up near diverter

PUMIpic for GITR Impurity Transport Code

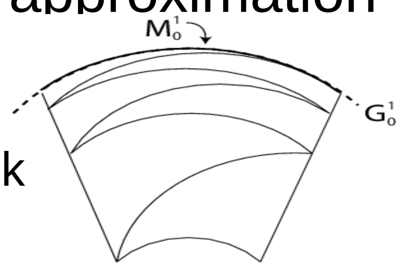
Fast and accurate wall interactions: layered mesh structure near the walls is being considered as an option

Close-up near diverter (with 4 layers)

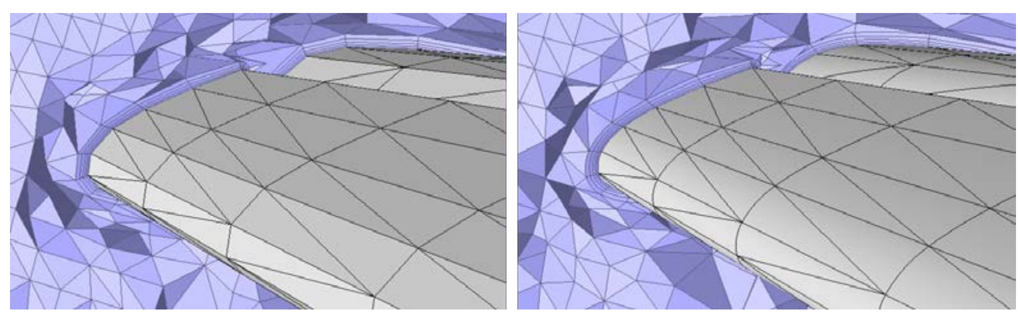


- Distance to wall is readily available and can be used for:
  - Predicting wall intersections (during particle push)
  - Applying physics in sheath region
- Any near-wall anisotropy can be exploited – leading to fewer elements for a given level of accuracy
- High-order/curved elements can be used to improve geometric approximation

Curved layered stack



Linear mesh (left) and high-order mesh (right)



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