Center for Tokamak Transients Simulation

Providing M3D-C1 Unstructured Mesh Technologies

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Providing M3D-C1 Unstructured Mesh Technologies

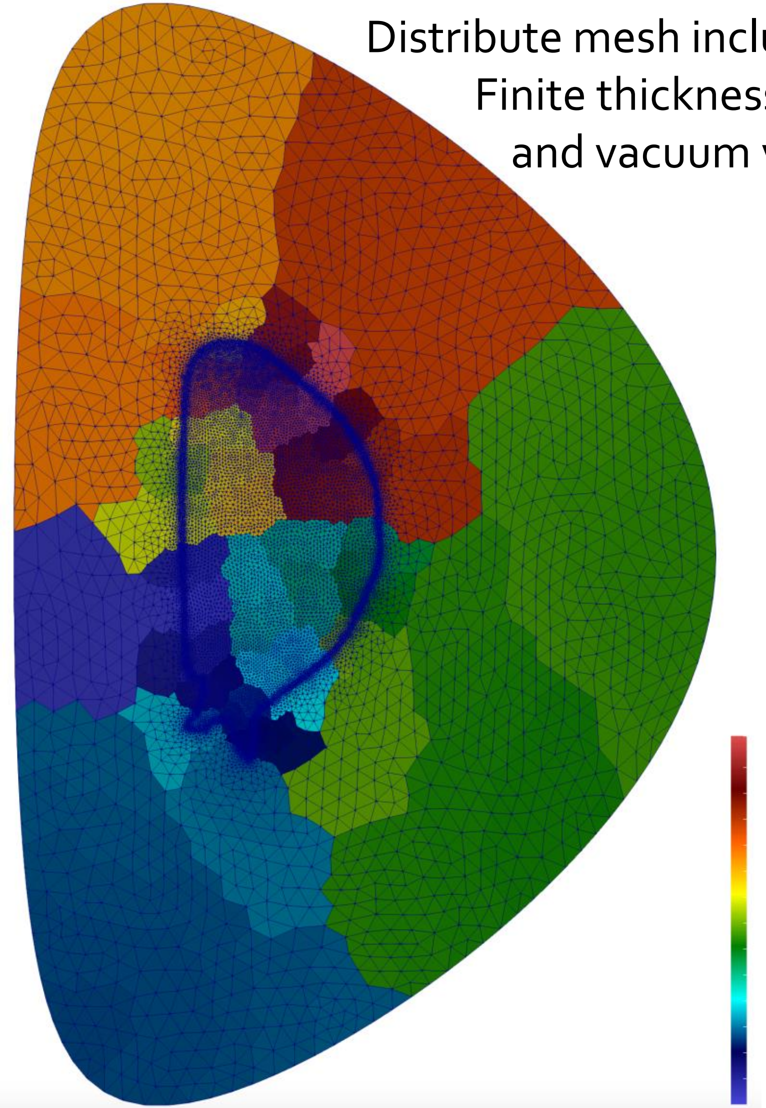
BUILDING ON FASTMATH DEVELOPED UNSTRUCTURED MESH TECHNOLOGIES THE RPI TEAM IS PROVIDING

- **Tokamak geometry construction**
- **Tokamak mesh generation**
- **Mesh infrastructure for M3D-C1**
- **Mesh control**
  - **Based on a priori information**
  - **Adaptation based on a posteriori error estimators**
- **Mesh support of M3D-C1 on HPC systems**

Tokamak Geometry Construction and Mesh Generation

TOOLS DEVELOPED TAKE ADVANTAGE OF

- **Simmetrix unstructured mesh generators**
- **Tokamak Model and Mesh Software (ToMMS) for which most of the developments were done to meet specific meshing requirements for HBPS**
- **ToMMS development for CTTS**
  - **Converting discrete segment tokamak geometry into proper topological model for meshing**
  - **Support for finite thickness wall mesh and vacuum vessel**

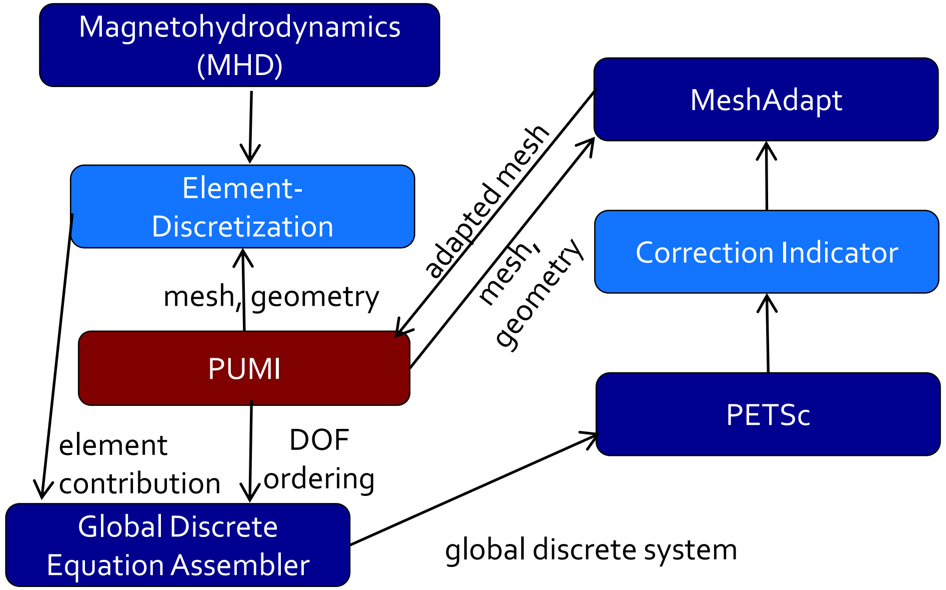


Distribute mesh including
Finite thickness wall
and vacuum vessel

Mesh Infrastructure for M3D-C1

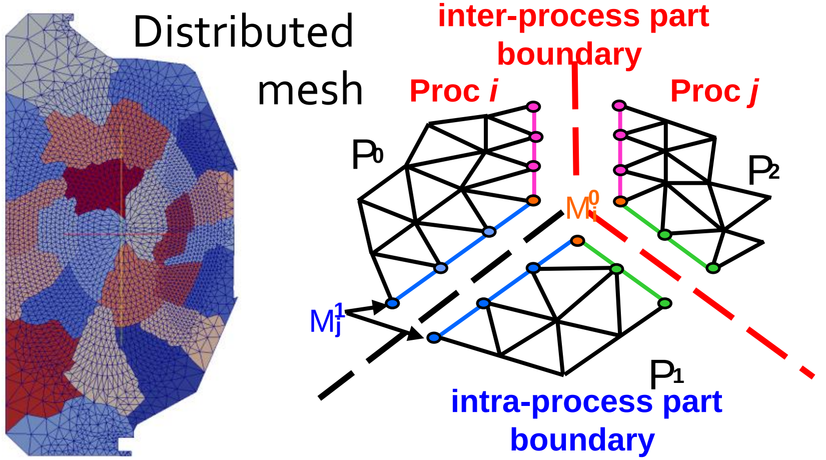
CORE M3D-C1 COMPONENTS

- **Overall M3D-C1 code, element level calculations (physics and its discretization) – Fortran code developed by CTTS core developers**
- **"Solver" technologies based on PETSc, MUMPS – C++ code enhanced for M3D-C1 use by NERSC team**
- **Mesh infrastructure – C++ code based on FASTMath unstructured mesh technologies**



MESH INFRASTRUCTURE BASED ON PUMI/MESHADAPT

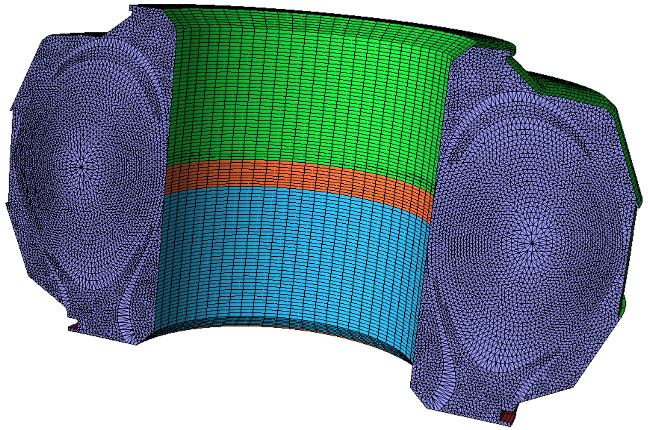
- **Supports parallel 2D and 3D unstructured meshes and associated fields**
- **Controls assembly of element vectors and matrices into the global system provided to PETSc**
- **Execute parallel mesh adaptation operations**



Mesh Infrastructure for M3D-C1

PARALLEL UNSTRUCTURED MESH INFRASTRUCTURE (PUMI)

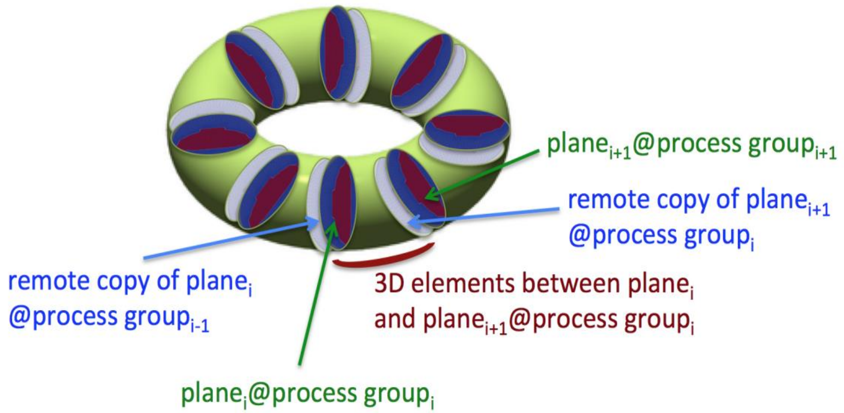
- **Supports mesh migration as needed by dynamic load balancing and mesh adaptation**
- **Includes dynamic load balancing and reordering algorithms**
- **Investigated alternative dof ordering procedures**



3D wedge mesh constructed by extruding a 2D triangular mesh

USE OF PUMI TO SUPPORT M3D-C1 WORKFLOWS

- **Construction of the 3D extruded mesh from the 2D mesh**
- **Support for converting from a 2D initial set of simulation steps to a fully 3D simulation steps**
- **Support of application of mesh adaptation with dynamic load rebalancing**
- **Adjacency based ordering**



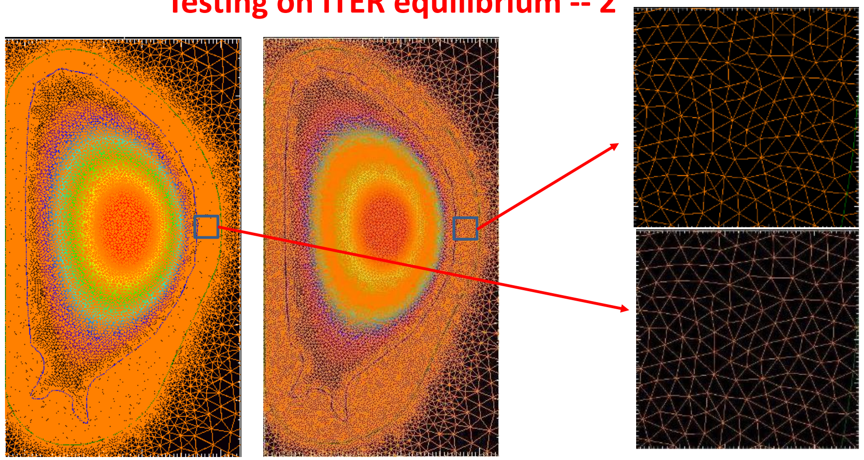
Conversion from 2D to 3D simulation

Mesh Control

BASED ON A PRIORI INFORMATION

- **Mesh size and gradation information set on model topological entities**
- **Setting mesh size fields and applying the mesh modification procedures used by PUMI/MeshAdapt**

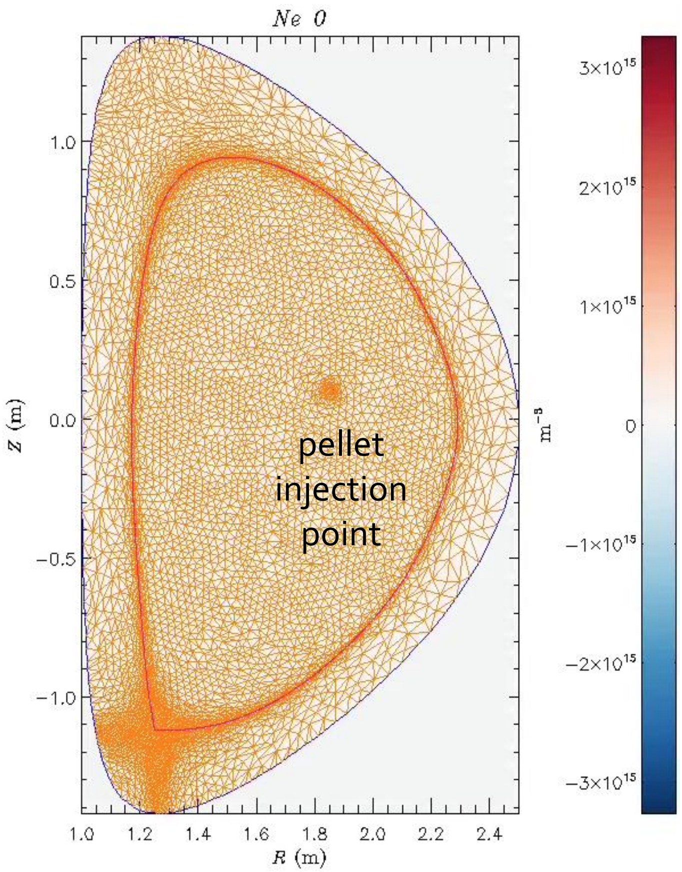
Testing on ITER equilibrium -- 2



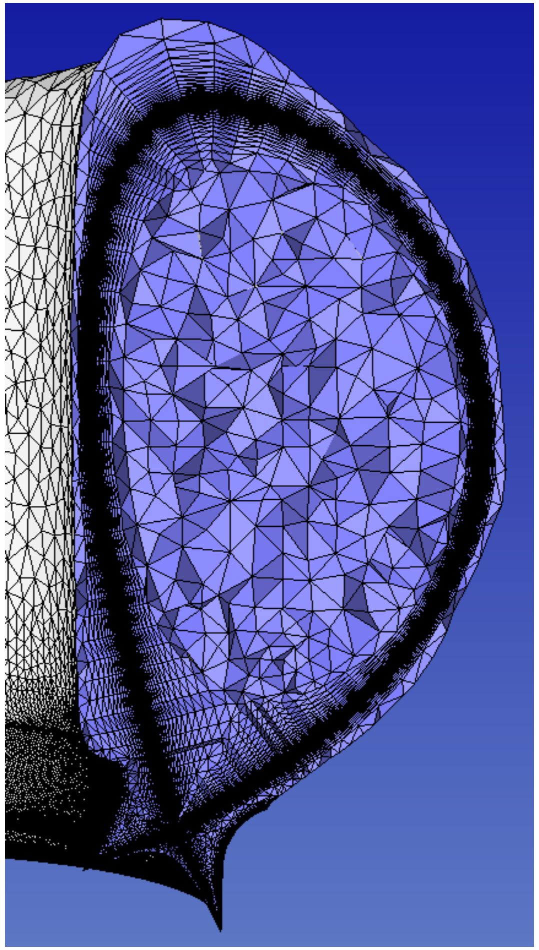
/p/tsc/m3dnl/ITER/NewMesh/Eq2 and .../Adapted

Leaves wall zones untouched!

Recently added a priori mesh control feature that provided an additional level of mesh control



Mesh size control based on mesh modification along the separatrix curve and a pellet injection point



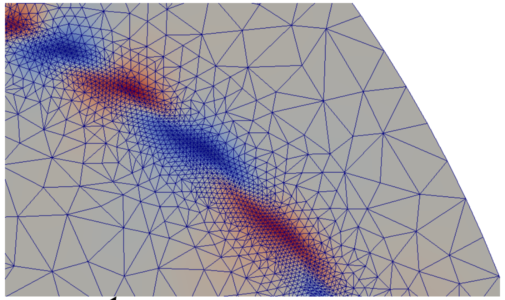
Mesh size control set on model entities including the separatrix curve as a model entity

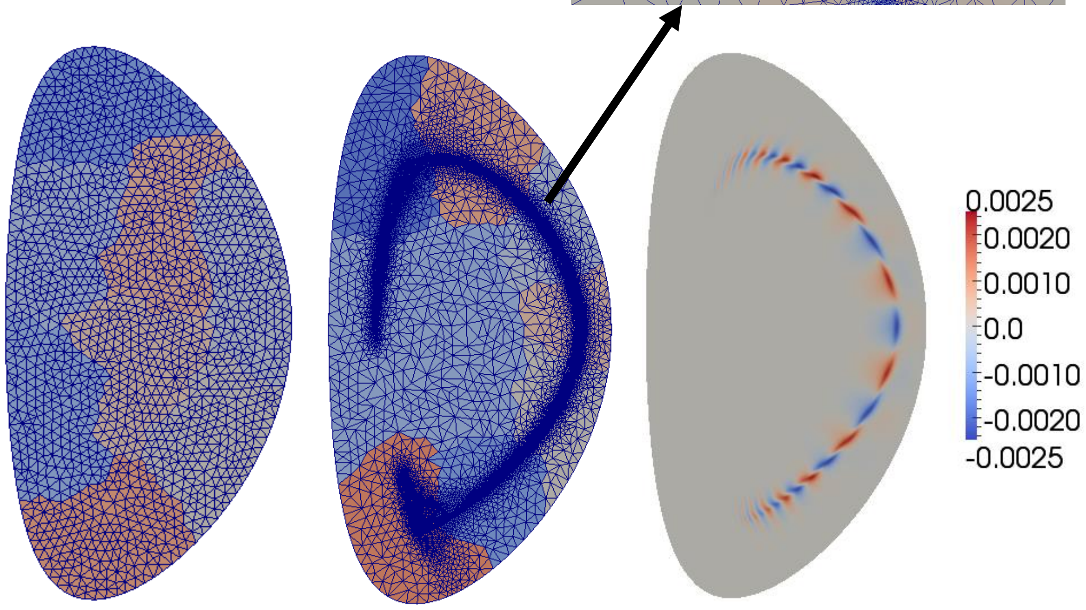
Mesh Control

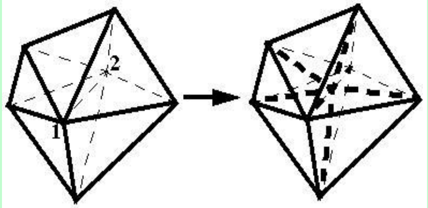
BASED ON A POSTERIORI INFORMATION

- **Simulation field information used by error indicator to estimate level of error in the current mesh entities**
- **Correction indicator used to set anisotropic mesh size field**
- **PUMI MeshAdapt used to modify mesh to match the mesh size field**

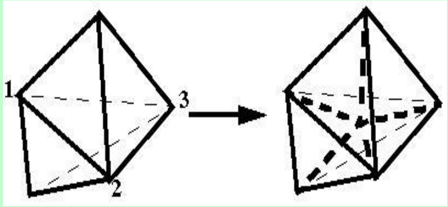
Mesh adapted based on a previously developed residual based error estimator





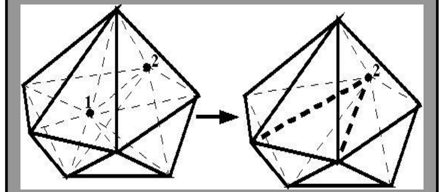


Edge split

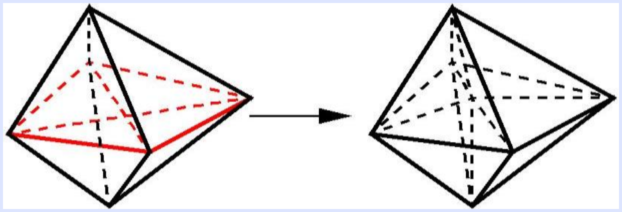


face split

Core MeshAdapt mesh modification operators



Edge collapse


Double split collapse

Error Indicator and Mesh Adaptation for Pellet Ablation Simulations

SPR-based patch-recovery error estimation

- Patch-recovery methods construct a C^0 (continuous) field from a C^{-1} (discontinuous) solution field using least square fits. We will use the 2nd derivative of the primary psi_field. (The m3dc1 finite element basis maintain continuity of the function and its 1st derivatives across element boundaries, hence the reason for using the second derivatives.)
- The recovered C^0 field can be shown to satisfy "super-convergence" and thus can be used to estimate discretization errors.
- By replacing the exact field with the recovered field we can find an estimate for element errors.

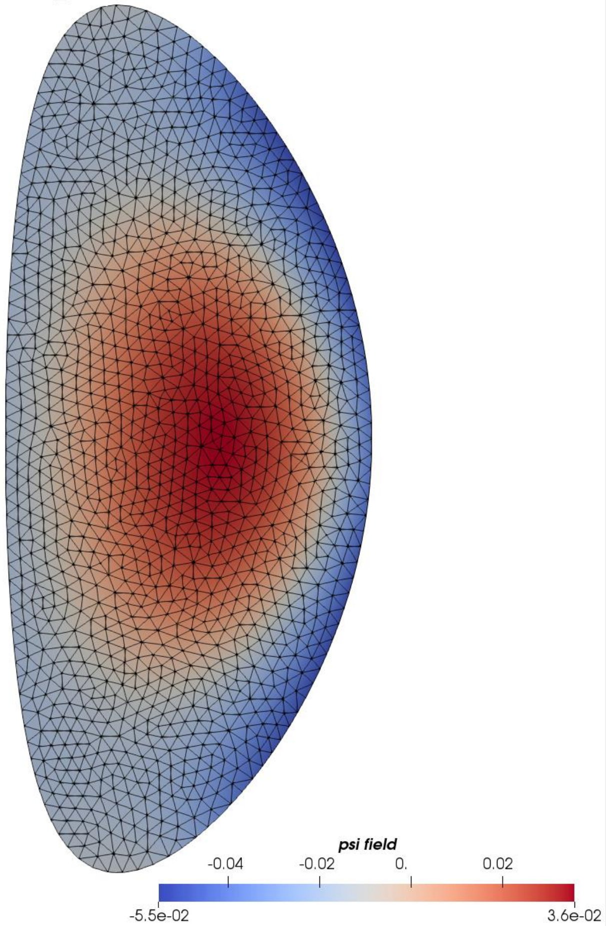
$$\|e\|_{\Omega_e} := \left[\int_{\Omega_e} (\underbrace{\boxed{\mathbf{E}}}_{\text{Exact}} - \underbrace{\boxed{\mathbf{E}_h}}_{\text{FEM}})^2 \, d\Omega\right]^{1/2} \xrightarrow{\sim} \|e^*\|_{\Omega_e} := \left[\int_{\Omega_e} (\underbrace{\boxed{\mathbf{E}^*}}_{\text{Recovered}} - \mathbf{E}_h)^2 \, d\Omega\right]^{1/2}$$

- Having computed individual element errors we can define the new desired sizes as $h^{desired} = h^{current} \times r$, with size factor "*r*" being selected to get a uniform distribution of errors in the new mesh.
- PUMI MeshAdapt tools can then be used to modify the mesh to obtain the desired sizes computed in the previous step.

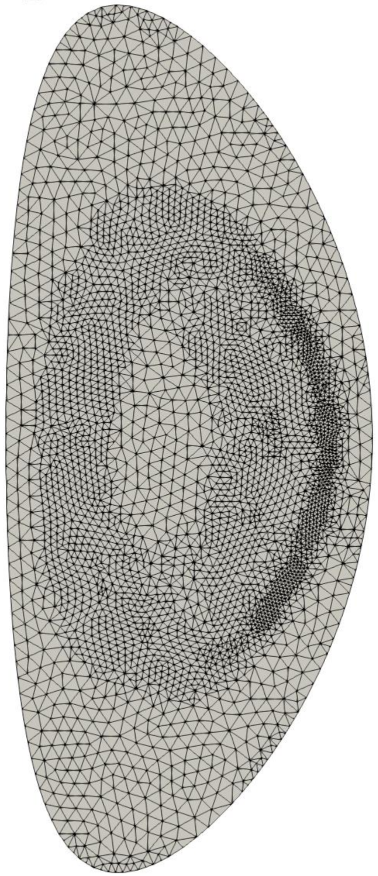
Error Indicator and Mesh Adaptation for Pellet Ablation Simulations

SPR-based patch-recovery error estimation initial debugging result

before adapt



after adapt



Mesh Support of M3D-C1 on HPC Systems

SUPPORTING UNSTRUCTURED MESH NEEDS ON HPC SYSTEMS

- **Installing Simmetrix, PUMI/MeshAdapt, Zoltan/ParMETIS, PETSC**

SYSTEMS PUMI AND MESHADPT IS SUPPORTED ON FOR M3D-C1

- **PPPL Portal RHEL6 and RHEL7**
- **NERSC Cori CPU & GPU**
- **ORNL Ascent**
- **Princeton Perseus, Perseus AMD, Stellar, Traverse GPU**
- **General Atomic Saturn**
- **LNCC Sdumont @ Brazil (http://sdumont.lncc.br)**
- **Cineca Marconi @ Italy (http://cineca.it)**
- **MPG Hydra @ Germany (http://mpcdf.mpg.de)**

Future Developments

DURING LAST YEAR OF SCIDAC 4

- **Completion of 2D and 3D adaptive procedures for pellet ablation simulations**
- **Examination of error indicators based on alternative solution parameters**
- **Develop correction indicator to set mesh anisotropy**

POSSIBLE SCIDAC 5 DEVELOPMENTS

- **Developed improved error estimators and anisotropic mesh size field correction indicators**
- **Move from PUMI CPU based mesh infrastructure to Omega GPU based mesh infrastructure**
  - **Support improved methods to do PETSc assembly for GPU based solves (coordinated with LBL team)**
  - **Develop GPU based mesh adaptation**
- **Use of FASTMath/SciDAC 4 FES Partnerships developed PUMIPic to support M3D-C1 PIC on distributed meshes (PUMIPic is GPU based and uses Omega)**
- **Build on work on stand alone coupling technologies being developed in ECP (coupled with Rapids for ADIOS2) for code coupling needs**