Unstructured Meshing Technologies

Presented to
ATPESC 2021 Participants

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U.S. DEPARTMENT OF ENERGY | Office of Science

ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

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Rensselaer

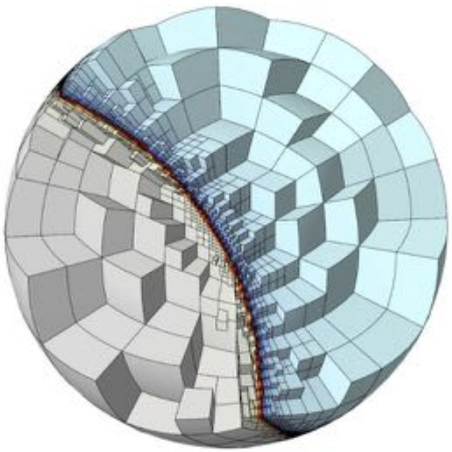
SMU

Finite elements are a good foundation for large-scale simulations on current and future architectures

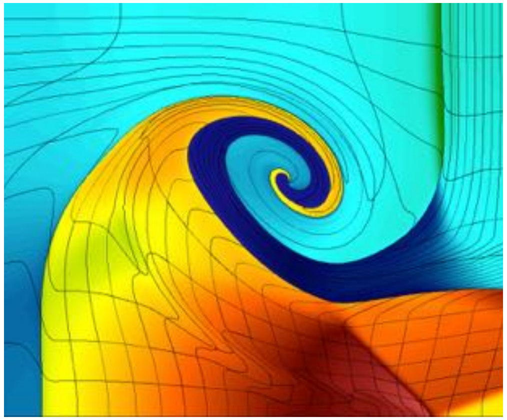
- Backed by well-developed theory.
- Naturally support unstructured and curvilinear grids.
- **High-order finite elements on high-order meshes**
  - Increased accuracy for smooth problems
  - Sub-element modeling for problems with shocks
  - Bridge unstructured/structured grids
  - Bridge sparse/dense linear algebra
  - FLOPs/bytes increase with the order
- Demonstrated match for compressible shock hydrodynamics (BLAST).
- Applicable to variety of physics (DeRham complex).

$$\underset{\text{“nodes”}}{\boxed{H(grad)}} \xrightarrow{\nabla} \underset{\text{“edges”}}{\boxed{H(curl)}} \xrightarrow{\nabla\times} \underset{\text{“faces”}}{\boxed{H(div)}} \xrightarrow{\nabla\cdot} \underset{\text{“zones”}}{\boxed{L_2}}$$

High-order kinematics	High-order MHD	High-order rad. diff.	High-order thermodynamics



Non-conforming mesh refinement on high-order curved meshes

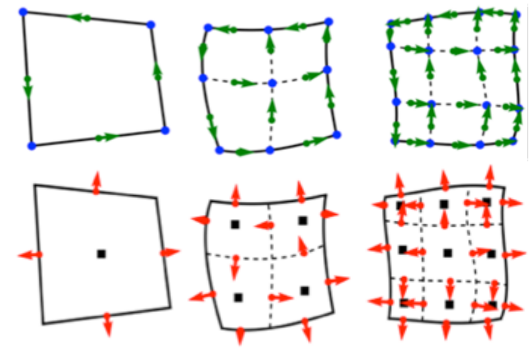


8^{th} order Lagrangian hydro simulation of a shock triple-point interaction

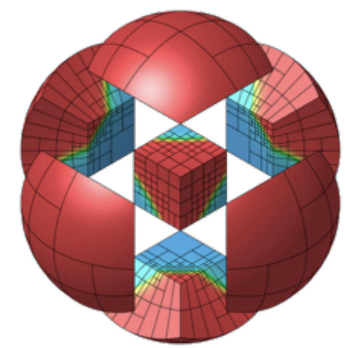
Modular Finite Element Methods (MFEM)

MFEM is an *open-source C++ library* for scalable FE research and fast application prototyping

- Triangular, quadrilateral, tetrahedral and hexahedral; volume and surface meshes
- Arbitrary order curvilinear mesh elements
- Arbitrary-order H1, H(curl), H(div)- and L2 elements
- Local conforming and non-conforming refinement
- NURBS geometries and discretizations
- Bilinear/linear forms for variety of methods (Galerkin, DG, DPG, Isogeometric, …)
- Integrated with: *HYPRE, SUNDIALS, PETSc, SUPERLU, PUMI, VisIt, Spack, xSDK, OpenHPC,* and more …
- Parallel and highly performant
- Main component of *ECP's co-design Center for Efficient Exascale Discretizations (CEED)*
- Native "in-situ" visualization: *GLVis*, glvis.org



Linear, quadratic and cubic finite element spaces on curved meshes



mfem.org
(v4.3, 2021)

Example 1 – Laplace equation

- Mesh

```cpp
   // 2. Read the mesh from the given mesh file. We can handle triangular,
   //    quadrilateral, tetrahedral, hexahedral, surface and volume meshes with
   //    the same code.
   Mesh *mesh;
   ifstream imesh(mesh_file);
   if (!imesh)
   {
      cerr << "\nCan not open mesh file: " << mesh_file << '\n' << endl;
      return 2;
   }
   mesh = new Mesh(imesh, 1, 1);
   imesh.close();
   int dim = mesh->Dimension();

   // 3. Refine the mesh to increase the resolution. In this example we do
   //    'ref_levels' of uniform refinement. We choose 'ref_levels' to be the
   //    largest number that gives a final mesh with no more than 50,000
   //    elements.
   {
      int ref_levels =
         (int)floor(log(50000./mesh->GetNE())/log(2.)/dim);
      for (int l = 0; l < ref_levels; l++)
         mesh->UniformRefinement();
   }
```

- Finite element space

```cpp
   // 4. Define a finite element space on the mesh. Here we use continuous
   //    Lagrange finite elements of the specified order. If order < 1, we
   //    instead use an isoparametric/isogeometric space.
   FiniteElementCollection *fec;
   if (order > 0)
      fec = new H1_FECollection(order, dim);
   else if (mesh->GetNodes())
      fec = mesh->GetNodes()->OwnFEC();
   else
      fec = new H1_FECollection(order = 1, dim);
   FiniteElementSpace *fespace = new FiniteElementSpace(mesh, fec);
   cout << "Number of unknowns: " << fespace->GetVSize() << endl;
```

- Initial guess, linear/bilinear forms

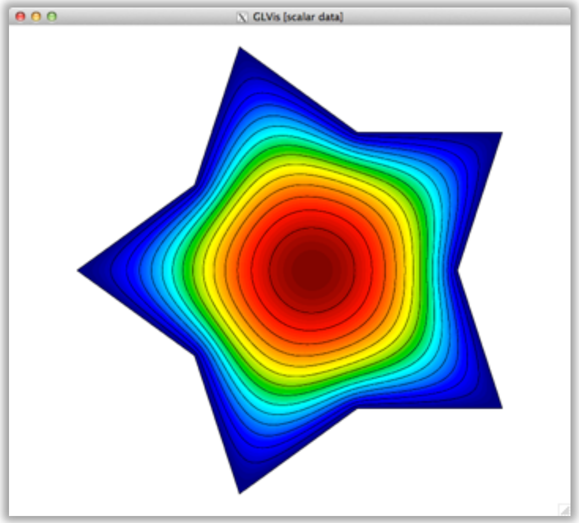
```cpp
   // 5. Set up the linear form b(.) which corresponds to the right-hand side of
   //    the FEM linear system, which in this case is (1,phi_i) where phi_i are
   //    the basis functions in the finite element fespace.
   LinearForm *b = new LinearForm(fespace);
   ConstantCoefficient one(1.0);
   b->AddDomainIntegrator(new DomainLFIntegrator(one));
   b->Assemble();

   // 6. Define the solution vector x as a finite element grid function
   //    corresponding to fespace. Initialize x with initial guess of zero,
   //    which satisfies the boundary conditions.
   GridFunction x(fespace);
   x = 0.0;

   // 7. Set up the bilinear form a(.,.) on the finite element space
   //    corresponding to the Laplacian operator -Delta, by adding the Diffusion
   //    domain integrator and imposing homogeneous Dirichlet boundary
   //    conditions. The boundary conditions are implemented by marking all the
   //    boundary attributes from the mesh as essential (Dirichlet). After
   //    assembly and finalizing we extract the corresponding sparse matrix A.
   BilinearForm *a = new BilinearForm(fespace);
   a->AddDomainIntegrator(new DiffusionIntegrator(one));
   a->Assemble();
   Array<int> ess_bdr(mesh->bdr_attributes.Max());
   ess_bdr = 1;
   a->EliminateEssentialBC(ess_bdr, x, *b);
   a->Finalize();
   const SparseMatrix &A = a->SpMat();
```

- Linear solve

```cpp
#ifndef MFEM_USE_SUITESPARSE
   // 8. Define a simple symmetric Gauss-Seidel preconditioner and use it to
   //    solve the system Ax=b with PCG.
   GSSmoother M(A);
   PCG(A, M, *b, x, 1, 200, 1e-12, 0.0);
#else
   // 8. If MFEM was compiled with SuiteSparse, use UMFPACK to solve the system.
   UMFPackSolver umf_solver;
   umf_solver.Control[UMFPACK_ORDERING] = UMFPACK_ORDERING_METIS;
   umf_solver.SetOperator(A);
   umf_solver.Mult(*b, x);
#endif
```

- Visualization

```cpp
   // 10. Send the solution by socket to a GLVis server.
   if (visualization)
   {
      char vishost[] = "localhost";
      int  visport   = 19916;
      socketstream sol_sock(vishost, visport);
      sol_sock.precision(8);
      sol_sock << "solution\n" << *mesh << x << flush;
   }
```



- works for any mesh & any H1 order
- builds without external dependencies

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   for (int l = 0; l < ref_levels; l++)
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```
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   LinearForm *b = new LinearForm(fespace);
   ConstantCoefficient one(1.0);
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   a->Assemble();
   Array<int> ess_bdr(mesh->bdr_attributes.Max());
   ess_bdr = 1;
   a->EliminateEssentialBC(ess_bdr, x, *b);
   a->Finalize();
   const SparseMatrix &A = a->SpMat();
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   umf_solver.Mult(*b, x);
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```

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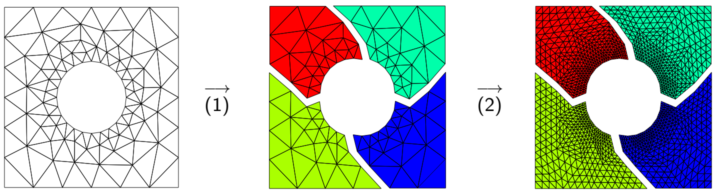
      socketstream sol_sock(vishost, visport);
      sol_sock.precision(8);
      sol_sock << "solution\n" << *mesh << x << flush;
   }
```

Example 1 – parallel Laplace equation

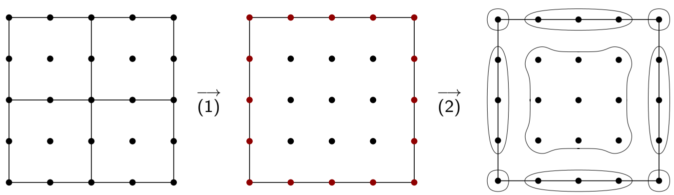
- Parallel mesh

```
// 5. Define a parallel mesh by a partitioning of the serial mesh. Refine
//    this mesh further in parallel to increase the resolution. Once the
//    parallel mesh is defined, the serial mesh can be deleted.
ParMesh *pmesh = new ParMesh(MPI_COMM_WORLD, *mesh);
delete mesh;
{
   int par_ref_levels = 2;
   for (int l = 0; l < par_ref_levels; l++)
      pmesh->UniformRefinement();
}
```



- Parallel finite element space

```
ParFiniteElementSpace *fespace = new ParFiniteElementSpace(pmesh, fec);
```



$$P : true\_dof \mapsto dof$$

- Parallel initial guess, linear/bilinear forms

```
ParLinearForm *b = new ParLinearForm(fespace);
ParGridFunction x(fespace);
ParBilinearForm *a = new ParBilinearForm(fespace);
```

- Parallel assembly

```
// 10. Define the parallel (hypre) matrix and vectors representing a(.,.),
//     b(.) and the finite element approximation.
HypreParMatrix *A = a->ParallelAssemble();
HypreParVector *B = b->ParallelAssemble();
HypreParVector *X = x.ParallelAverage();
```

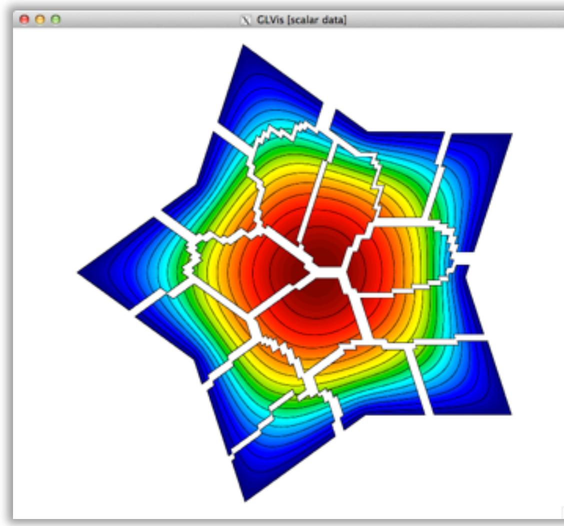
$$A = P^T a P \qquad B = P^T b \qquad x = PX$$

- Parallel linear solve with AMG

```
// 11. Define and apply a parallel PCG solver for AX=B with the BoomerAMG
//     preconditioner from hypre.
HypreSolver *amg = new HypreBoomerAMG(*A);
HyprePCG *pcg = new HyprePCG(*A);
pcg->SetTol(1e-12);
pcg->SetMaxIter(200);
pcg->SetPrintLevel(2);
pcg->SetPreconditioner(*amg);
pcg->Mult(*B, *X);
```

- Visualization

```
// 14. Send the solution by socket to a GLVis server.
if (visualization)
{
   char vishost[] = "localhost";
   int  visport   = 19916;
   socketstream sol_sock(vishost, visport);
   sol_sock << "parallel " << num_procs << " " << myid << "\n";
   sol_sock.precision(8);
   sol_sock << "solution\n" << *pmesh << x << flush;
}
```



- highly scalable with minimal changes
- build depends on *hypre* and METIS

MFEM example codes – mfem.org/examples


MFEM v3.0

Main Page

Example Codes

This file provides a brief overview of the MFEM example codes. For detailed documentation of the MFEM sources, including the examples, build the Doxygen documentation in the doc/ directory, or browse the online version.

Clicking on any of the categories below displays examples that contain the described feature. *All examples support (arbitrarily) high-order meshes and finite element spaces.* The numerical results from the example codes can be visualized using the GLVis visualization tool (based on MFEM). See the GLVis website, for more details.

Users are encouraged to submit any example codes that they have created and would like to share. *Contact a member of the MFEM team to report bugs or post questions or comments.*

Equation (PDE)
- All
- Laplace
- Elasticity
- Definite Maxwell
- grad-div
- Darcy
- Advection

Finite Elements
- All
- L_2 discontinuous elements
- H^1 nodal elements
- $H(curl)$ Nedelec elements
- $H(div)$ Raviart-Thomas elements
- $H^{-\frac{1}{2}}$ interfacial elements

Discretization
- All
- Galerkin FEM
- Mixed FEM
- Discontinuous Galerkin (DG)
- Discontinuous Petrov-Galerkin (DPG)
- Isogeometric analysis (NURBS)
- Adaptive mesh refinement (AMR)

Solver
- All
- Jacobi
- Gauss-Seidel
- PCG
- MINRES
- Algebraic Multigrid (BoomerAMG)
- Auxiliary-space Maxwell Solver (AMS)
- Auxiliary-space Divergence Solver (ADS)
- UMFPACK (serial direct)
- Newton method (nonlinear solver)
- Explicit Runge-Kutta (ODE integration)
- Implicit Runge-Kutta (ODE integration)

Example 1: Laplace Problem

This example code demonstrates the use of MFEM to define a simple isoparametric finite element discretization of the Laplace problem

$$-\Delta u = 1$$

with homogeneous Dirichlet boundary conditions. Specifically, we discretize with the FE space coming from the mesh (linear by default, quadratic for quadratic curvilinear mesh, NURBS for NURBS mesh, etc.)

The example highlights the use of mesh refinement, finite element grid functions, as well as linear and bilinear forms corresponding to the left-hand side and right-hand side of the discrete linear system. We also cover the explicit elimination of boundary conditions on all boundary edges, and the optional connection to the GLVis tool for visualization.

The example has a serial (ex1.cpp) and a parallel (ex1p.cpp) version.

Example 2: Linear Elasticity

This example code solves a simple linear elasticity problem describing a multi-material cantilever beam. Specifically, we approximate the weak form of

$$-\mathrm{div}(\sigma(\mathbf{u})) = 0$$

where

$$\sigma(\mathbf{u}) = \lambda \mathrm{div}(\mathbf{u})\, I + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$$

is the stress tensor corresponding to displacement field $\mathbf{u}$, and λ and μ are the material Lame constants. The boundary conditions are $\mathbf{u} = 0$ on the fixed part of the boundary with attribute 1, and $\sigma(\mathbf{u}) \cdot n = f$ on the remainder with f being a constant pull down vector on boundary elements with attribute 2, and zero otherwise. The geometry of the domain is assumed to be as follows:

Discretization Demo & Lesson

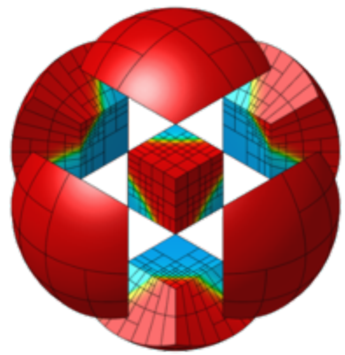
https://xsdk-project.github.io/MathPackagesTraining2021/lessons/mfem_convergence/

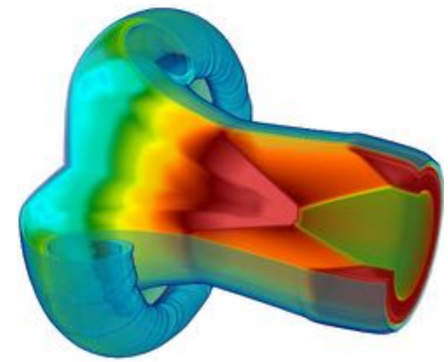
Application to high-order ALE shock hydrodynamics

hypre: *Scalable linear solvers library*

MFEM: *Modular finite element methods library*

BLAST: *High-order ALE shock hydrodynamics research code*





www.llnl.gov/casc/hypre

mfem.org

www.llnl.gov/casc/blast

- *hypre* provides scalable algebraic multigrid solvers
- MFEM provides finite element discretization abstractions
  - uses *hypre*’s parallel data structures, provides finite element info to solvers
- BLAST solves the Euler equations using a high-order ALE framework
  - combines and extends MFEM’s objects

BLAST models shock hydrodynamics using high-order FEM in both Lagrangian and Remap phases of ALE

Lagrange phase

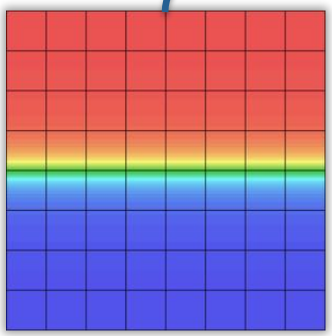
Physical time evolution

Based on physical motion

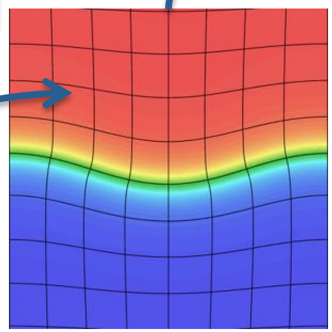
Remap phase

Pseudo-time evolution

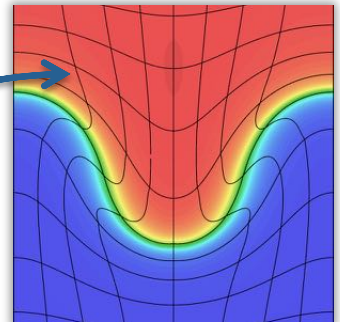
Based on mesh motion



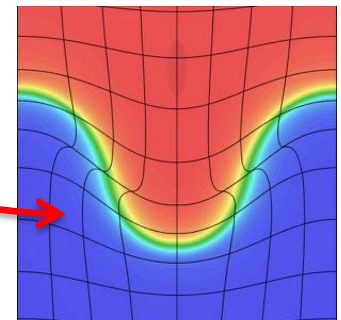
$t = 0$



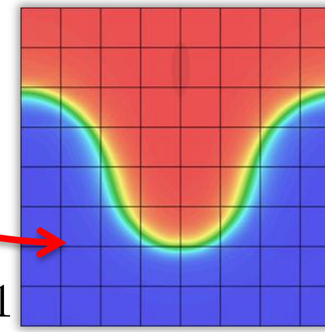
$t = 1.5$



$t = 3.0 \quad \tau = 0$



$\tau = 0.5$

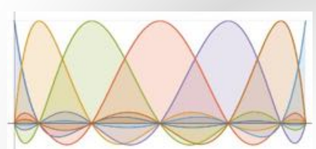


$\tau = 1$

Lagrangian phase ($\vec{c} = \vec{0}$)

Momentum Conservation:	$\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \nabla \cdot \sigma$
Mass Conservation:	$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \vec{v}$
Energy Conservation:	$\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \sigma : \nabla \vec{v}$
Equation of Motion:	$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$

- Galerkin FEM



Gauss-Lobatto basis

- Discont. Galerkin

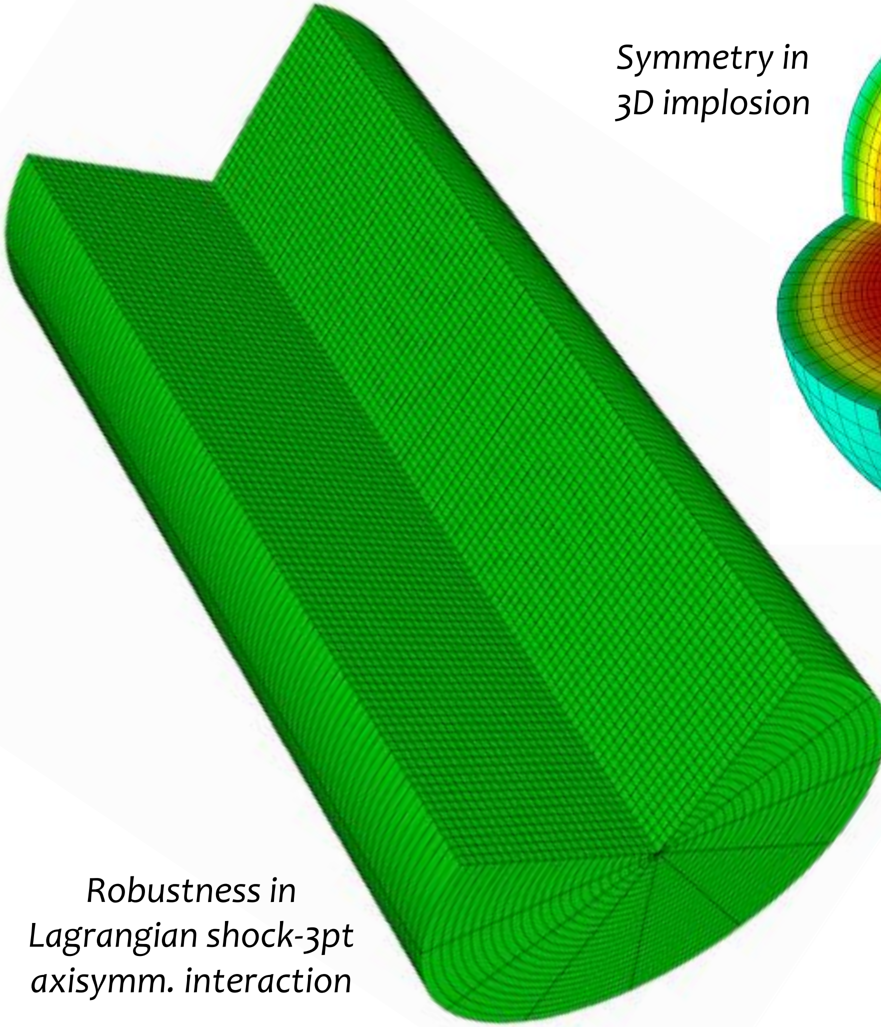
Bernstein basis

Advection phase ($\vec{c} = -\vec{v}_m$)

Momentum Conservation:	$\frac{\mathrm{d}(\rho\vec{v})}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho\vec{v})$
Mass Conservation:	$\frac{\mathrm{d}\rho}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla\rho$
Energy Conservation:	$\frac{\mathrm{d}(\rho e)}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho e)$
Mesh velocity:	$\vec{v}_m = \frac{\mathrm{d}\vec{x}}{\mathrm{d}\tau}$

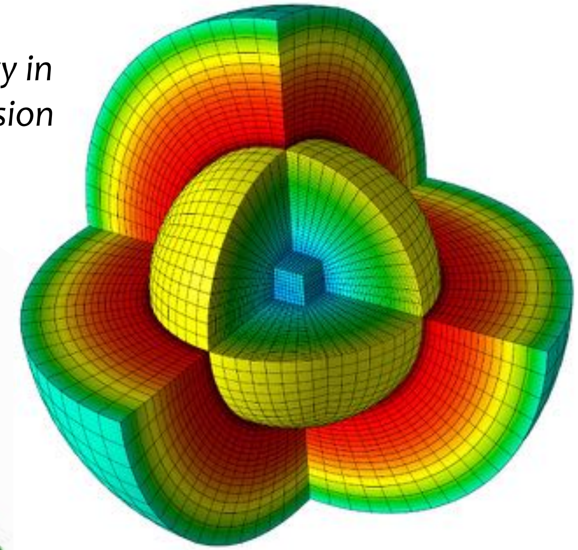
High-order finite elements lead to more accurate, robust and reliable hydrodynamic simulations

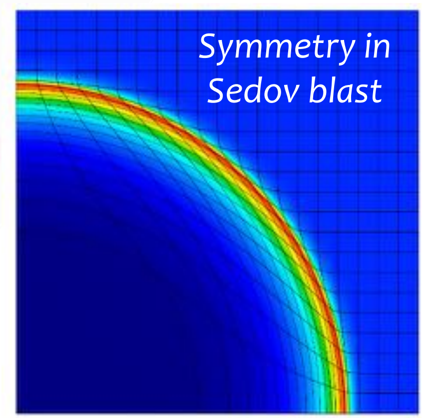
Parallel ALE for Q4 Rayleigh-Taylor instability (256 cores)



Robustness in Lagrangian shock-3pt axisymm. interaction

Symmetry in 3D implosion

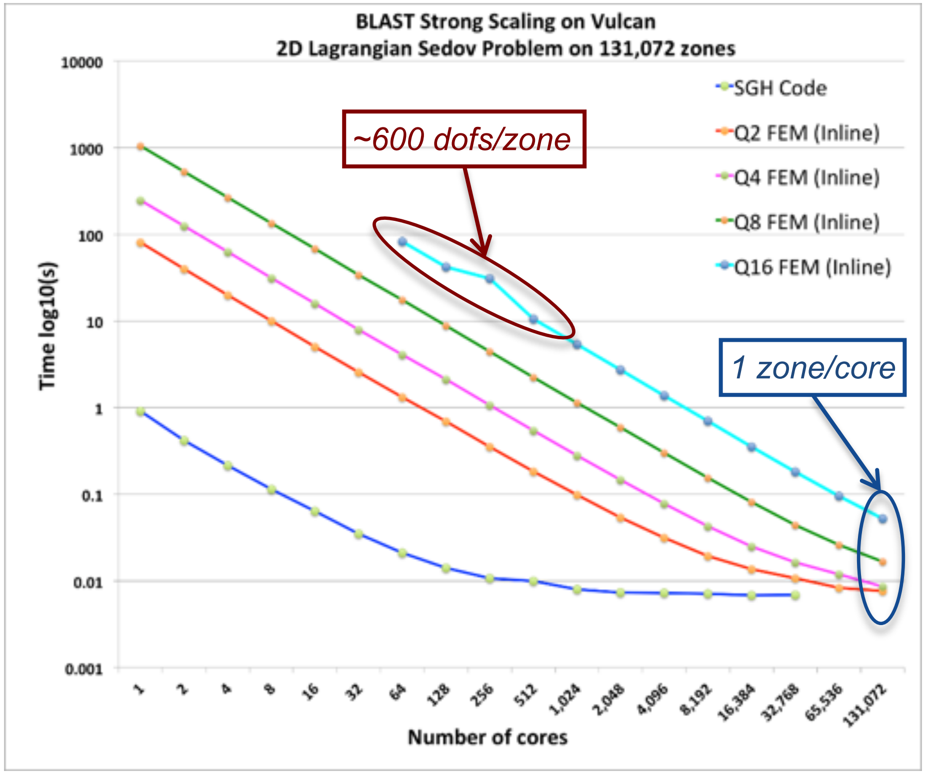




Symmetry in Sedov blast

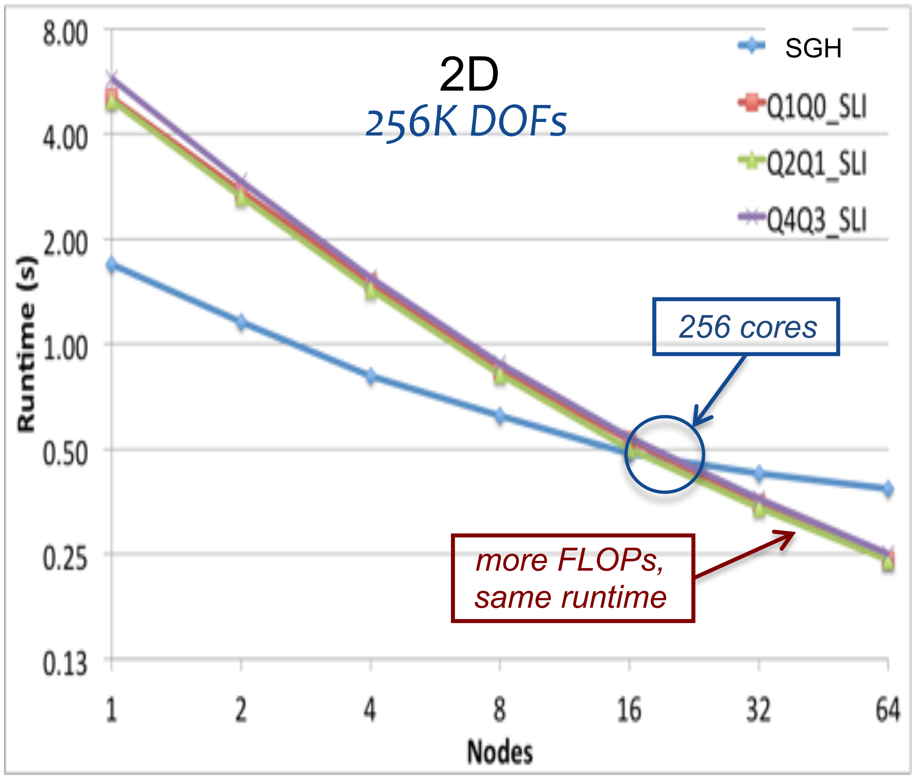
High-order finite elements have excellent strong scalability

Strong scaling, p-refinement



Finite element partial assembly

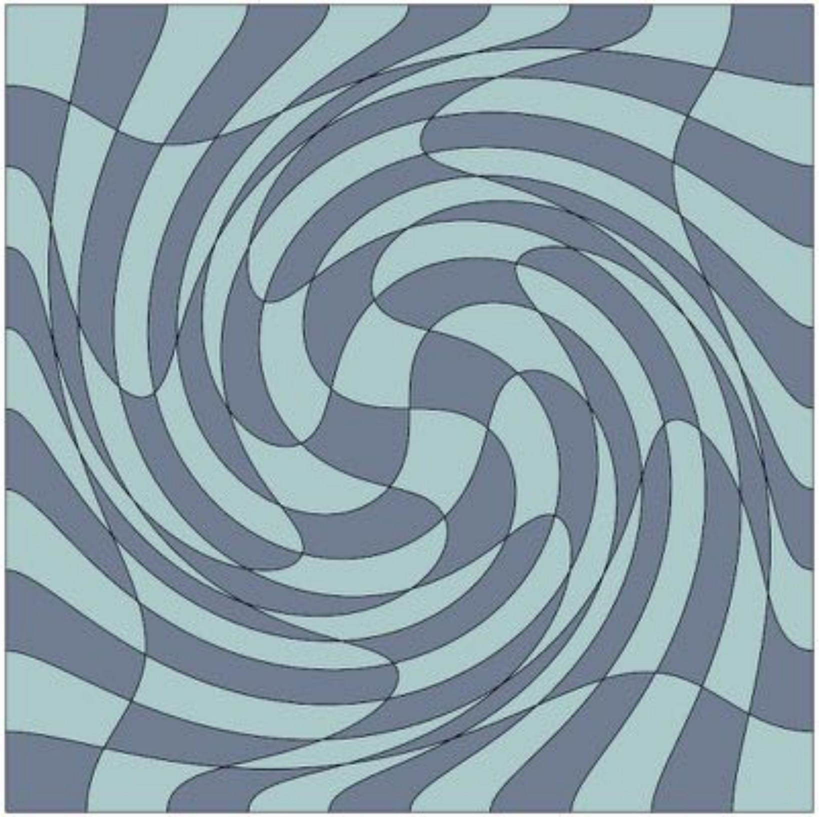
Strong scaling, fixed #dofs



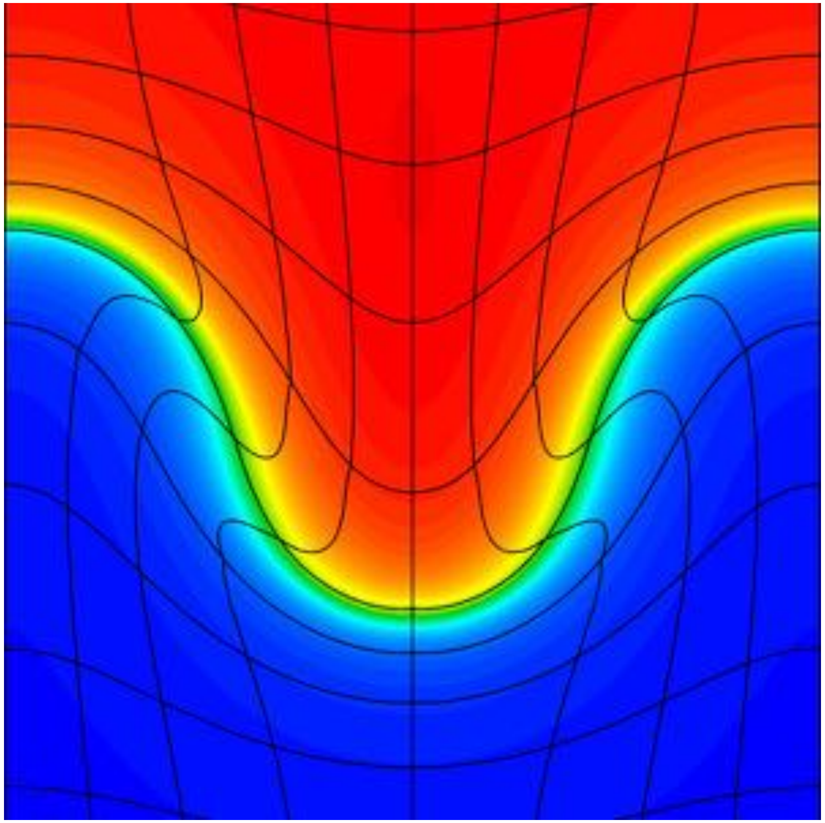
FLOPs increase faster than runtime

Unstructured Mesh R&D: Mesh optimization and high-quality interpolation between meshes

We target *high-order curved elements* + *unstructured meshes* + *moving meshes*



High-order mesh relaxation by neo-Hookean evolution (Example 10, ALE remesh)

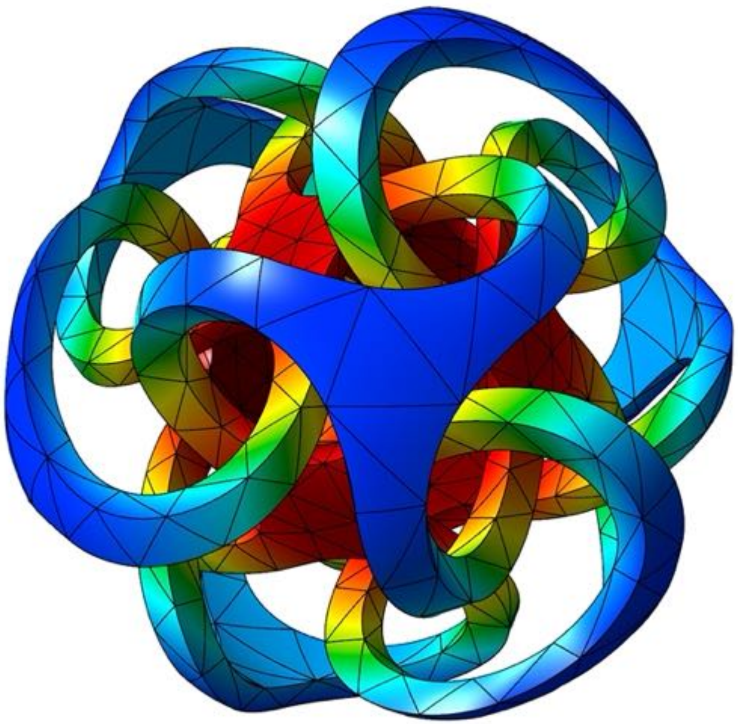


DG advection-based interpolation (ALE remap, Example 9, radiation transport)

Accurate and flexible finite element visualization

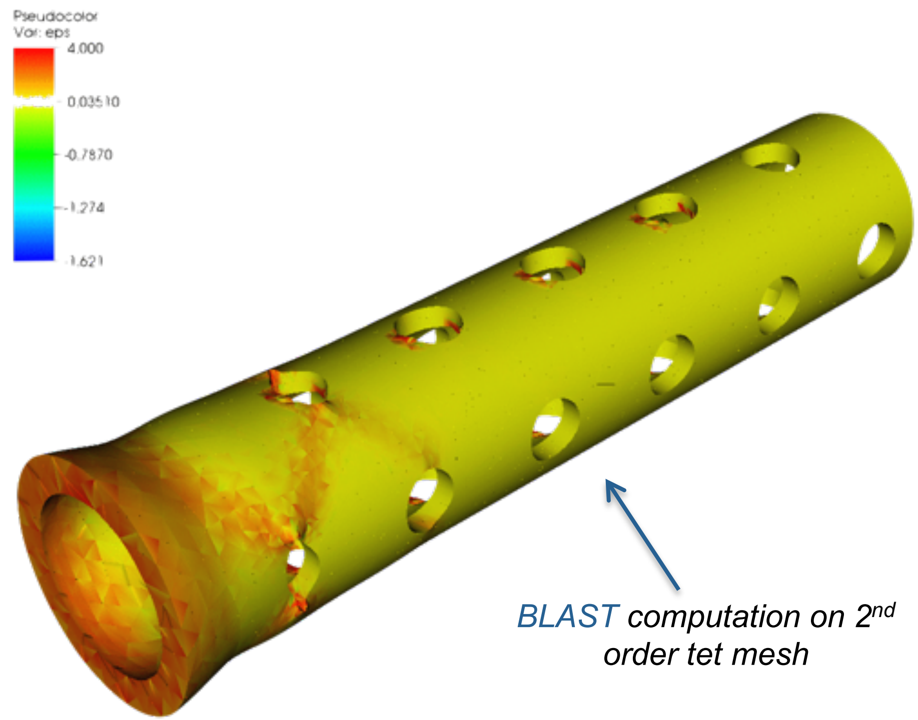
Two visualization options for high-order functions on high-order meshes

GLVis: *native MFEM lightweight OpenGL visualization tool*



glvis.org

VisIt: *general data analysis tool, MFEM support since version 2.9*



visit.llnl.gov

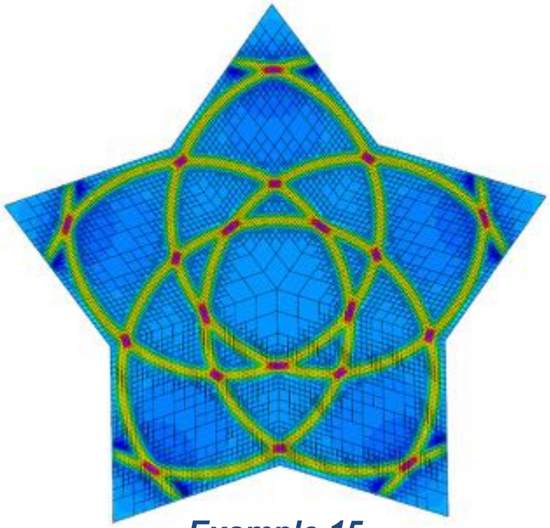
MFEM's unstructured AMR infrastructure

Adaptive mesh refinement on library level:

- Conforming local refinement on simplex meshes
- ***Non-conforming refinement for quad/hex meshes***
- h-refinement with fixed p

General approach:

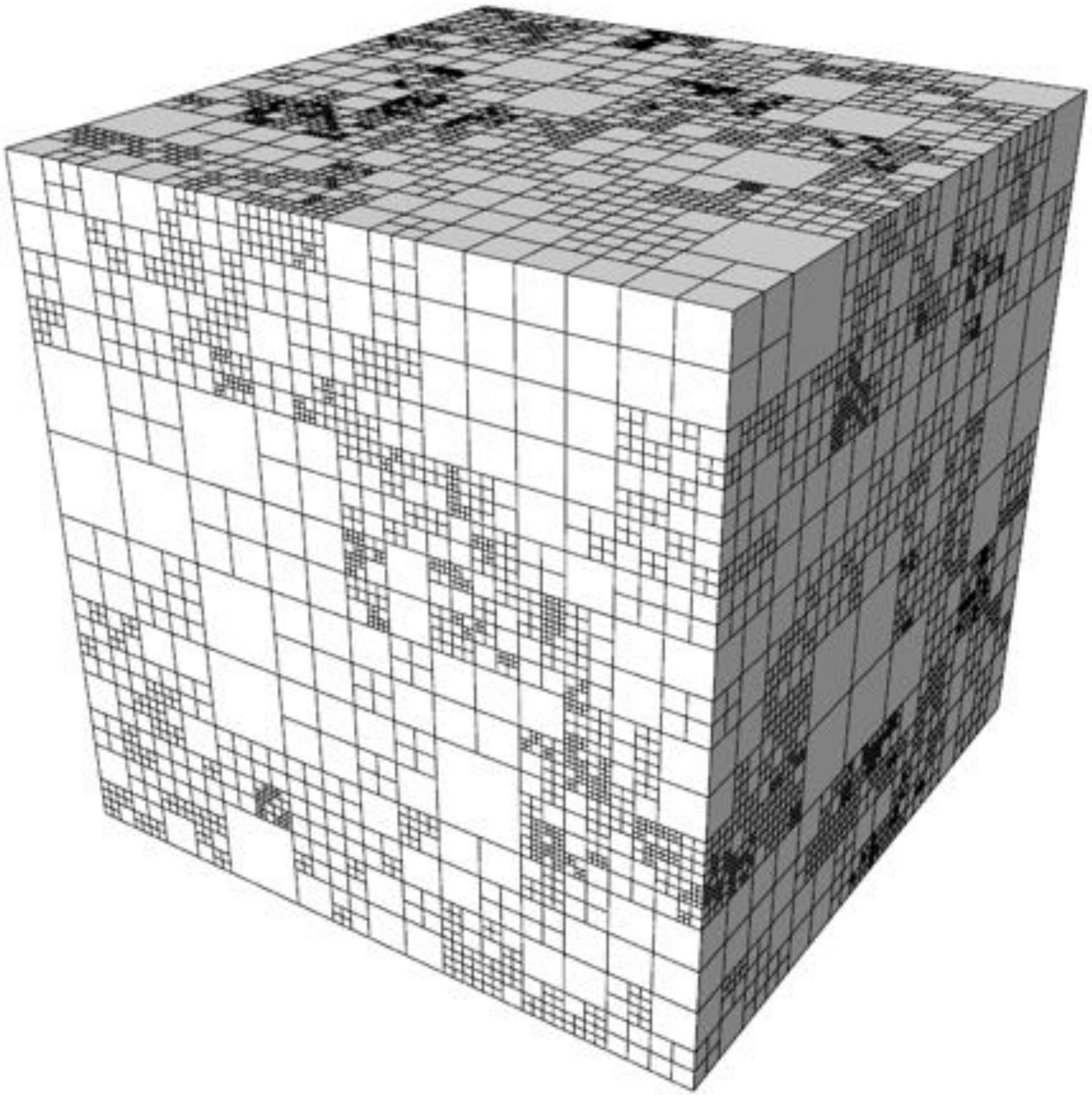
- any high-order finite element space, H1, H(curl), H(div), … , on any high-order curved mesh
- 2D and 3D
- arbitrary order hanging nodes
- anisotropic refinement
- derefinement
- serial and parallel, including parallel load balancing
- independent of the physics (easy to incorporate in applications)



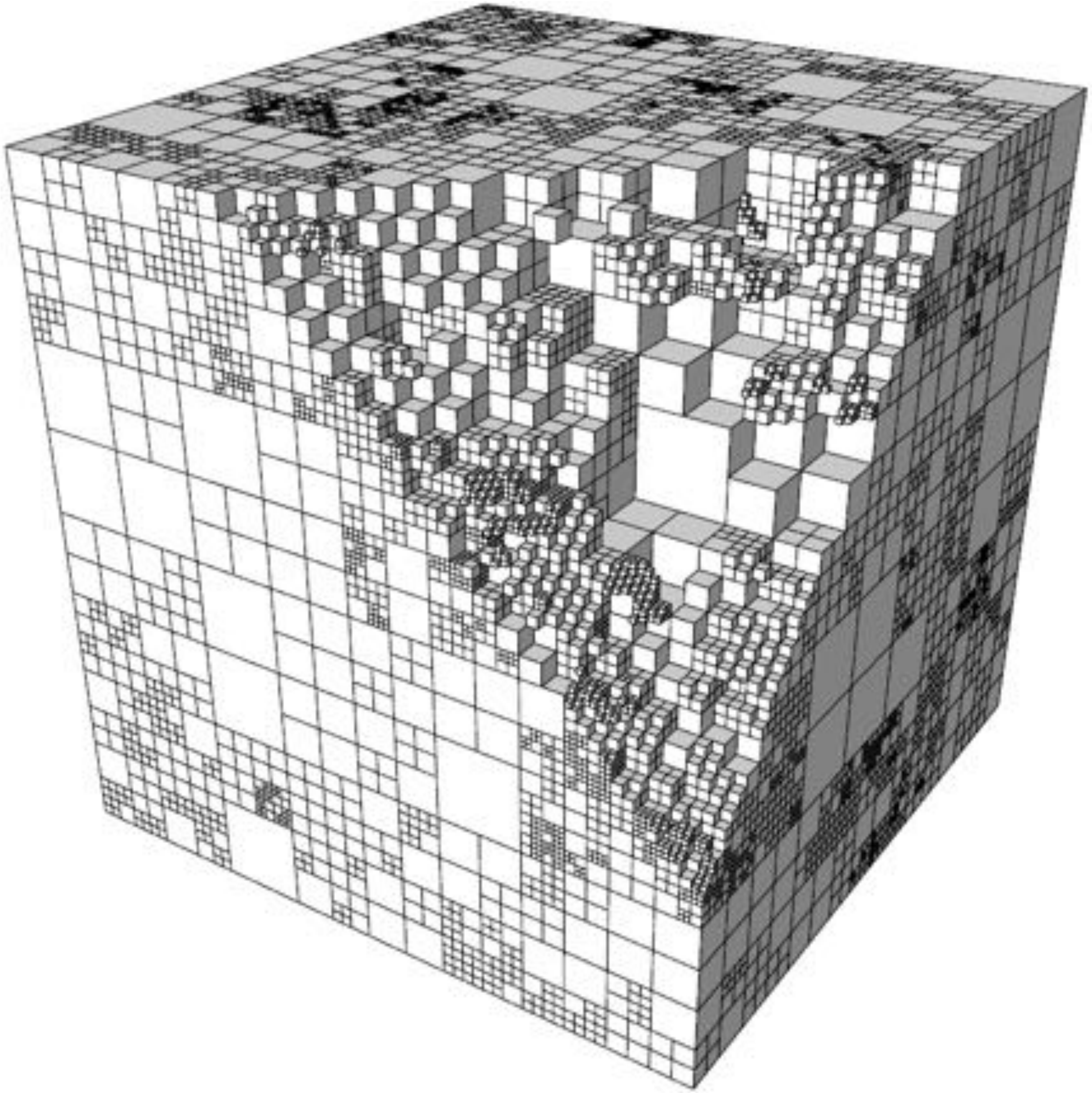
Example 15

Shaper miniapp

Nonconforming variational restriction

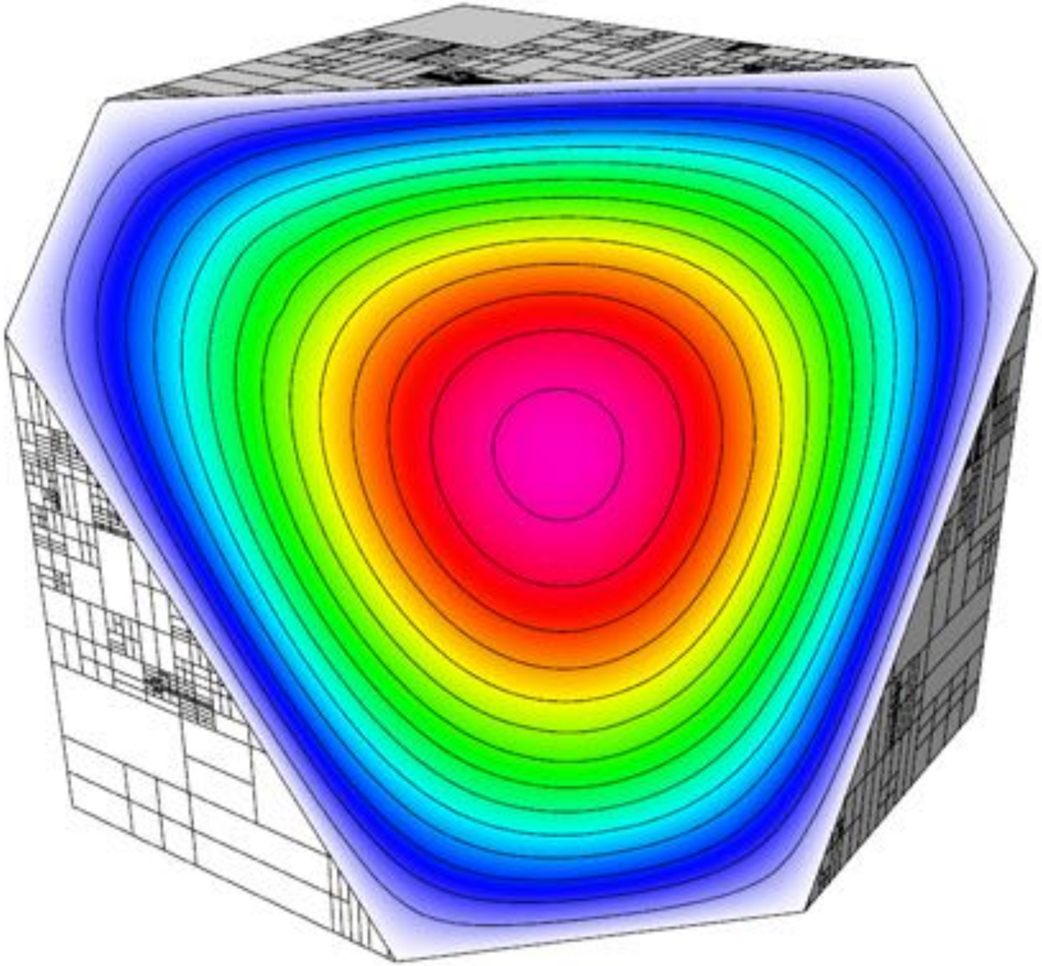


Nonconforming variational restriction



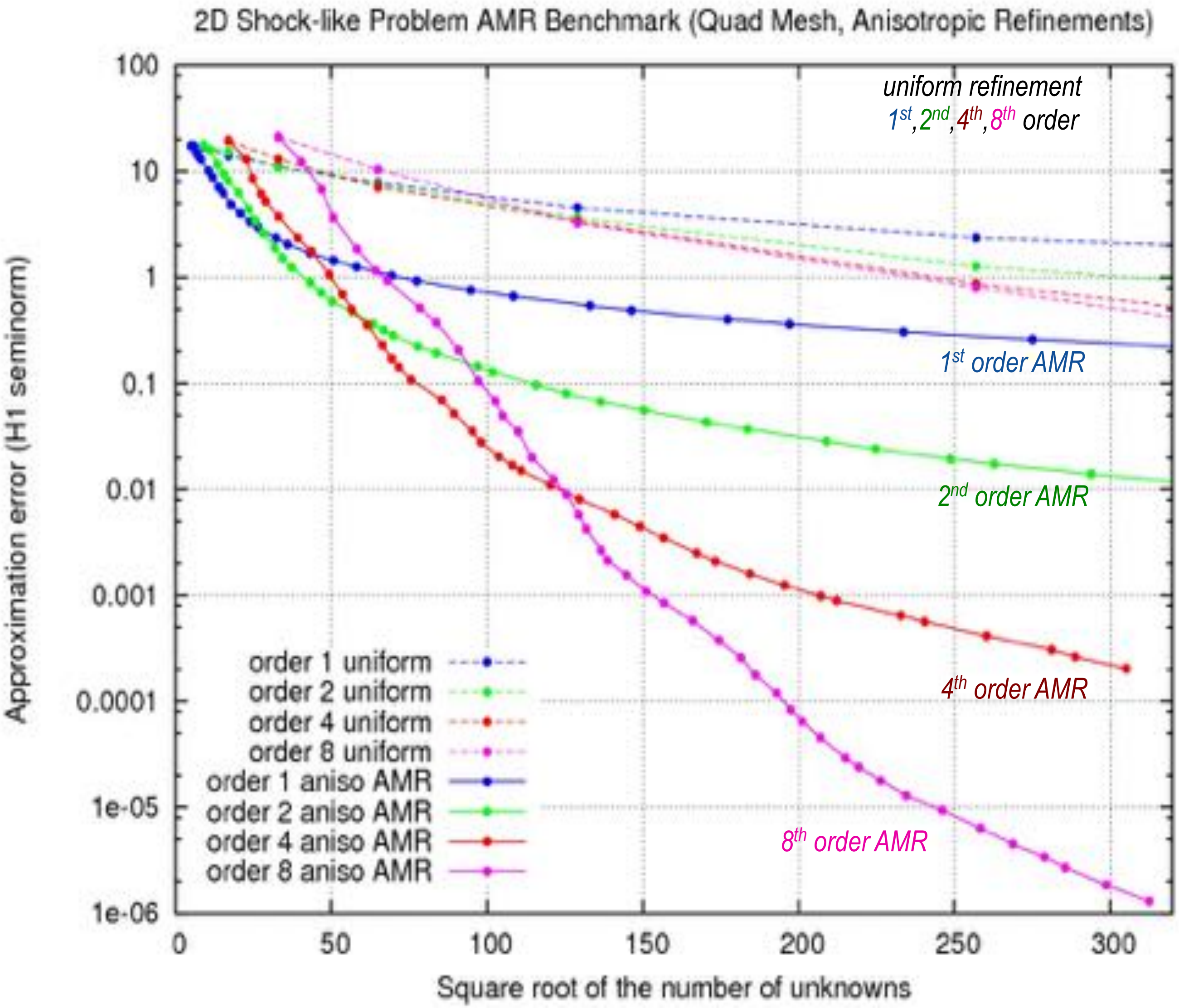
Regular assembly of A on the elements of the (cut) mesh

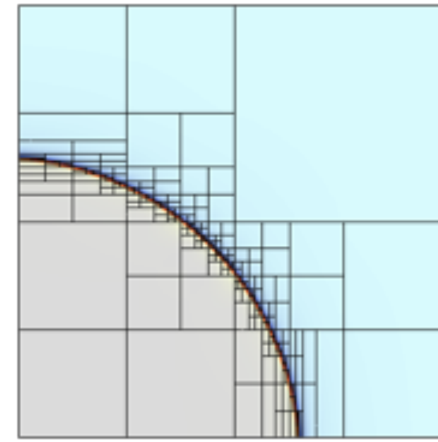
Nonconforming variational restriction

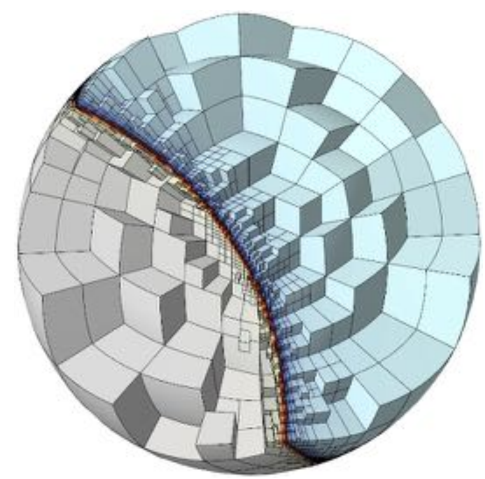


Conforming solution $y = P\,x$

AMR = smaller error for same number of unknowns

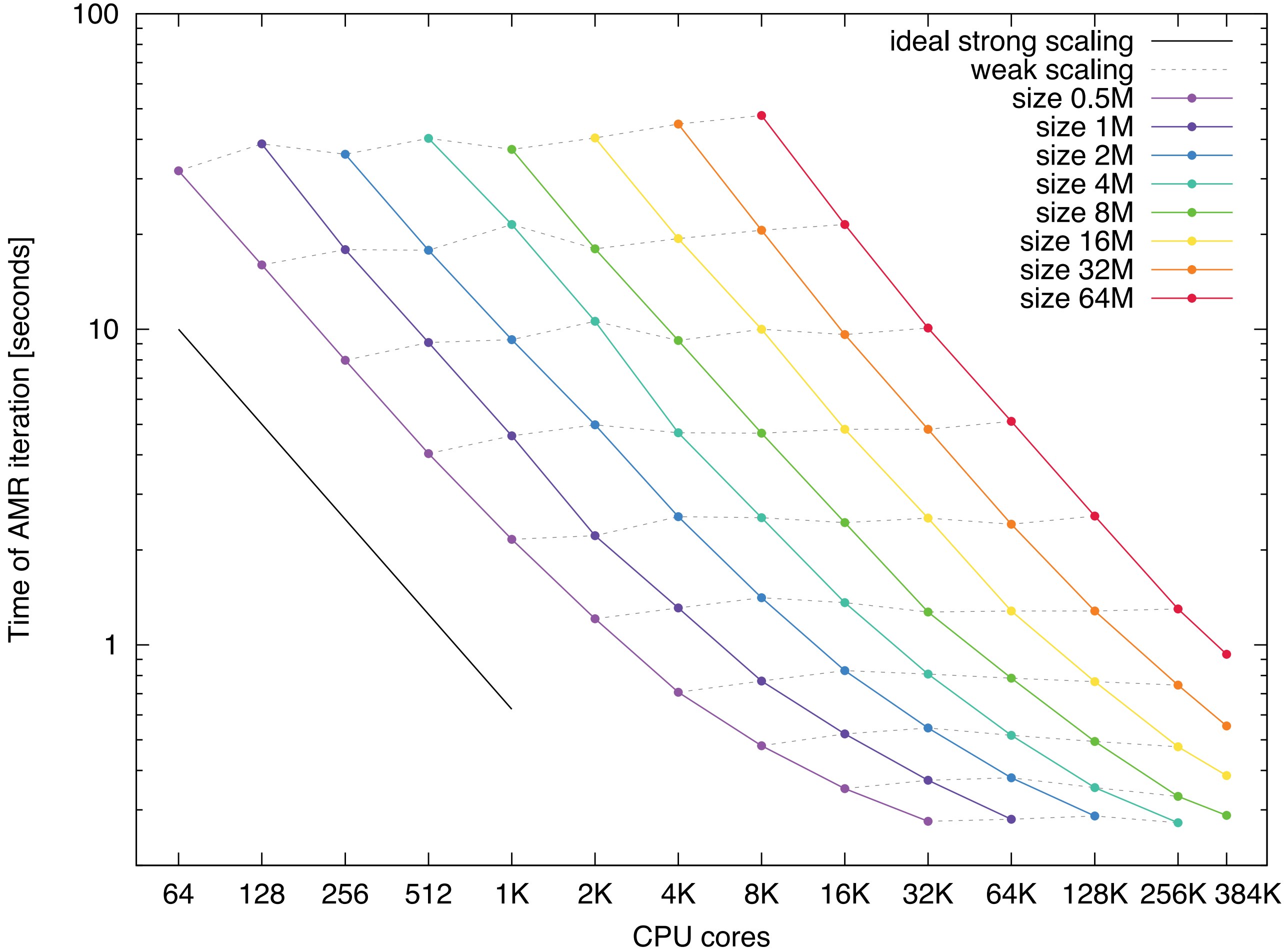


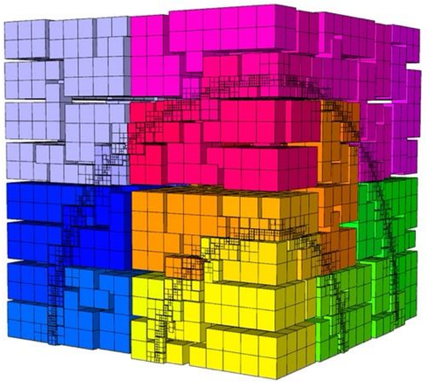




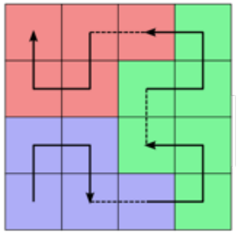
Anisotropic adaptation to shock-like fields in 2D & 3D

Parallel AMR scaling to ~400K MPI tasks



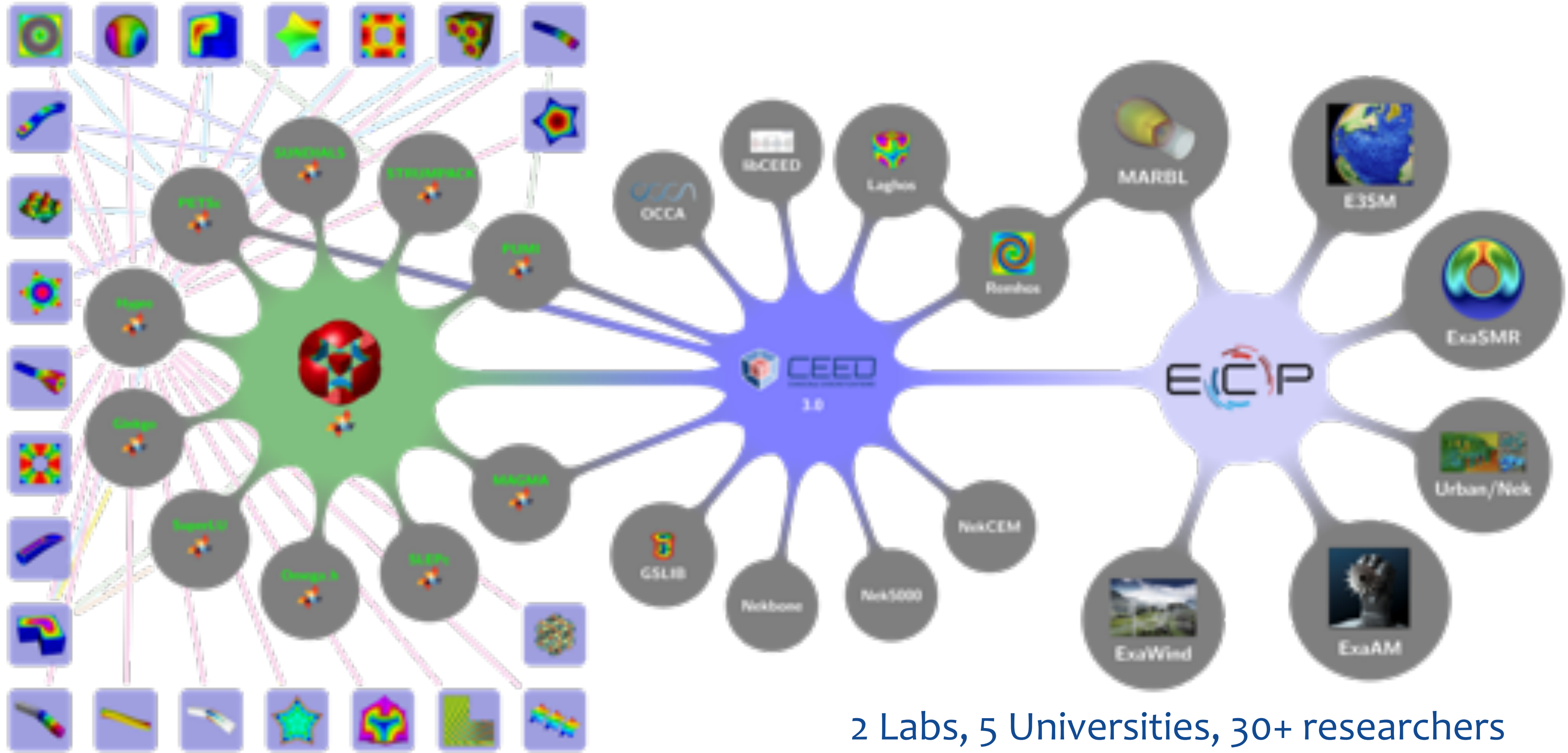


Parallel decomposition (2048 domains shown)



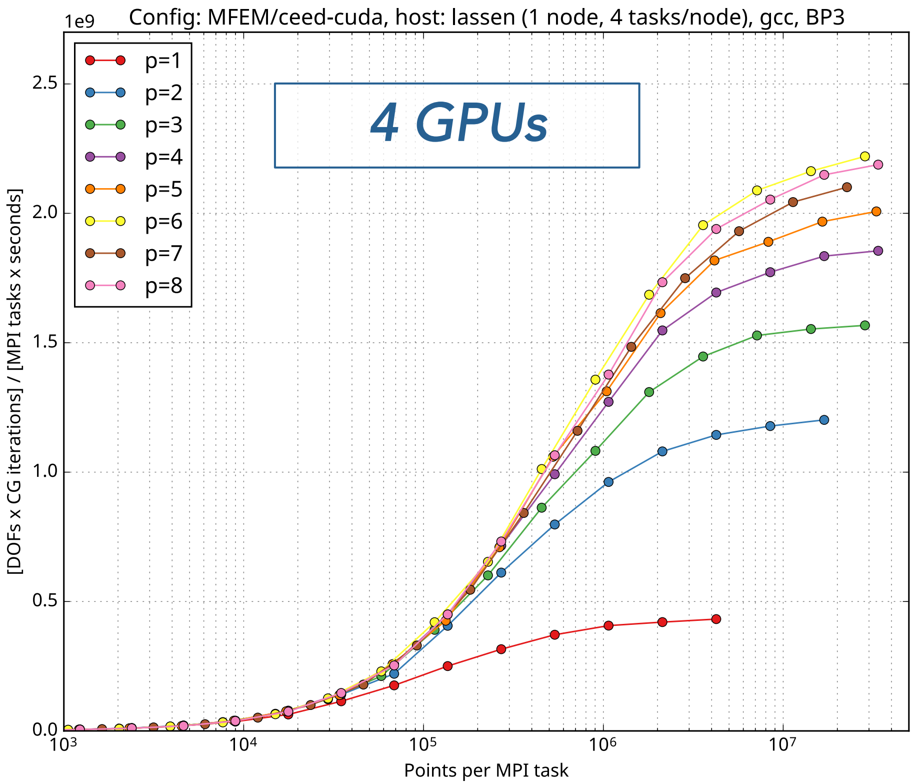
Parallel partitioning via Hilbert curve

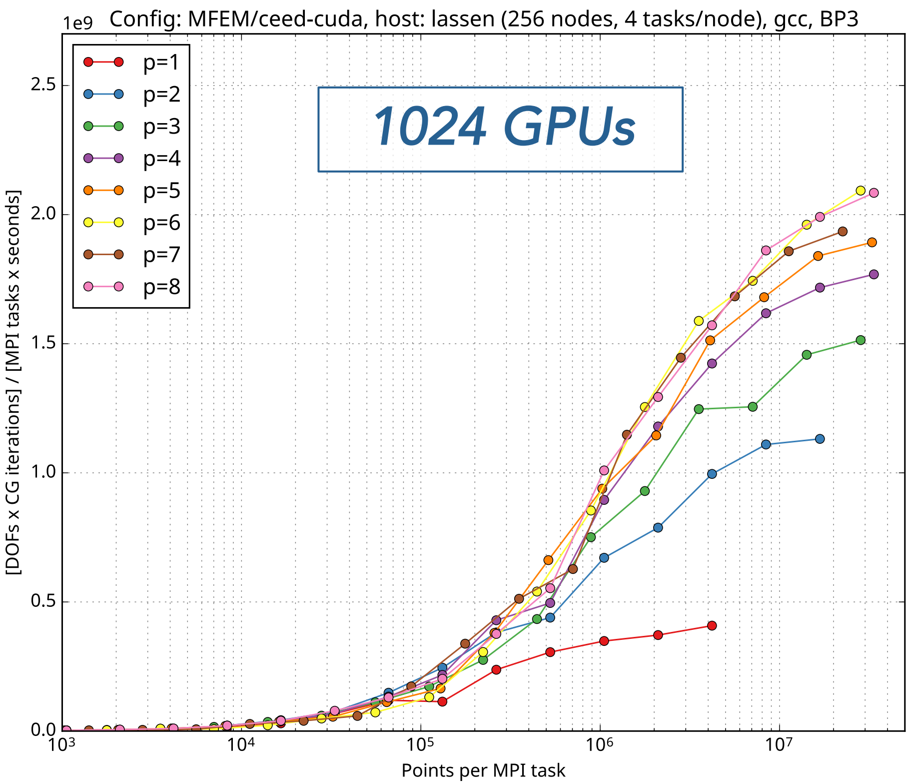
- weak+strong scaling up to ~400K MPI tasks on BG/Q
- **measure AMR only components:** interpolation matrix, assembly, marking, refinement & rebalancing (no linear solves, no "physics")



2 Labs, 5 Universities, 30+ researchers

MFEM Scaling on Multiple GPUs





Largest problem size: 34 billion; Best total performance: **2.1 TDOF/s**

MFEM-BP3, 3D, Lassen 4 x V100 GPUs / node

Resources

- **More information and publications**
  - MFEM – **mfem.org**
  - MFEM Project - **github.com/mfem**
  - MFEM Repo - **github.com/mfem/mfem**
  - MFEM Issues - **github.com/mfem/mfem/issues**
  - BLAST – **computation.llnl.gov/projects/blast**
  - CEED – **ceed.exascaleproject.org**
- **Virtual Community Workshop (Oct 20, 2021)**
  - Website – **mfem.org/workshop**
  - Technical presentations from MFEM team
  - Contributed talks from application devs
  - Demos of MFEM through python , and Jupyter notebooks
  - Discussions of development roadmap, and application areas

Q4 Rayleigh-Taylor single-material ALE on 256 processors

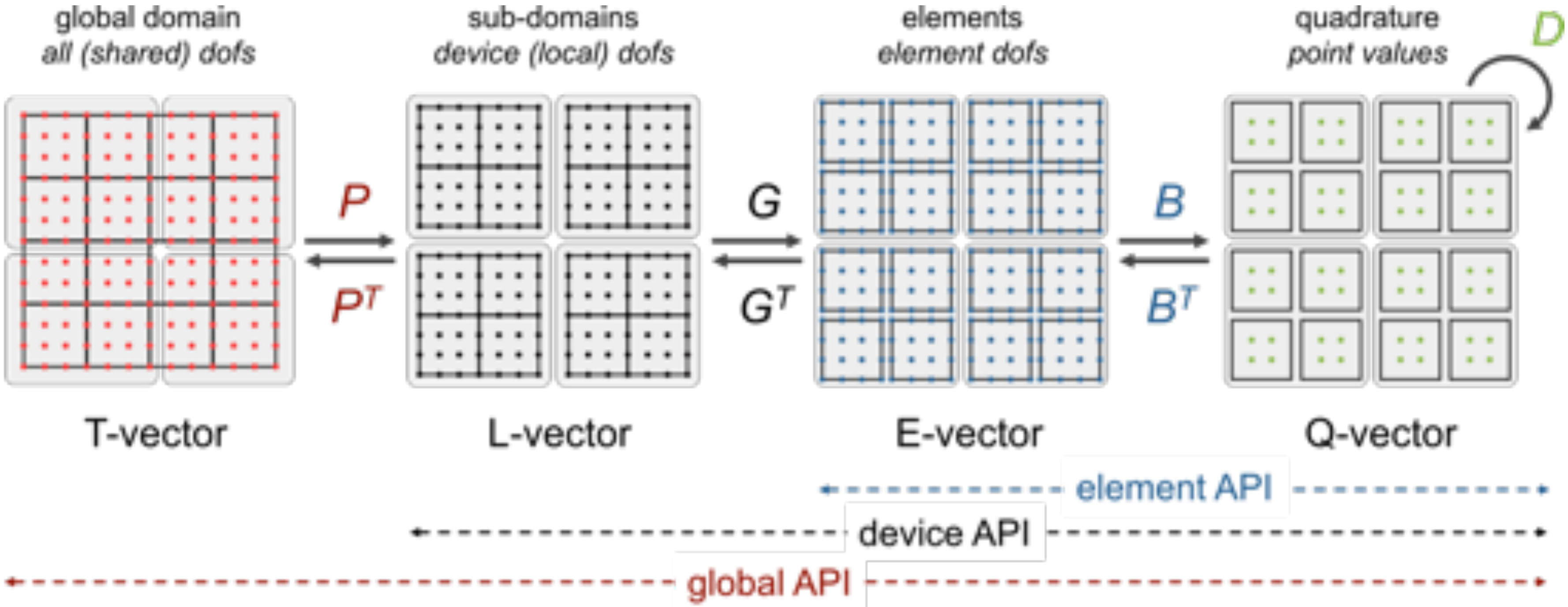
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
LLNL-PRES-755924

Lawrence Livermore National Laboratory

Fundamental finite element operator decomposition

The assembly/evaluation of FEM operators can be decomposed into **parallel**, **mesh topology**, **basis**, and geometry/physics components:

$$\boxed{A = P^T G^T B^T D B G P}$$



- ***partial assembly*** = store only D, evaluate B (tensor-product structure)
- better representation than A: *optimal memory*, *near-optimal FLOPs*
- purely algebraic, applicable to many apps

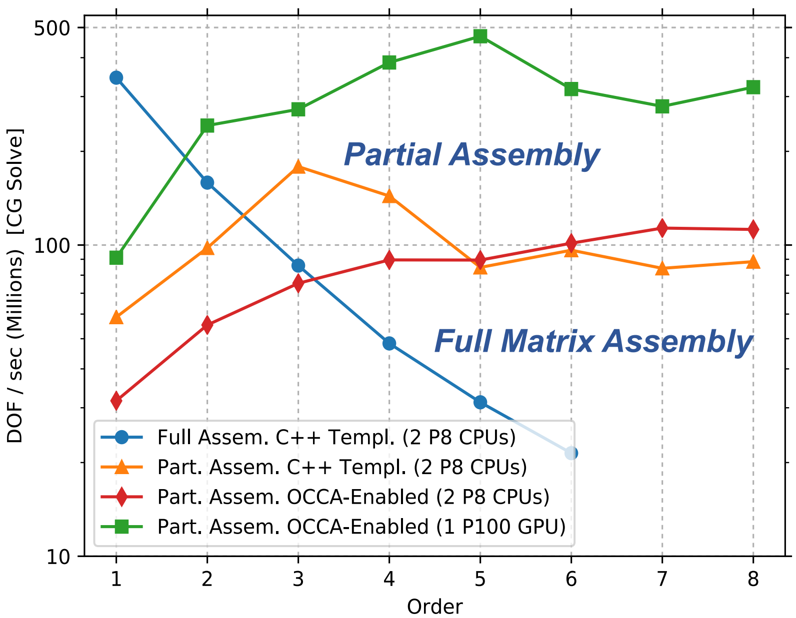
Tensorized partial assembly

$$B_{ki} = \varphi_i(q_k) = \varphi^{1d}_{i_1}(q_{k_1})\varphi^{1d}_{i_2}(q_{k_2}) = B^{1d}_{k_1 i_1} B^{1d}_{k_2 i_2} \qquad U_{k_1 k_2} = B^{1d}_{k_1 i_1} B^{1d}_{k_2 i_2} V_{i_1 i_2} \mapsto U = B^{1d} V (B^{1d})^T$$

p – order, d – mesh dim, $O(p^d)$ – dofs

Method	Memory	Assembly	Action
Full Matrix Assembly	$O(p^{2d})$	$O(p^{3d})$	$O(p^{2d})$
Partial Assembly	$O(p^d)$	$O(p^d)$	$O(p^{d+1})$

Storage and floating point operation scaling for different assembly types



Poisson CG solve performance with different assembly types (higher is better)

Full matrix performance drops sharply at high orders while partial assembly scales well!

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
LLNL-PRES-755924

Lawrence Livermore National Laboratory

FASTMath Unstructured Mesh Technologies

K.D. Devine[1], V. Dobrev[2], D.A. Ibanez[1], T. Kolev[2], K.E. Jansen[3], O. Sahni[4], M.S. Shephard[4], G.M. Slota[4], C.W. Smith[4]

[1]Sandia National Laboratories

[2]Lawrence Livermore National Laboratory

[3]University of Colorado

[4]Rensselaer Polytechnic Institute

U.S. DEPARTMENT OF ENERGY | Office of Science

ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

Unstructured Mesh Methods

Unstructured mesh – a spatial domain discretization composed of topological entities with general connectivity and shape

Advantages

- Automatic mesh generation for any level of geometric complexity
- Can provide the highest accuracy on a per degree of freedom basis
- General mesh anisotropy possible
- Meshes can easily be adaptively modified
- Given a complete geometry, with analysis attributes defined on that model, the entire simulation work flow can be automated

Disadvantages

- More complex data structures and increased program complexity, particularly in parallel
- Requires careful mesh quality control (level depend required a function of the unstructured mesh analysis code)
- Poorly shaped elements increase condition number of global system – makes matrix solves harder
- Non-tensor product elements not as computationally efficient

Unstructured Mesh Methods

Goal of FASTMath unstructured mesh developments include:

- Provide unstructured mesh components that are easily used by application code developers to extend their simulation capabilities
- Ensure those components execute on exascale computing systems and support performant exascale application codes
- Develop components to operate through multi-level APIs that increase interoperability and ease of integration
- Address technical gaps by developing tools that address needs and/or eliminate/minimize disadvantages of unstructured meshes
- Work with DOE application developers on integration of these components into their codes

FASTMath Unstructured Mesh Developments

Technology development areas:

- Unstructured Mesh Analysis Codes – Support application's PDE solution needs – MFEM library is a key example
- Performant Mesh Adaptation – Parallel mesh adaptation to integrate into analysis codes to ensure solution accuracy
- Dynamic Load Balancing and Task Management – Technologies to ensure load balance and effectively execute by optimal task placement
- Unstructured Mesh for PIC – Tools to support PIC on unstructured meshes
- Unstructured Mesh ML and UQ – ML for data reduction, adaptive mesh UQ
- In Situ Vis and Data Analytics – Tools to gain insight as simulations execute

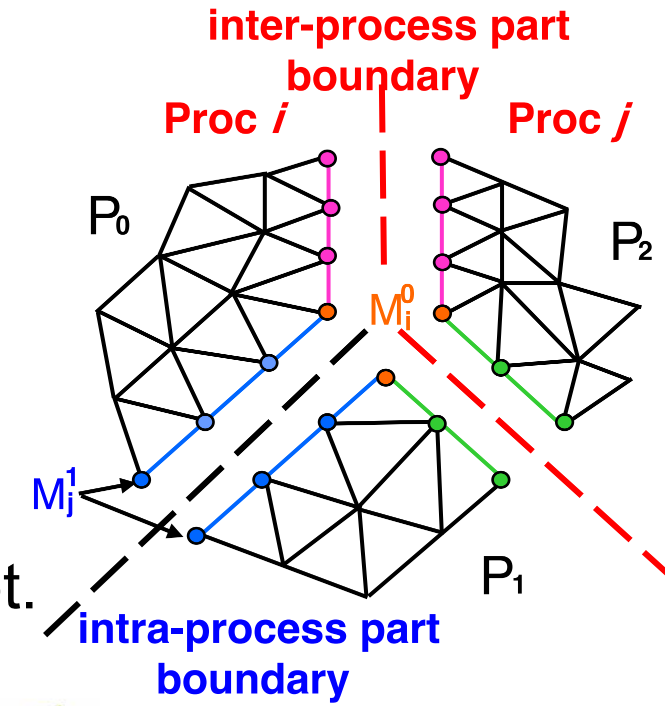
FASTMath Unstructured Mesh Tools and Components

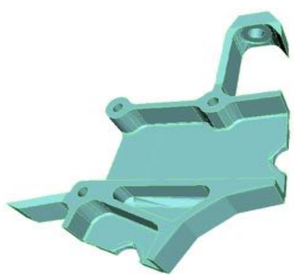
- FE Analysis codes
  - MFEM (https://mfem.org/)
  - LGR (https://github.com/SNLComputation/lgrtk)
  - PHASTA (https://github.com/phasta/phasta)
- Unstructured Mesh Infrastructure
  - Omega_h (https://github.com/SNLComputation/omega_h)
  - PUMI/MeshAdapt (https://github.com/SCOREC/core)
  - PUMIpic (https://github.com/SCOREC/pumi-pic)
- Load balancing, task placement
  - Zoltan (https://github.com/sandialabs/Zoltan)
  - Zoltan2 (https://github.com/trilinos/Trilinos/tree/master/packages/zoltan2)
  - Xtra-PULP (https://github.com/HPCGraphAnalysis/PuLP)
  - EnGPar (http://scorec.github.io/EnGPar/)
- Unstructured Mesh PIC applications
  - XGCm (https://github.com/SCOREC/xgcm) – private repo
  - GITRm (https://github.com/SCOREC/gitrm) – private repo

Parallel Unstructured Mesh Infrastructure

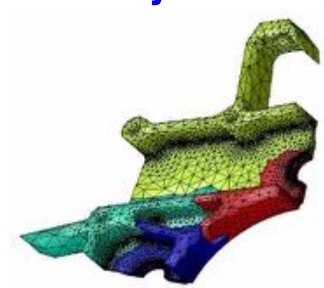
Support unstructured mesh interactions on exascale systems
- Mesh hierarchy to support interrogation and modification
- Maintians linkage to original geometry
- Conforming mesh adaptation
- Inter-process communication
- Supports field operations

Tools
- Omega_h – full CPU/GPU support
- PUMI – CPU based curved mesh adapt.
- PUMIPic – Unstructured mesh with particles for GPU implementations




Geometric model

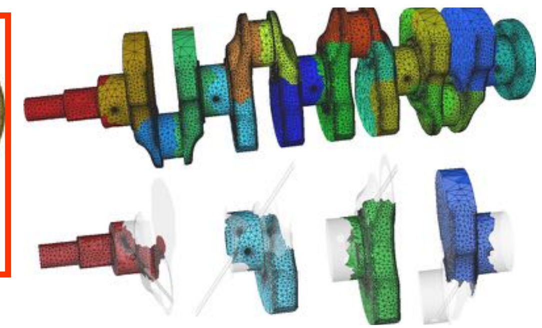

Partition model


Distributed mesh

Mesh Generation and Control

Mesh Generation:

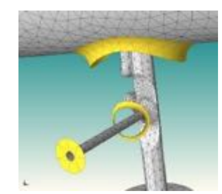
- Automatically mesh complex domains – should work directly from CAD, image data, etc.

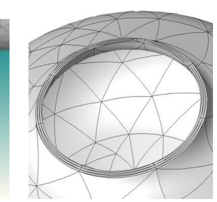


- Use tools like Gmsh, Simmetrix, etc.

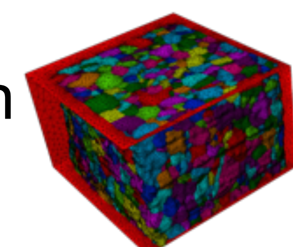
Mesh control:

- Use *a posteriori* information to improve mesh





- Curved geometry and curved mesh entities
- Support full range of mesh modifications – vertex motion, mesh entity curving, cavity based refinement and coarsening, etc. anisotropic adaptation

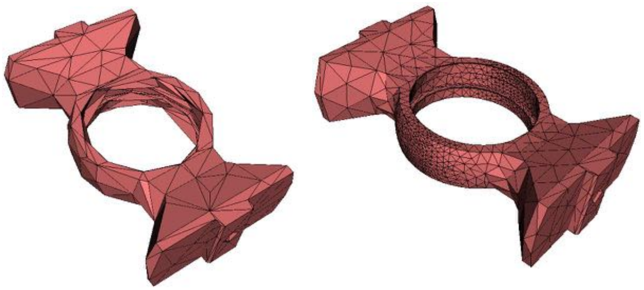


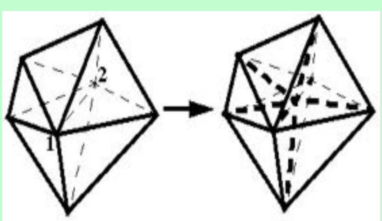
- Control element shapes as needed by the various discretization methods for maintaining accuracy and efficiency

Parallel execution of all functions is critical on large meshes

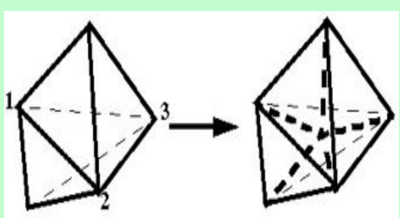
General Mesh Modification for Mesh Adaptation

- Driven by an anisotropic mesh size field that can be set by any combination of criteria
- Employ a “complete set” of mesh modification operations to alter the mesh into one that matches the given mesh size field
- Advantages
  - Supports general anisotropic meshes
  - Can obtain level of accuracy desired
  - Can deal with any level of geometric domain complexity
  - Solution transfer can be applied incrementally - provides more control to satisfy conservation constraints

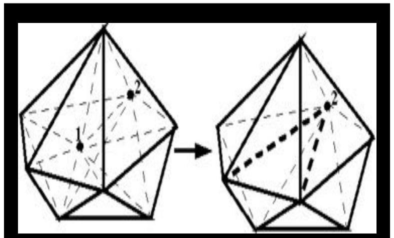


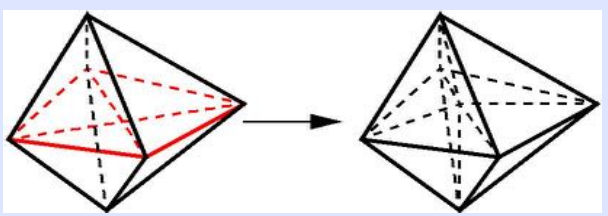


Edge split



face split

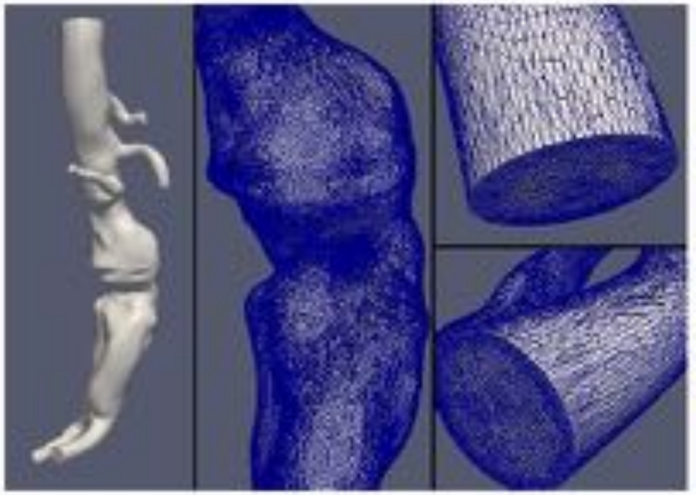


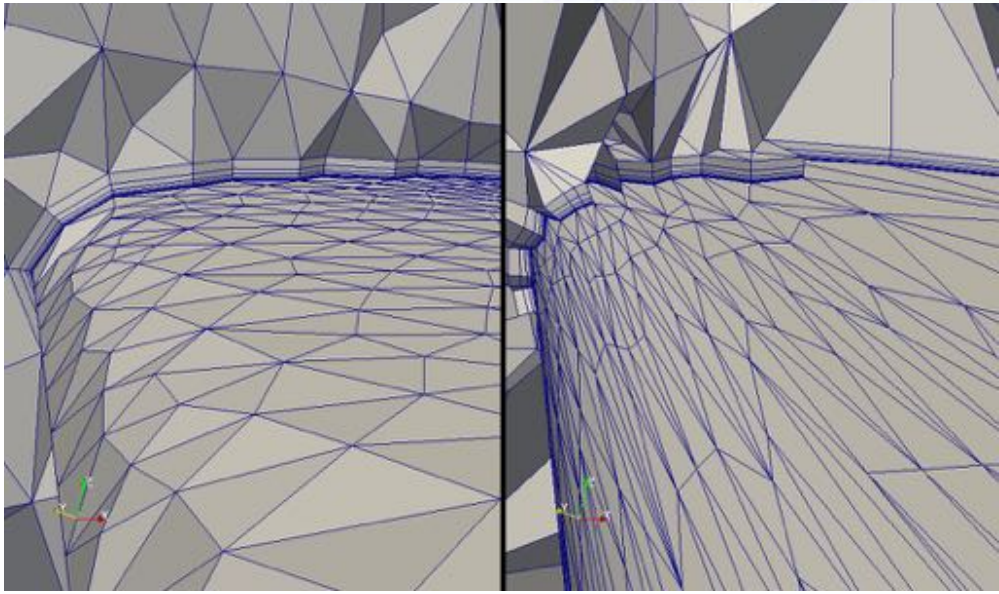


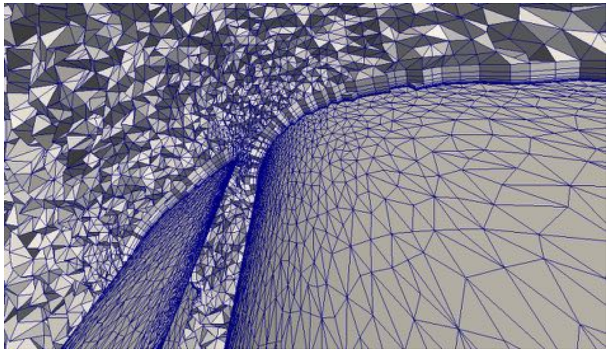
Double split collapse to remove sliver

Mesh Adaptation Status

- Applied to very large scale models – 92B elements on 3.1M processes on ¾ million cores
- Local solution transfer supported through callback
- Effective storage of solution fields on meshes
- Supports adaptation with boundary layer meshes





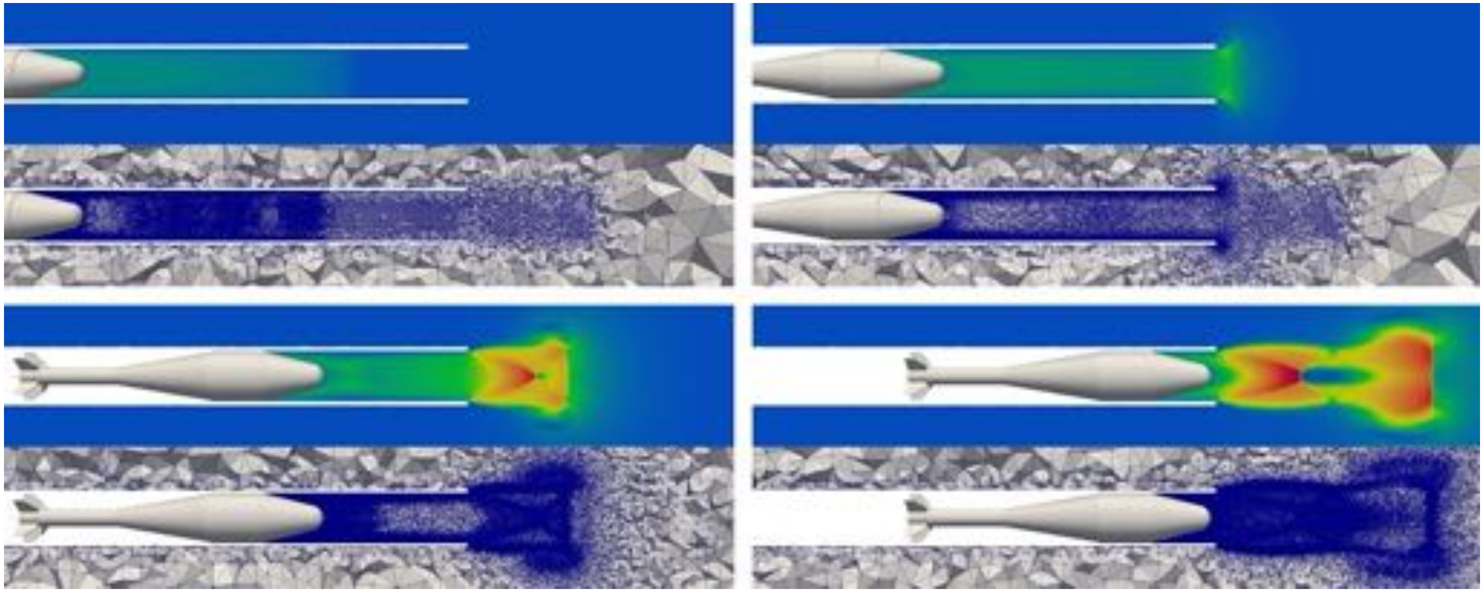


Mesh Adaptation of Evolving Geometry Problems

Many applications have geometry that evolves as a function of the results – Effective adaptive loops combine mesh motion and mesh modification

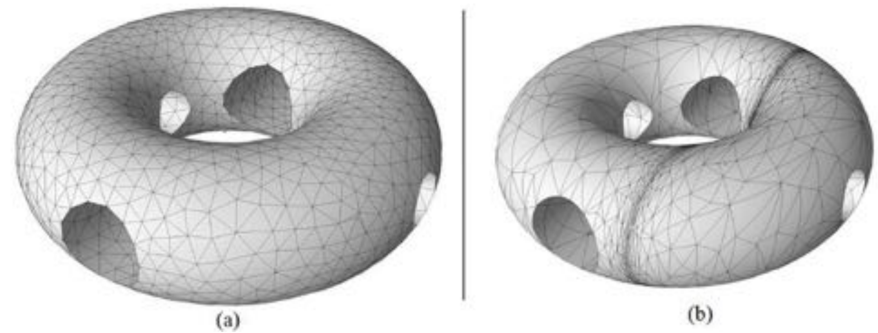
Adaptive loop:

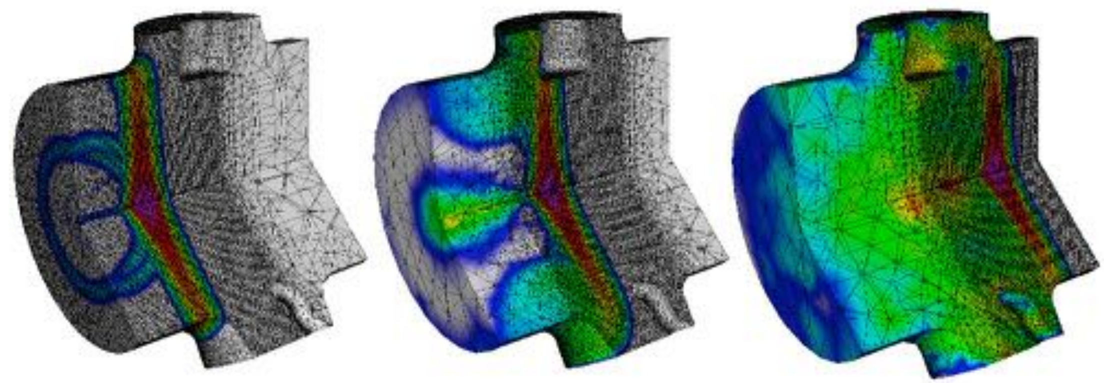
1. Initialize analysis case, generate initial mesh, start time stepping loop
2. Perform time steps employing mesh motion - monitor element quality and discretization errors
3. When element quality is not satisfactory or discretization errors too large – set mesh size field and perform mesh modification
4. Return to step 2.

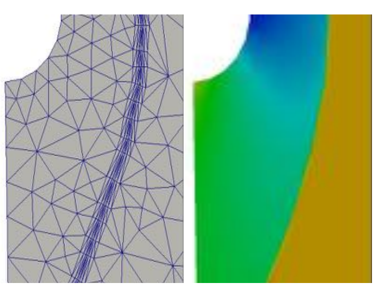


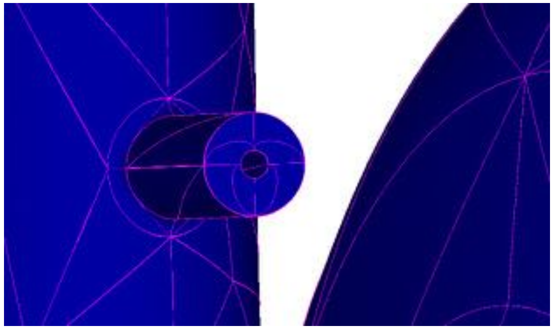
Mesh Adaptation

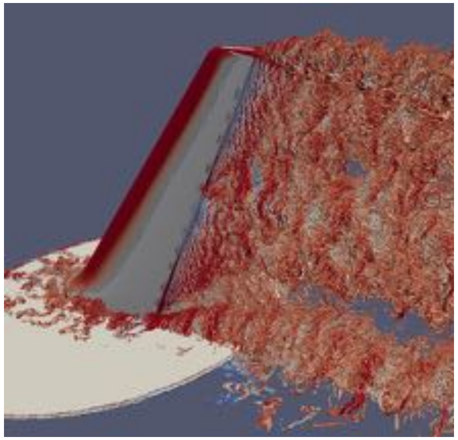
- Supports adaptation of curved elements
- Adaptation based on multiple criteria, examples
  - Level sets at interfaces
  - Tracking particles
  - Discretization errors
  - Controlling element shape in evolving geometry





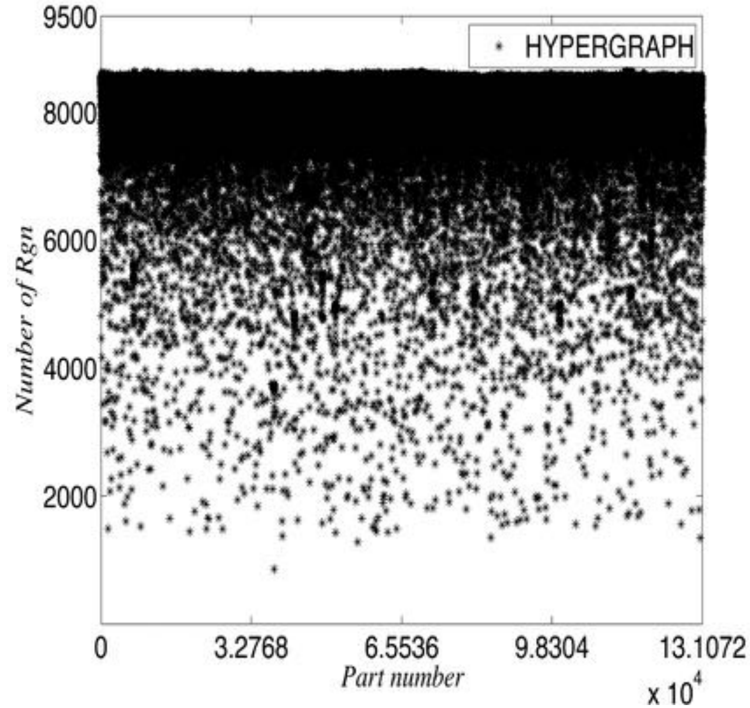






Load Balancing, Dynamic Load balancing

- Purpose: Balance, rebalance computational load while controlling communications
  - Equal “work load” with minimum inter-process communications



- FASTMath load balancing tools
  - Zoltan/Zoltan2 libraries provide multiple dynamic partitioners with general control of partition objects and weights
  - EnGPar diffusive multi-criteria partition improvement
  - XtraPuLP multi-constraint multi-objective label propagation-based graph partitioner

Architecture-aware partitioning and task mapping

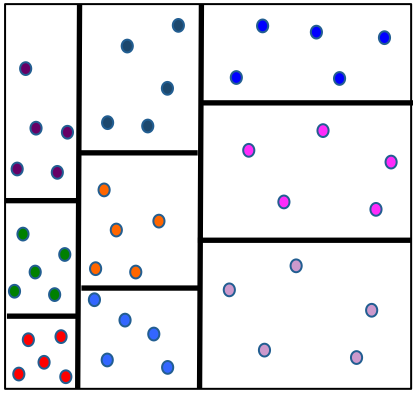
Reduce application communication time at extreme scale

- *Partitioning and load balancing*: assign work to processes in ways that avoid process idle time and minimize communication
- *Task mapping*: assign processes to cores in ways that reduce messages distances and network congestion
- *Important in extreme-scale systems*:
  - Small load imbalances can waste many resources
  - Large-scale networks can cause messages to travel long routes and induce congestion
- *Challenge* to develop algorithms that…
  - account for underlying architectures & hierarchies
  - run effectively side-by-side with application across many platforms (multicore, GPU)

Zoltan/Zoltan2 Toolkits: Partitioners

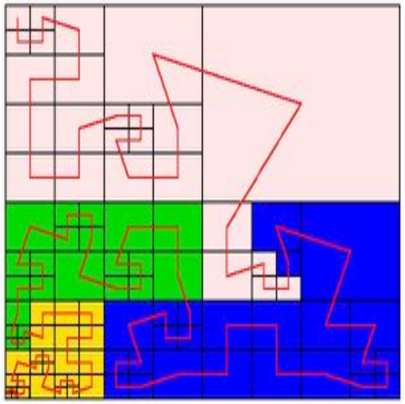
Suite of partitioners supports a wide range of applications; no single partitioner is best for all applications.

Geometric

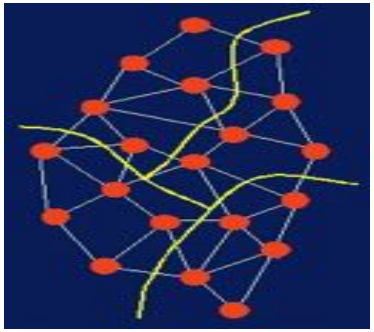


Recursive Coordinate Bisection
Recursive Inertial Bisection
Multi-Jagged Multi-section

Space Filling Curves

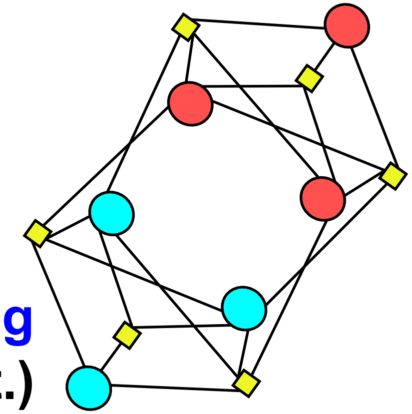


Topology-based



PHG Graph Partitioning
Interface to ParMETIS (U. Minnesota)
Interface to PT-Scotch (U. Bordeaux)

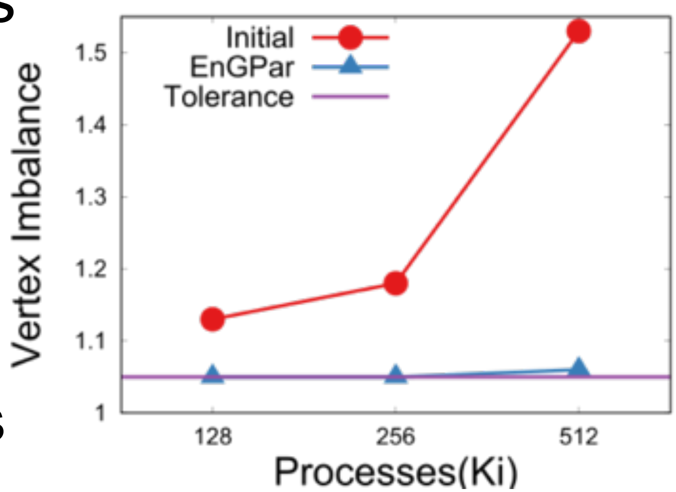
PHG Hypergraph Partitioning
Interface to PaToH (Ohio St.)

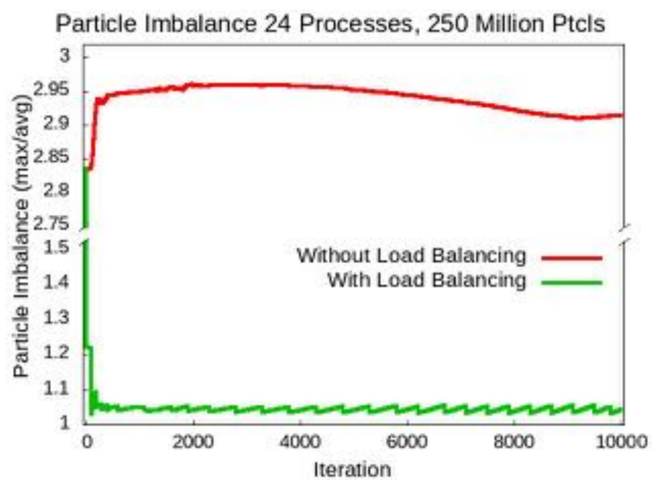


EnGPar Dynamic Load Balancing

Quickly reduces large imbalances on (hyper)graphs with billions of edges on up to 512K processes

- Multi-(hyper)graph supports multiple dependencies (edges) between application work/data items (vertices)
- Application defined vertex and edges
- Diffusion sends from heavily loaded parts to lighter parts
- On a 1.3B element mesh, in 8 seconds EnGPar reduces a 53% vtx imbalance to 6%, elm imbalance of 5%, edge cut increase by 1%
- Applied to PIC calculations to support particle balance – flexibility of vertex and edge definition critical to attaining 20% reduction in total run time



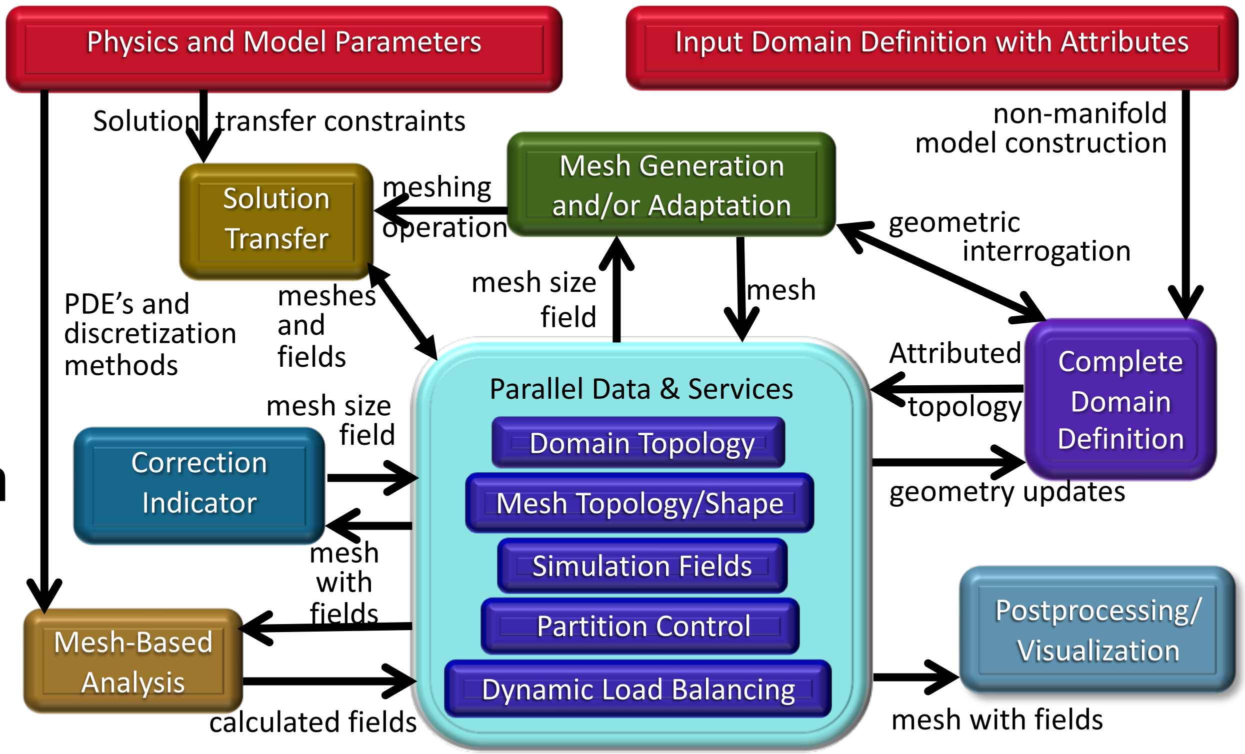


Application of EnGPar particle dynamic load balancing in a GITRm impurity transport simulation

Creation of Parallel Adaptive Loops

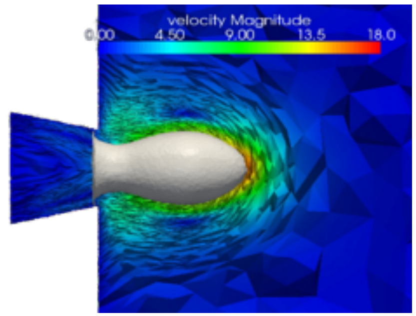
Parallel data and services are the core

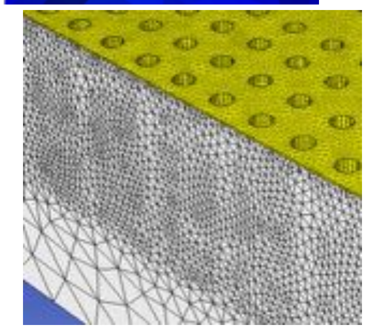
- Geometric model topology for domain linkage
- Mesh topology – it must be distributed
- Simulation fields distributed over geometric model and mesh
- Partition control
- Dynamic load balancing required at multiple steps
- API's to link to
  - CAD
  - Mesh generation and adaptation
  - Error estimation
  - etc

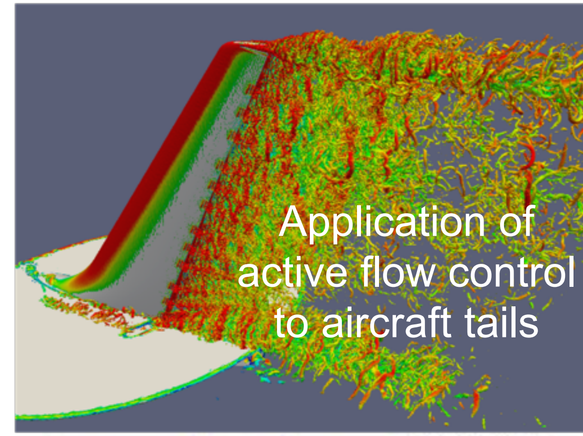


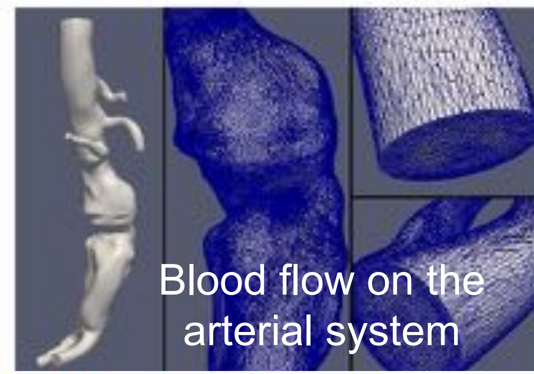
Parallel Adaptive Simulation Workflows

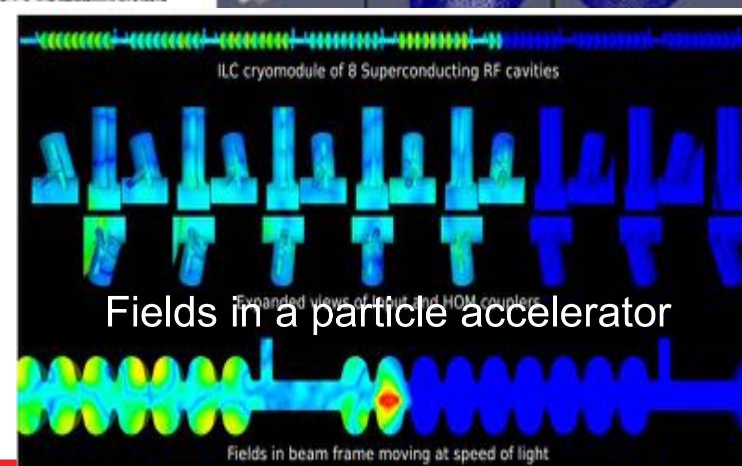
- Automation and adaptive methods critical to reliable simulations
- In-memory examples
  - MFEM – High order FE framework
  - PHASTA – FE for NS
  - FUN3D – FV CFD
  - Proteus – multiphase FE
  - Albany – FE framework
  - ACE3P – High order FE electromagnetics
  - M3D-C1 – FE based MHD
  - Nektar++ – High order FE flow






Application of active flow control to aircraft tails

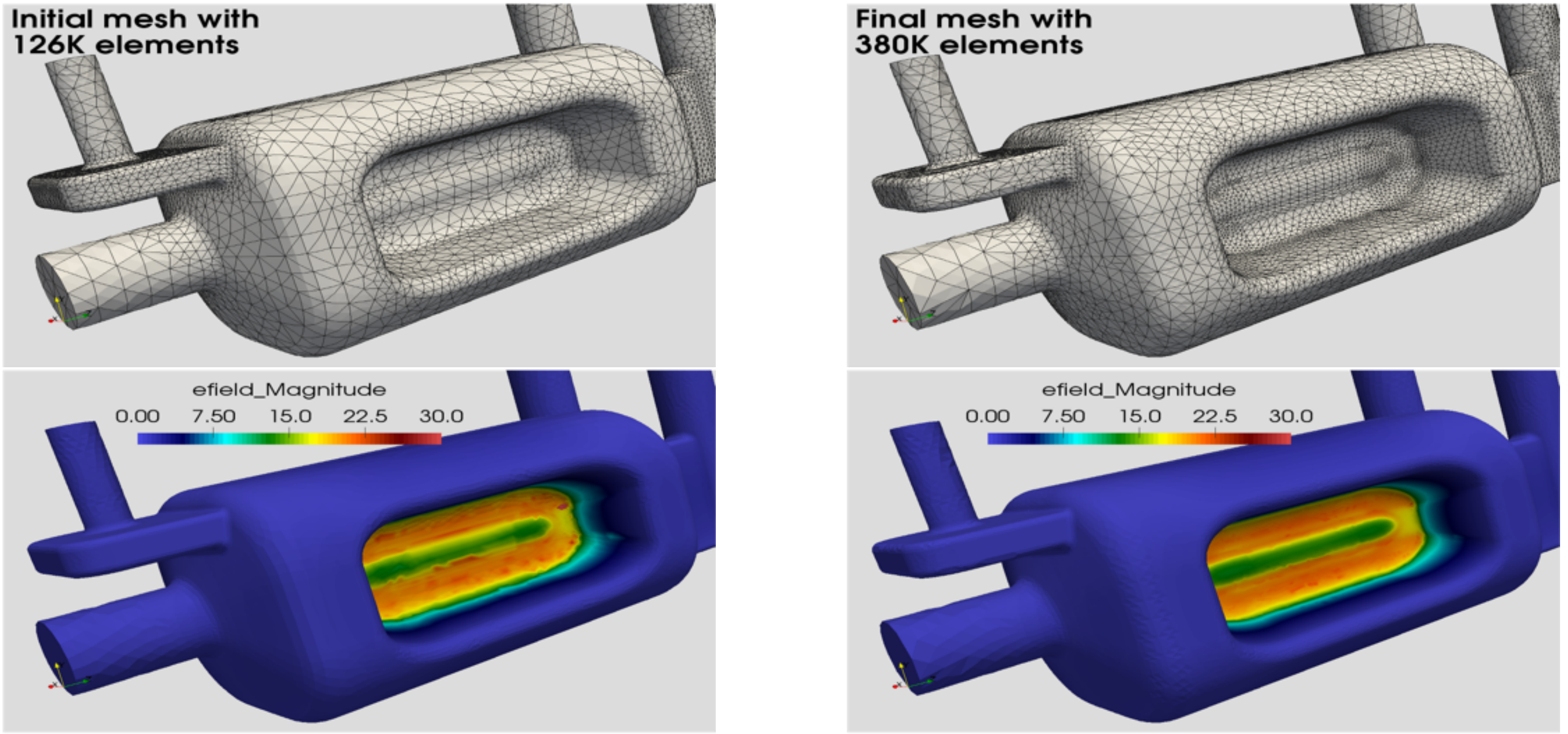

Blood flow on the arterial system



Fields in a particle accelerator

Application interactions – Accelerator EM

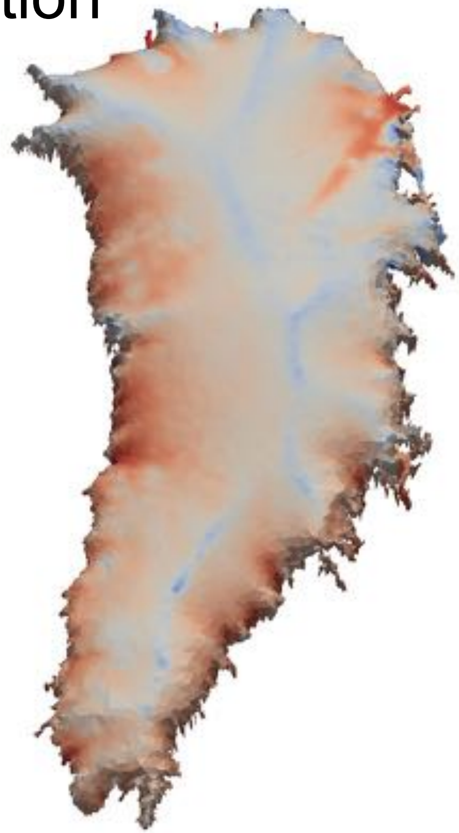
Omega3P Electro Magnetic Solver (second-order curved meshes)

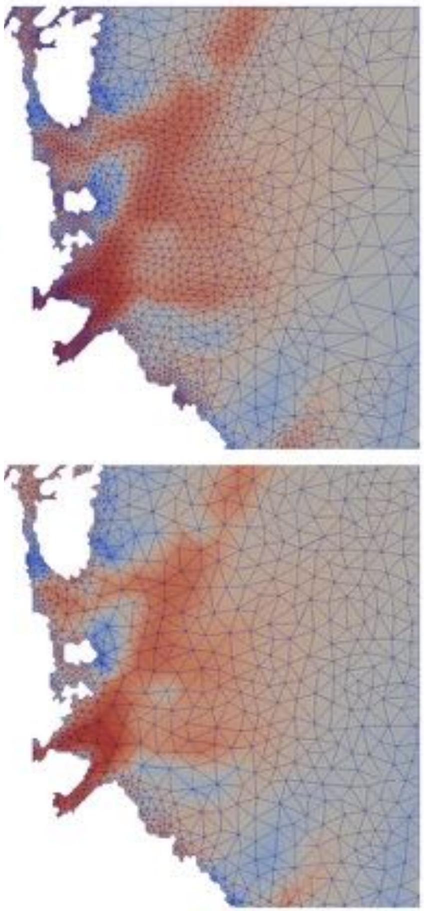


This figure shows the adaptation results for the CAV17 model. (top left) shows the initial mesh with ~126K elements, (top right) shows the final (after 3 adaptation levels) mesh with ~380K elements, (bottom left) shows the first eigenmode for the electric field on the initial mesh, and (bottom right) shows the first eigenmode of the electric field on the final (adapted) mesh.

Application interactions – Land Ice

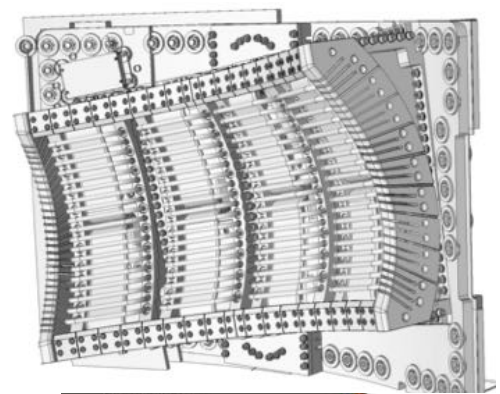
- FELIX, a component of the Albany framework is the analysis code
- Omega_h parallel mesh adaptation is integrated with Albany to do:
  - Estimate error
  - Adapt the mesh
- Ice sheet mesh is modified to minimize degrees of freedom
- Field of interest is the ice sheet velocity



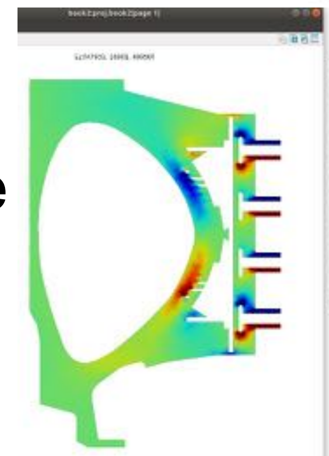


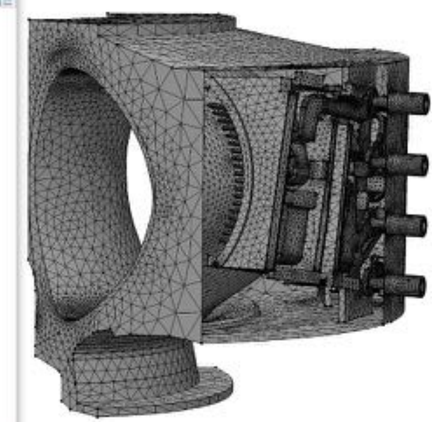
Application interactions – RF Fusion

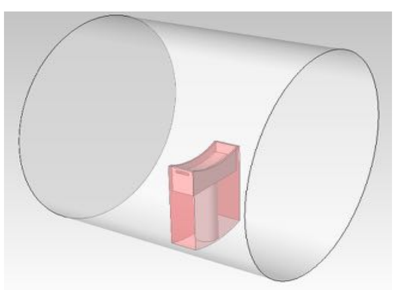
- Accurate RF simulations require
  - Detailed antenna CAD geometry
  - CAD geometry defeaturing
  - Extracted physics curves from EFIT
  - Faceted surface from coupled mesh
  - Analysis geometry combining CAD, physics geometry and faceted surface
  - 3D meshes for accurate FE calculations in MFEM
  - Projection based error estimator
  - Conforming mesh adaptation with PUMI

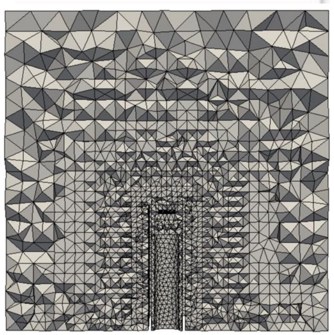


CAD model of antenna array

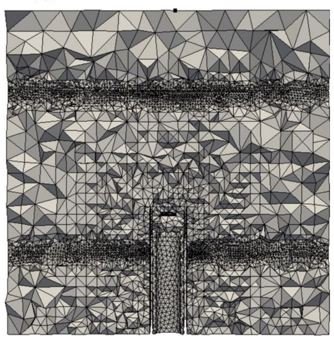








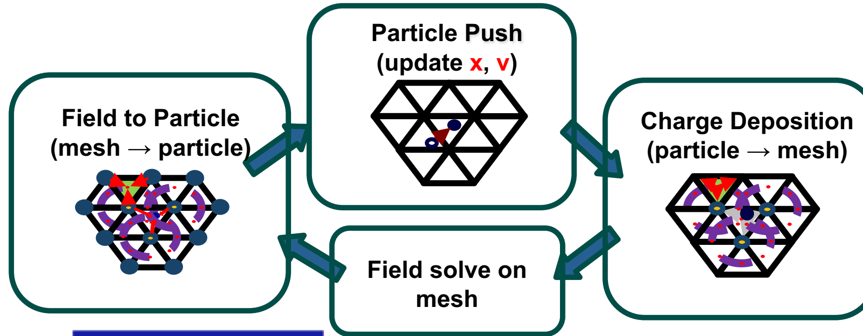
Initial Mesh

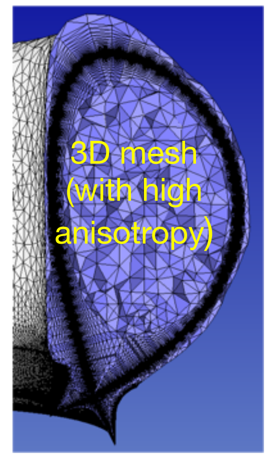


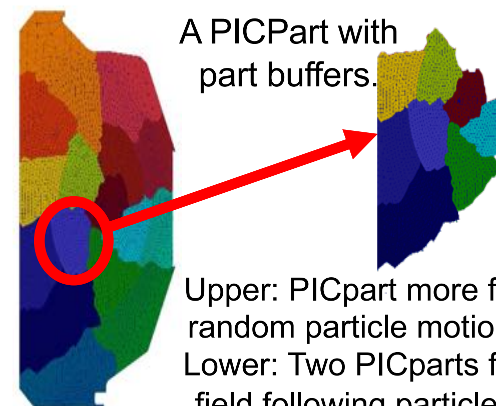
Final Adapted

Supporting Unstructured Mesh for Particle-in-Cell Calculations

PUMIPic data structures are mesh centric
- Mesh is distributed as needed by the application in terms of PICparts
- Mesh can be graded and anisotropic
- Particle data associated with elements
- Operations take advantage of distributed mesh topology
- Mesh distributed in PICparts
  - Start with a partition of mesh into a set of "core parts"
  - A PICpart is defined by a "core part" and sufficient buffer to keep particles on process for one or more pushes
  - GPU version defines buffer as set of neighboring parts – dramatic reduction in memory and communication costs

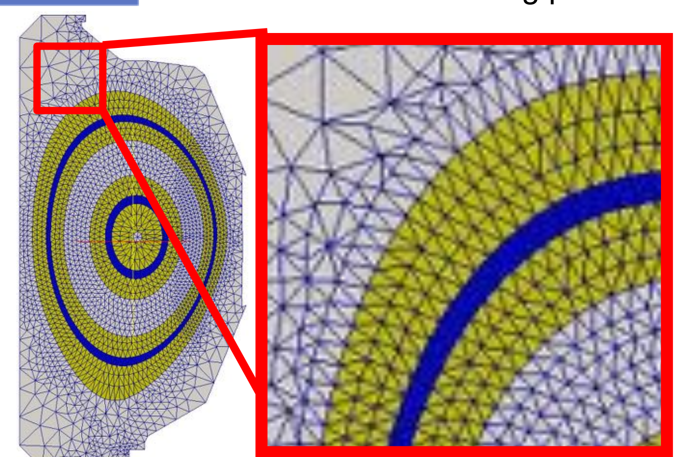






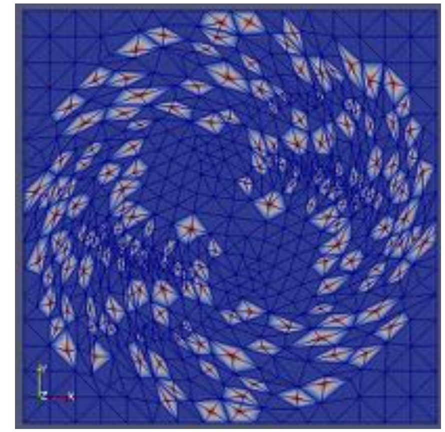
A PICPart with part buffers.

Upper: PICpart more for random particle motion.
Lower: Two PICparts for field following particles



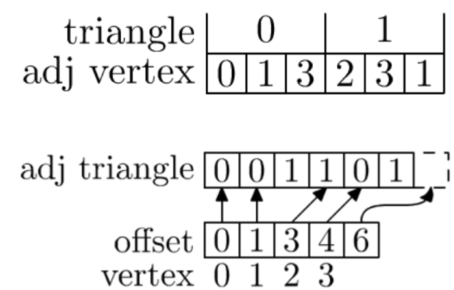
Mesh Data Structure for Heterogeneous Systems

- Mesh topology/adaptation tool - Omega
  - Conforming mesh adaptation (coarsening past initial mesh, refinement, swap)
  - Manycore and GPU parallelism using Kokkos, CUDA, or HIP
  - Distributed mesh via mesh partitions with MPI communications
  - Support for mesh-based fields

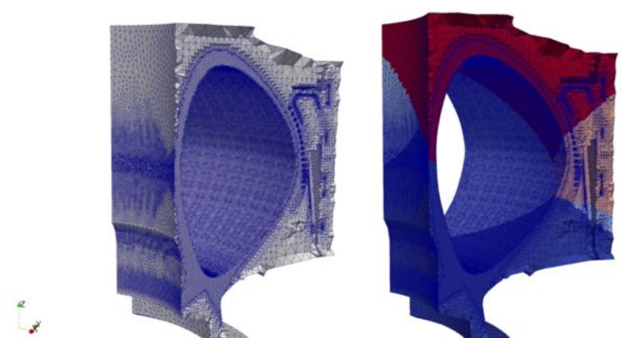


Adaptation following rotating flow field.

- Recent RPI developments:
  - Mixed mesh adjacency storage and query
  - Two-way mesh matching for periodic BC
- Ported and tested on AMD GPUs using HIP



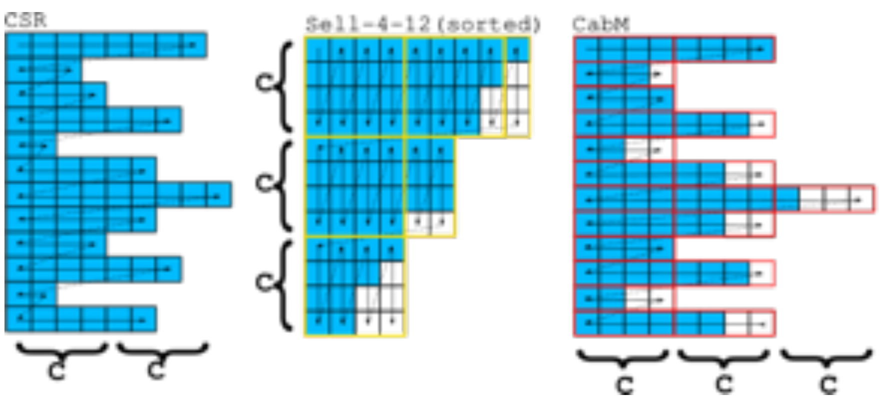
Mesh entity adjacency arrays.



Serial and RIB partitioned mesh of RF antenna and vessel model.

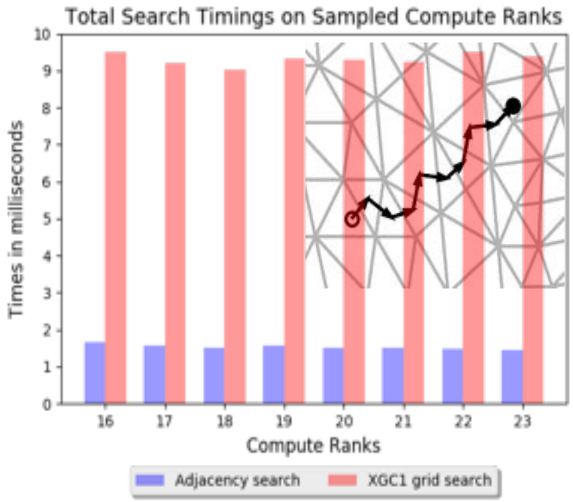
PUMIPic Particle Data Structures

- Layout of particles in memory is critical to performance. Requirements:
  - Optimizes push (sort/rebuild), scatter, and gather operations
  - Associates particles with mesh elements
  - Changes in the number of particles per element
  - Evenly distributes work with a range of particle distributions (e.g. uniform, Gaussian, exponential, etc.)
  - Stores a lot of particles per GPU – low overhead
- Particle data structure interface and implementation
  - API abstracts implementation for PIC code developers
  - CSR, Sell-C-σ, CabanaM
  - Performance is a function of particle distribution
  - Cabana AoSoA w/a CSR index of elements-to-particles are promising



Left to Right: CSR, SCS with vertical slicing (yellow boxes), CabanaM (red boxes are SOAs). C is a team of threads.

PIC Operations Supported by PUMIPic



- Particle push
- Adjacency based search
  - Faster than grid based search
- Element-to-particle association update
- Particle Migration
- Particle path visualization
- Mesh partitioning w/buffer regions
- Mesh field association
- Poisson field solve using PETSc DMPlex on GPUs
- Checkpoint/restart of particle and mesh data – supports customization for each application

2020 PUMIPic Paper: https://www.scorec.rpi.edu/REPORTS/2020-2.pdf

PUMIPic based XGCm Edge Plasma Code

XGCm is a version of XGC being built on PUMIPic

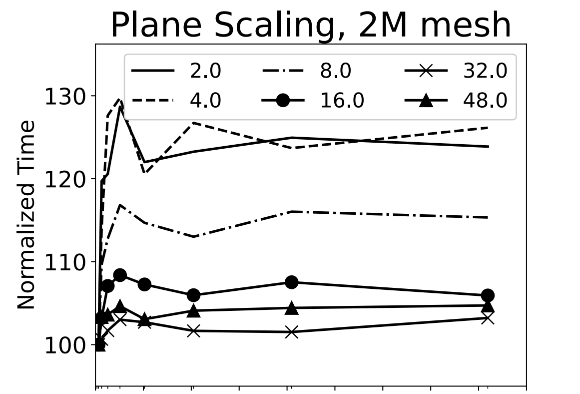
- targeting execution of all operations on GPUs

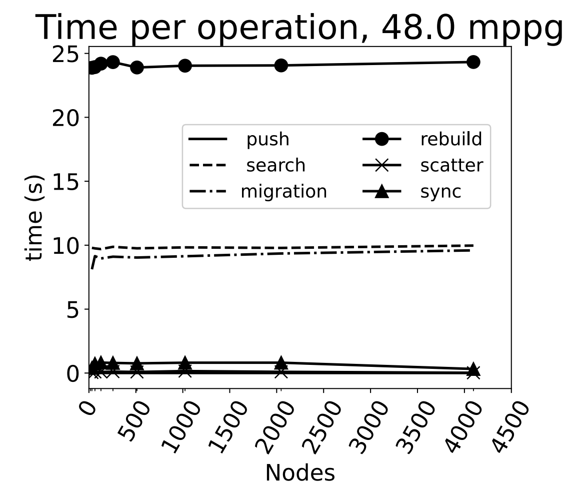
Testing of PUMIPic for use in XGC like push

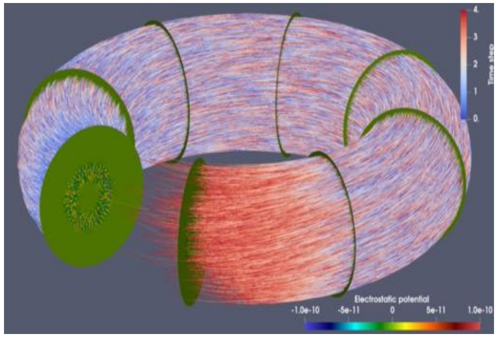
- 2M elements, 1M vertices, 2 to 128 poloidal planes
- Pseudo push and particle-to-mesh gyro scatter
- Tested on up to 24,576 GPUs of Summit with 1.1 trillion particles, for 100 iterations: push, adjacency
- Weak scaling up to 24576 GPUs (4096 nodes) with 48 million particles per GPU

XGCm status: All operations on GPU

- Ion and electron charge scatter and push
- Electrostatic potential calculation
- Gyro-kinetic electric field calculation and gather
- Poisson solve

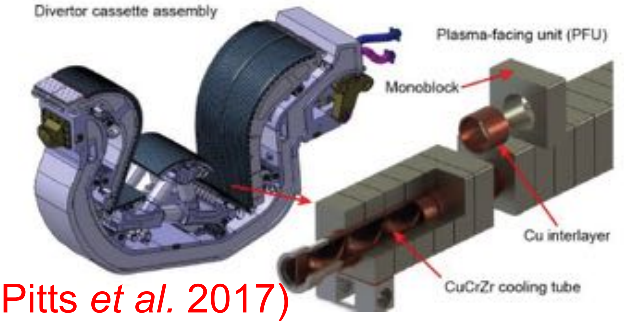




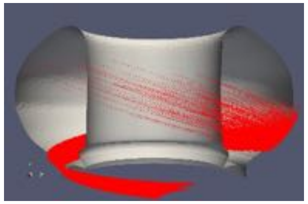


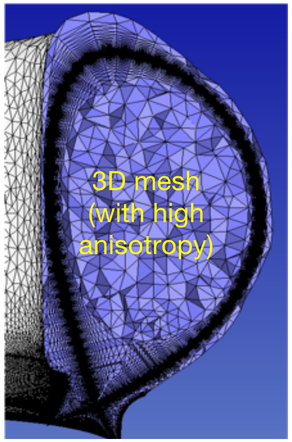
PUMIPic based GITRm Impurity Transport Code

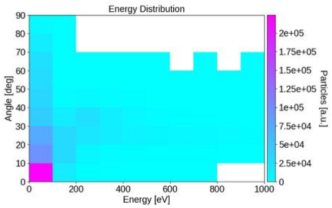
- Incorporates impurity transport capabilities of GITR
- 3D mesh for cases such including divertor cassettes, tiles, limiters, specific diagnostics/probes etc.
- Status
  - Physics equivalent to GITR
  - Particle initialization directly on 3D mesh
  - 3D mesh design/control including anisotropy to properly represent the background fields
  - Field transfer from SOLPS to 3D mesh
  - Non-uniform particle distribution – evolves quickly in time
  - Load balancing particles via EnGPar
  - Distance to boundary for sheath E field
  - Post-processing on 3D unstructured mesh

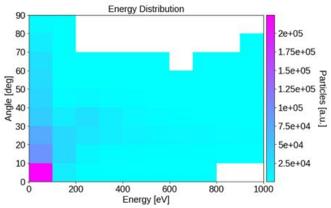


(Pitts *et al.* 2017)





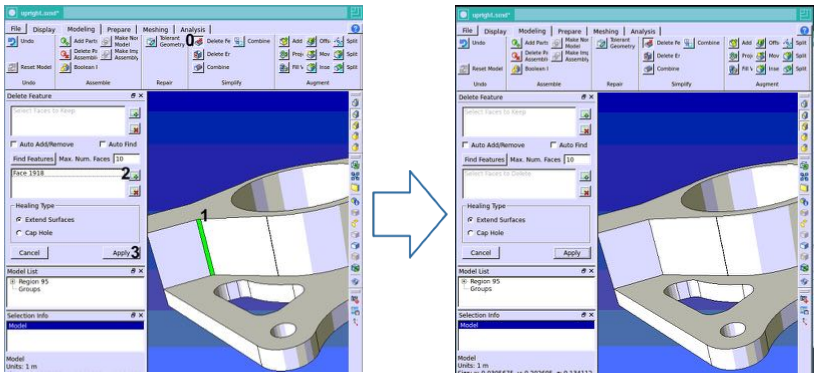




Statistical comparison for 1million particles, 100k timesteps

Hands-on Exercise

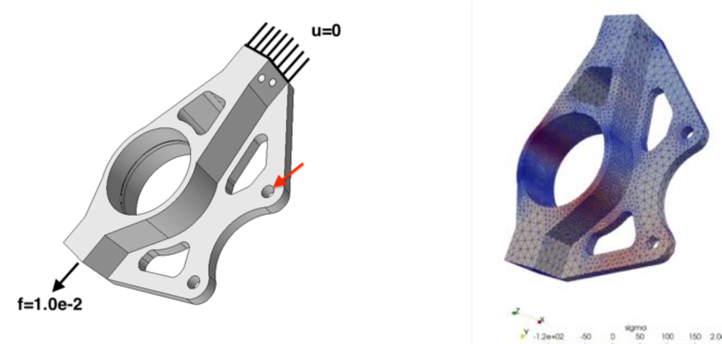
Exercising Simmetrix and PUMI tools for model preparation, mesh generation, partitioning, and adaptive MFEM analysis on a complex CAD model



Removing small model faces.

Initial mesh generation.

Mesh partitioning.



Problem definition and adaptive analysis.

https://xsdk-project.github.io/MathPackagesTraining2021/lessons/pumi/