FASTMath Unstructured Mesh Technologies

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

[1]Sandia National Laboratories
[2]Lawrence Livermore National Laboratory
[3]University of Colorado
[4]Rensselaer Polytechnic Institute

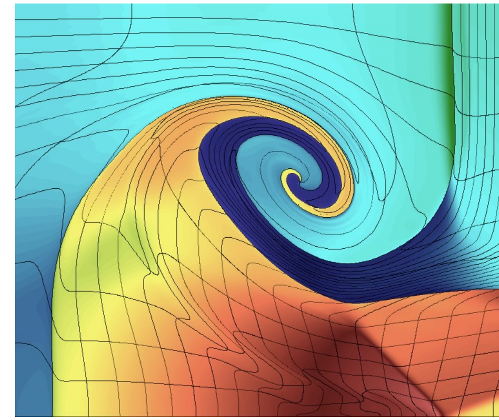
Finite elements are a good foundation for large-scale simulations on current and future architectures

- Backed by well-developed theory
- Naturally support unstructured and curvilinear grids.
- ***Finite elements naturally connect different physics***

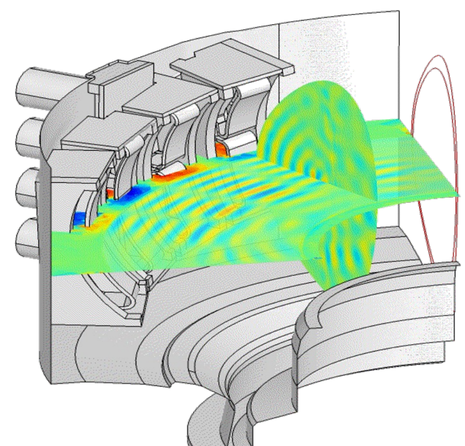
$$H(grad) \xrightarrow{\nabla} H(curl) \xrightarrow{\nabla\times} H(div) \xrightarrow{\nabla\cdot} L_2$$

$H(grad)$	$H(curl)$	$H(div)$	L_2
"nodes"	"edges"	"faces"	"elems"
High-order kinematics	High-order MHD	High-order rad. diffusion	High-order thermodynamics

- ***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
  - HPC utilization, FLOPs/bytes increase with the order
- ***Need new (interesting!) R&D for full benefits***
  - meshing, discretizations, solvers, AMR, UQ, visualization, …



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



Core-Edge tokamak EM wave propagation

FASTMATH

Modular Finite Element Methods (MFEM)

Flexible discretizations on unstructured grids

- Triangular, quadrilateral, tetrahedral, hexahedral, prism; volume, surface and topologically periodic meshes
- Bilinear/linear forms for: Galerkin methods, DG, HDG, DPG, IGA, …
- Local conforming and non-conforming AMR, mesh optimization
- Hybridization and static condensation

High-order methods and scalability

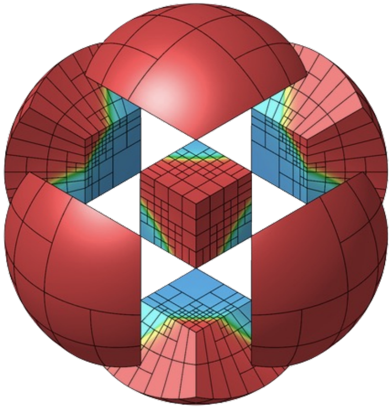
- Arbitrary-order H1, H(curl), H(div)- and L2 elements
- Arbitrary order curvilinear meshes
- MPI scalable to millions of cores + GPU accelerated
- Enables development from laptops to exascale machines.

Solvers and preconditioners

- Integrated with: HYPRE, SUNDIALS, PETSc, SLEPc, SUPERLU, VisIt, …
- AMG solvers for full de Rham complex on CPU+GPU, geometric MG
- Time integrators: SUNDIALS, PETSc, built-in RK, SDIRK, ...

Open-source software

- Open-source (GitHub) with 114 *contributors*, 50 *clones/day*
- Part of FASTMath, ECP/CEED, xSDK, OpenHPC, E4S, …
- 75+ example codes & miniapps: mfem.org/examples



mfem.org
(v4.7, May 2024)

Example 1 – Laplace equation

- Mesh

```
// 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

```
// 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

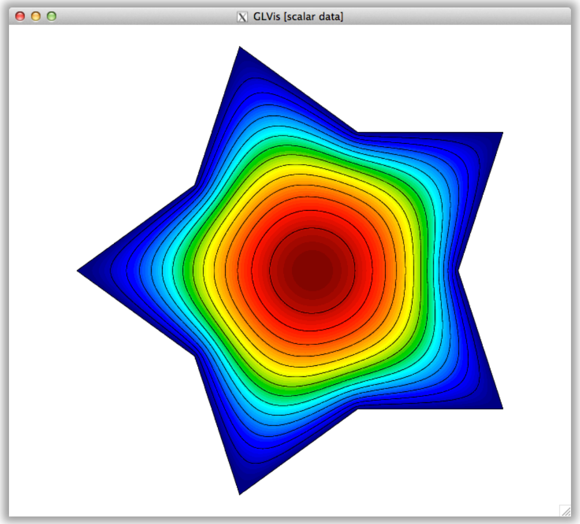
```
// 5. Set up the linear form b(.) which corresponds to the right-hand side of
//    the FEM linear system, which in this case is (1,phi_i) where phi_i are
//    the basis functions in the finite element fespace.
LinearForm *b = new LinearForm(fespace);
ConstantCoefficient one(1.0);
b->AddDomainIntegrator(new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

```
#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

```
   // 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

Example 1 – Laplace equation

- Mesh

```
// 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();
}
```

Example 1 – Laplace equation

- Finite element space

```
// 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;
```

Example 1 – Laplace equation

- Initial guess, linear/bilinear forms

```
   // 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();
```

Example 1 – Laplace equation

- Linear solve

```
#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
```

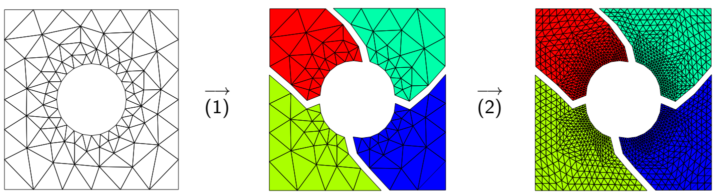
- Visualization

```
   // 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;
   }
```

Example 1 – parallel Laplace equation

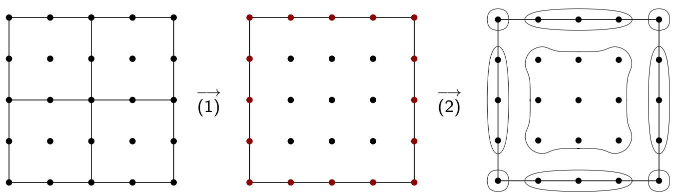
- Parallel mesh

```
// 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();
```

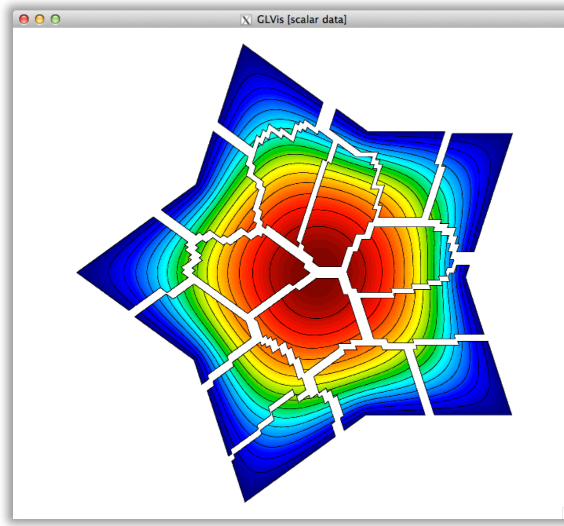
$$A = P^T a P \qquad B = P^T b \qquad x = PX$$

- 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

Example 1 – parallel Laplace equation

```
// 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();
}
```

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

```
ParLinearForm *b = new ParLinearForm(fespace);
```

```
ParGridFunction x(fespace);
```

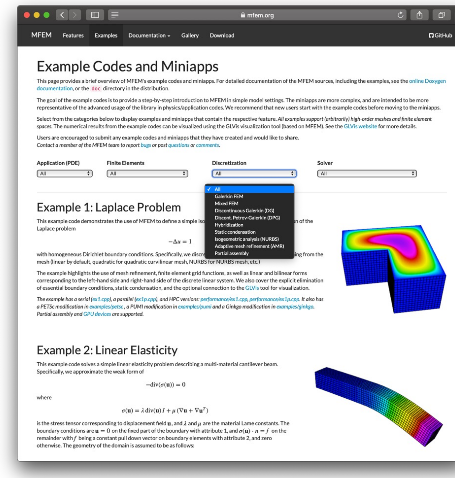
```
ParBilinearForm *a = new ParBilinearForm(fespace);
```

```
// 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();
```

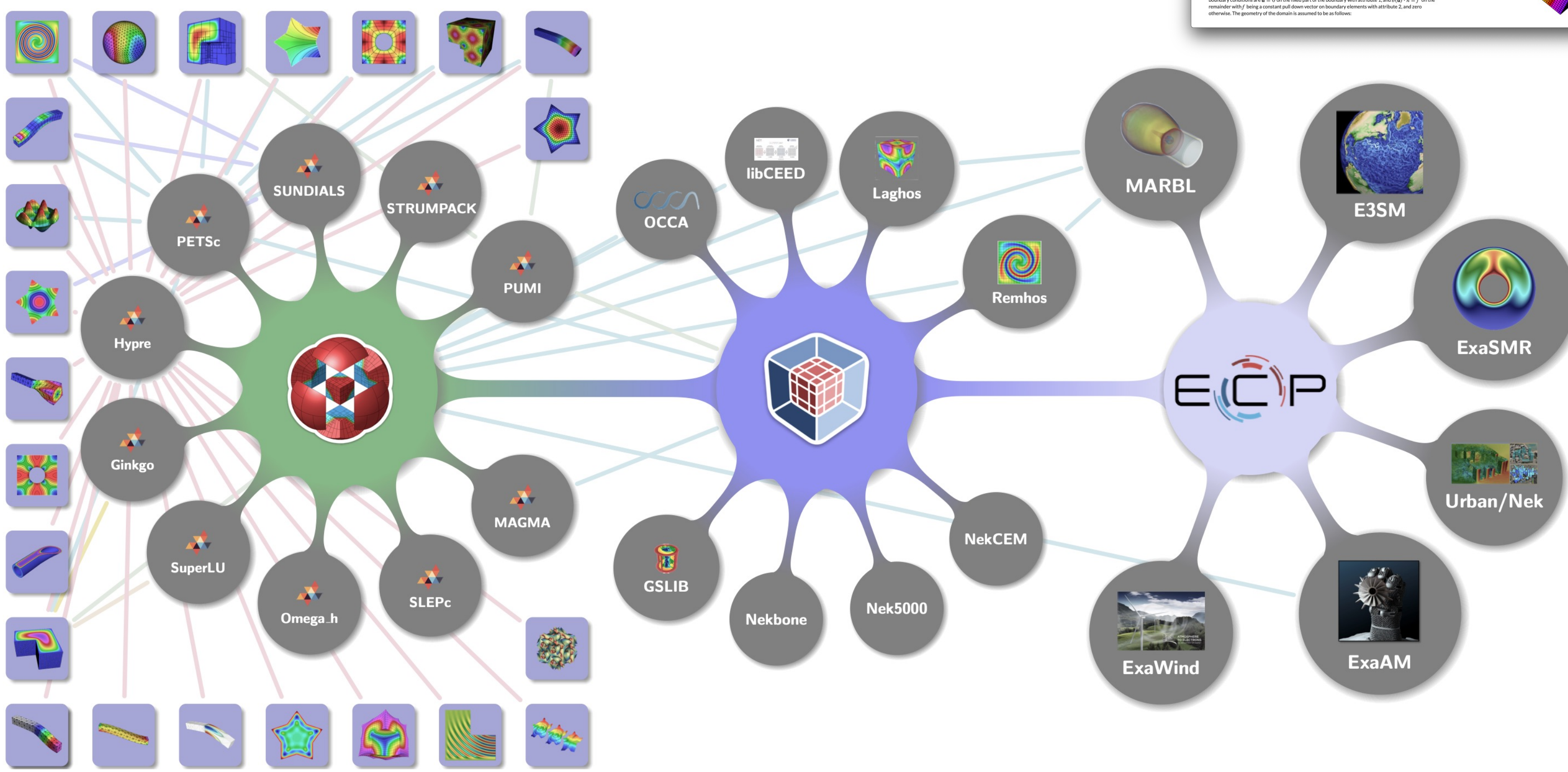
```
// 11. Define and apply a parallel PCG solver for AX=B with the BoomerAMG
//     preconditioner from hypre.
HypreSolver *amg = new HypreBoomerAMG(*A);
HyprePCG *pcg = new HyprePCG(*A);
pcg->SetTol(1e-12);
pcg->SetMaxIter(200);
pcg->SetPrintLevel(2);
pcg->SetPreconditioner(*amg);
pcg->Mult(*B, *X);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

```
   sol_sock << "parallel " << num_procs << " " << myid << "\n";
   sol_sock.precision(8);
   sol_sock << "solution\n" << *pmesh << x << flush;
```

MFEM example codes: mfem.org/examples



- 40+ example codes, most with both serial + parallel versions
- Tutorials to learn MFEM features
- Starting point for new applications
- Show integration with many external packages
- Miniapps: more advanced, ready-to-use physics solvers



Demo

https://xsdk-project.github.io/MathPackagesTraining2024/lessons/mfem_convergence/

Convergence Study Source Code

The `mfem_convergence/` directory contains the `convergence.cpp` source code for solving the Poisson problem using a variety of grids and orders. You can also view the code online on **GitHub**.

To define the system we need to solve, we need three things. First, we need to define our basis functions which live on the computational mesh.

```
// order is the FEM basis functions polynomial order
FiniteElementCollection *fec = new H1_FECollection(order, dim);

// pmesh is the parallel computational mesh
ParFiniteElementSpace *fespace = new ParFiniteElementSpace(pmesh, fec);
```

This defines a collection of H1 functions (meaning they have well-defined gradient) of a given polynomial order on a parallel computational mesh `pmesh`. Next, we need to define the integrals in Equation (5)

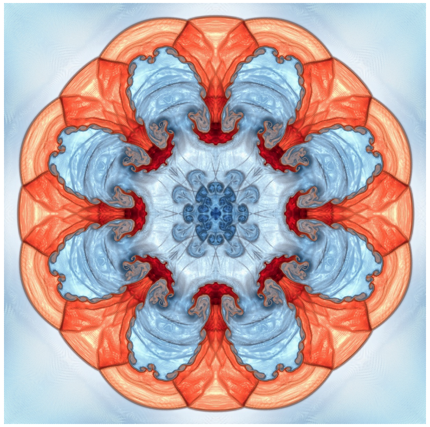
```
ParBilinearForm *a = new ParBilinearForm(fespace);
ConstantCoefficient one(1.0);
a->AddDomainIntegrator(new DiffusionIntegrator(one));
a->Assemble();
```

and Equation (6)

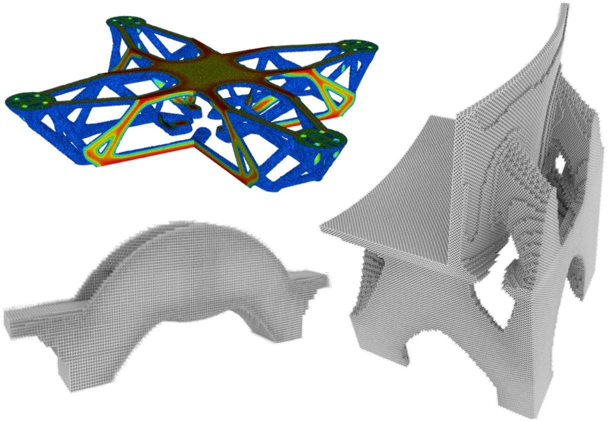
```
// f_exact is a C function defining the source
FunctionCoefficient f(f_exact);
ParLinearForm *b = new ParLinearForm(fespace);
b->AddDomainIntegrator(new DomainLFIntegrator(f));
b->Assemble();
```

This defines the matrix A and the vector b. We then solve the linear system for our solution vector x using **AMG-preconditioned** PCG iteration.

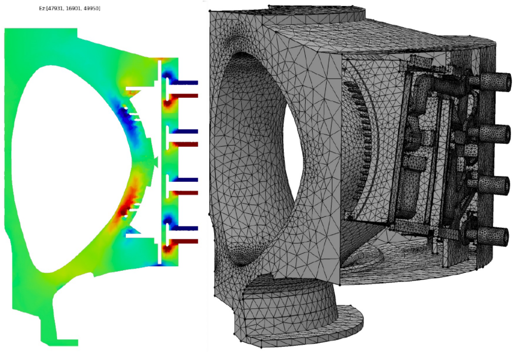
Some large-scale simulation codes powered by MFEM



Inertial confinement
fusion (BLAST)

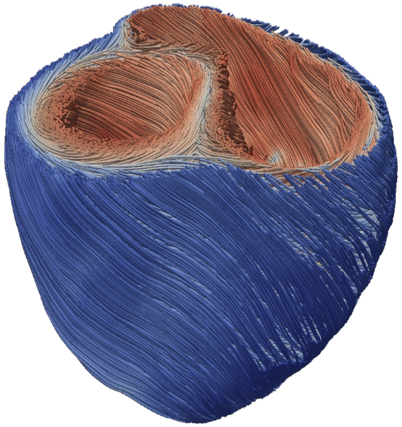


Topology optimization for
additive manufacturing (LiDO)

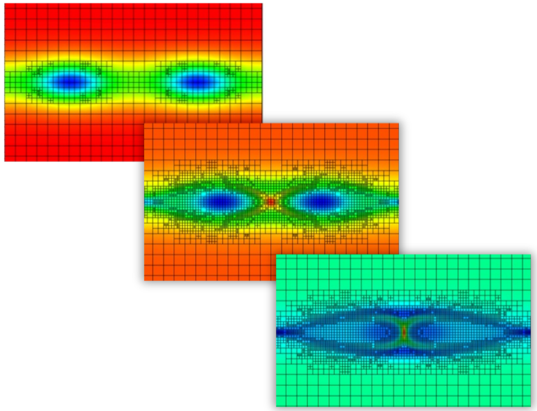


Core-edge tokamak EM
wave propagation (SciDAC, RPI)

MRI modeling (Harvard Medical)



Heart modeling (Cardioid)



Adaptive MHD island
coalescence (SciDAC, LANL)

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

Lagrange phase

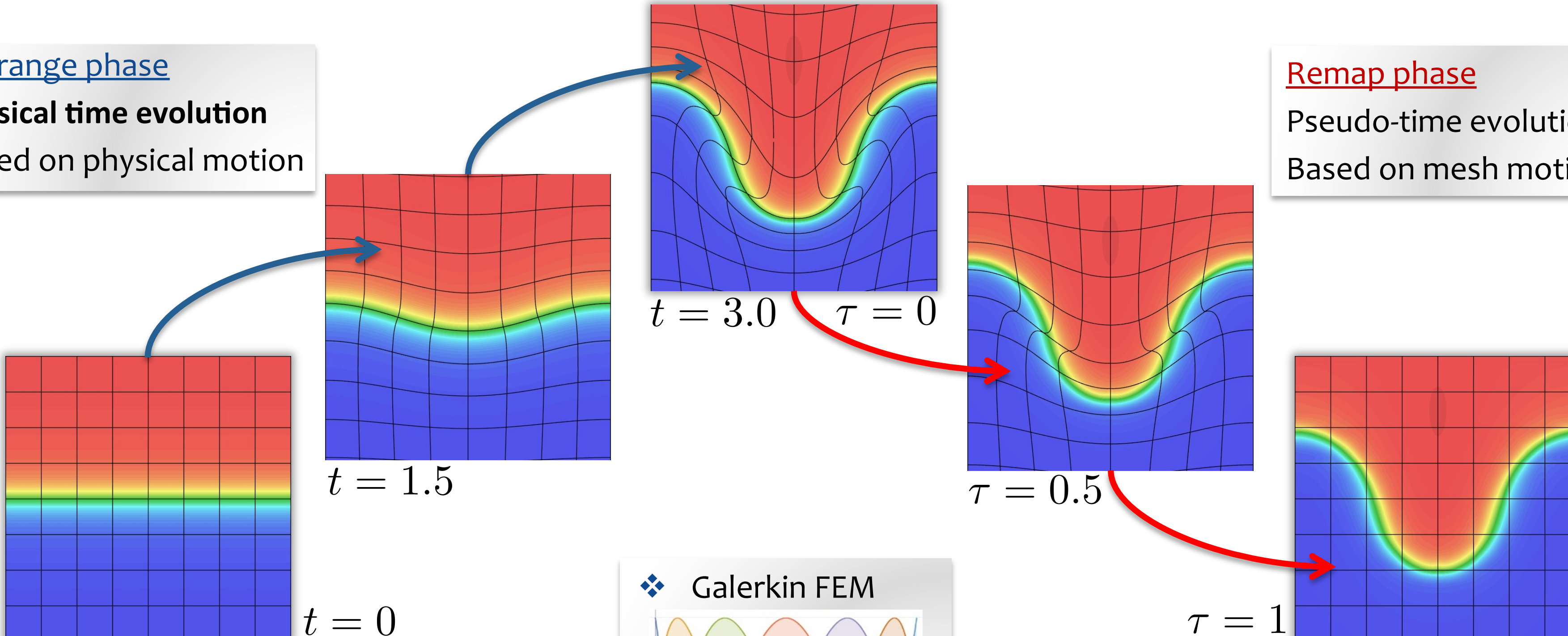
Physical time evolution

Based on physical motion

Remap phase

Pseudo-time evolution

Based on mesh motion



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

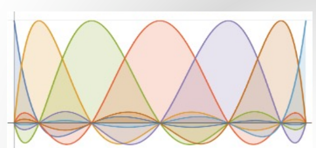
Momentum Conservation: $\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \nabla \cdot \sigma$

Mass Conservation: $\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \vec{v}$

Energy Conservation: $\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \sigma : \nabla \vec{v}$

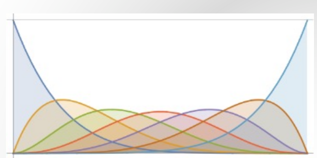
Equation of Motion: $\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$

- Galerkin FEM



Gauss-Lobatto basis

- Discont. Galerkin



Bernstein basis

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

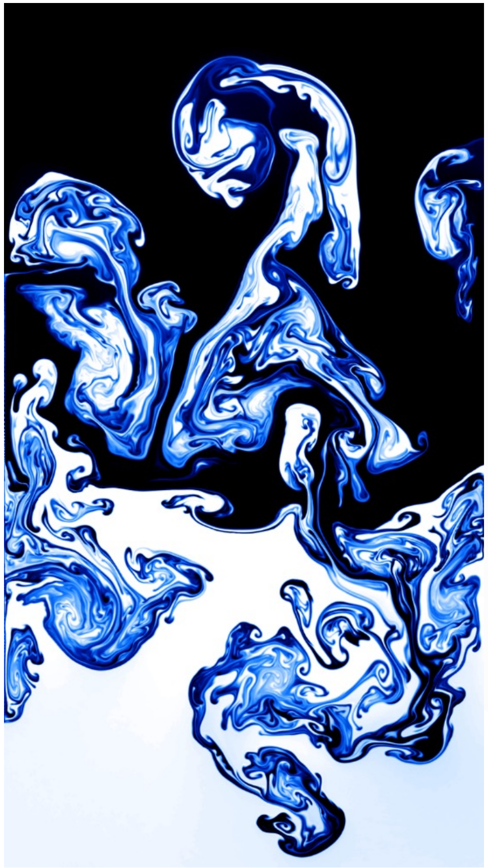
Momentum Conservation: $\frac{\mathrm{d}(\rho\vec{v})}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho\vec{v})$

Mass Conservation: $\frac{\mathrm{d}\rho}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla \rho$

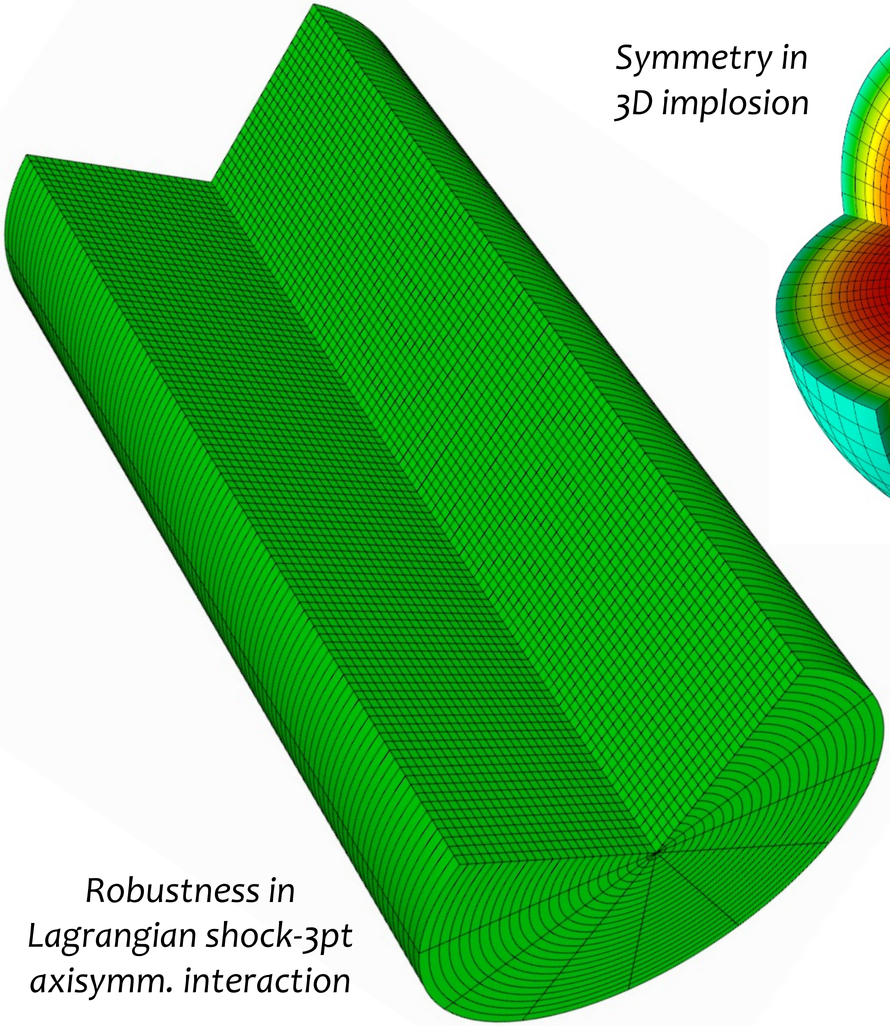
Energy Conservation: $\frac{\mathrm{d}(\rho e)}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho e)$

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

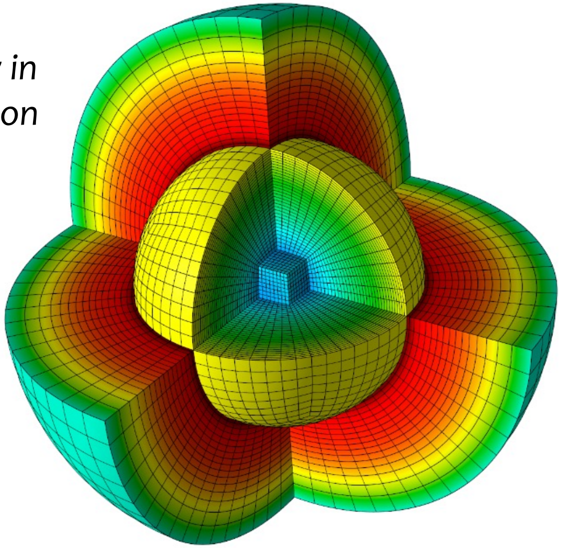


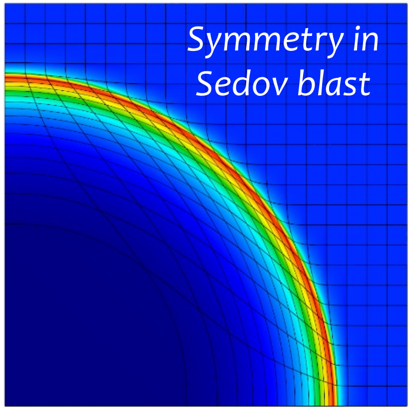
Parallel ALE for Q4 Rayleigh-Taylor instability (256 cores)



Robustness in Lagrangian shock-3pt axisymm. interaction

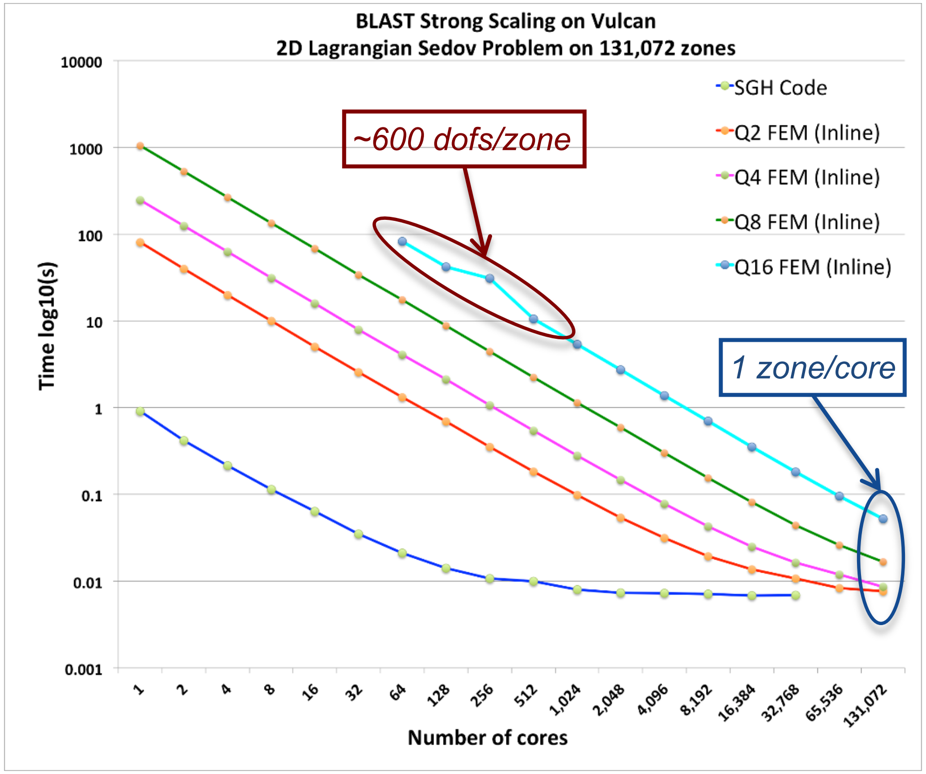
Symmetry in 3D implosion





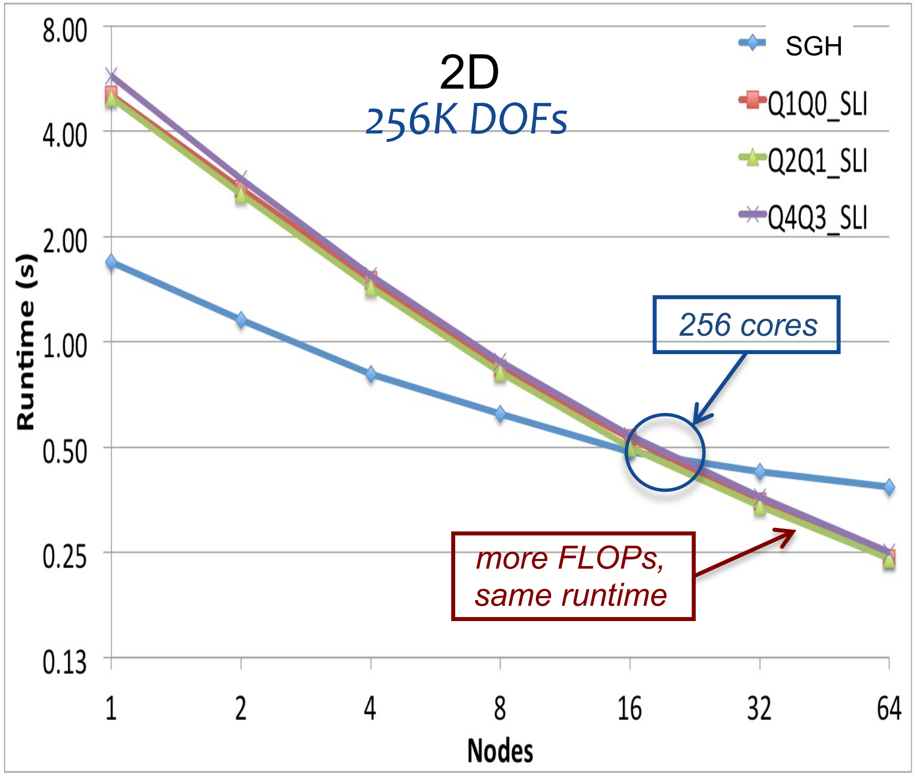
High-order finite elements have excellent strong scalability

Strong scaling, p-refinement



Finite element partial assembly

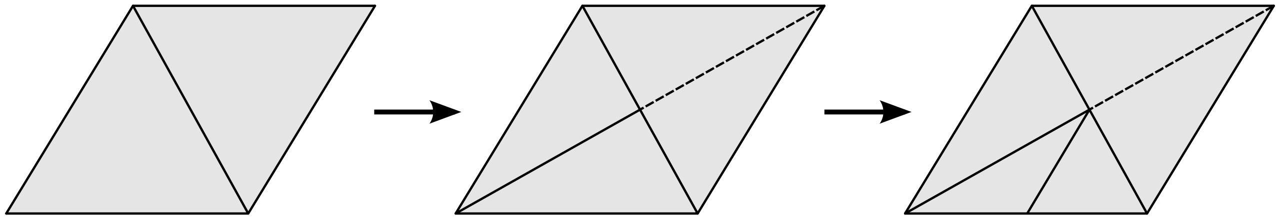
Strong scaling, fixed #dofs



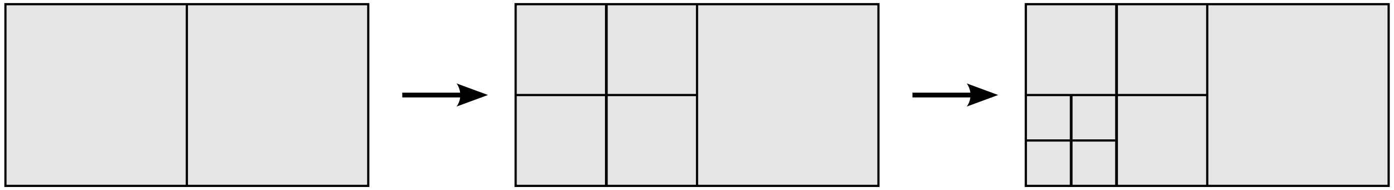
FLOPs increase faster than runtime

Conforming & Nonconforming Mesh Refinement

- Conforming refinement



- Nonconforming refinement



  - Natural for quadrilaterals and hexahedra

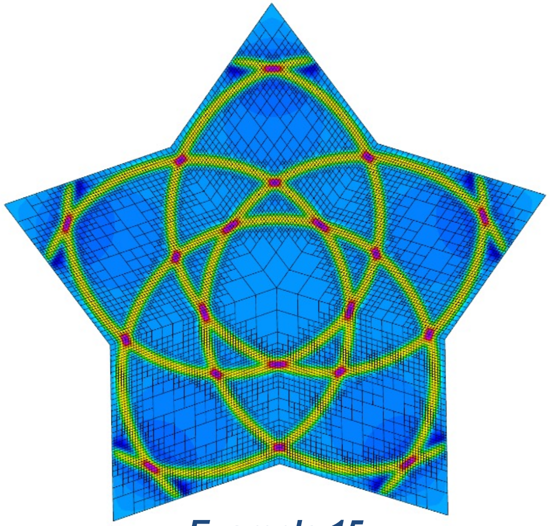
MFEM's unstructured AMR infrastructure

Adaptive mesh refinement on library level:

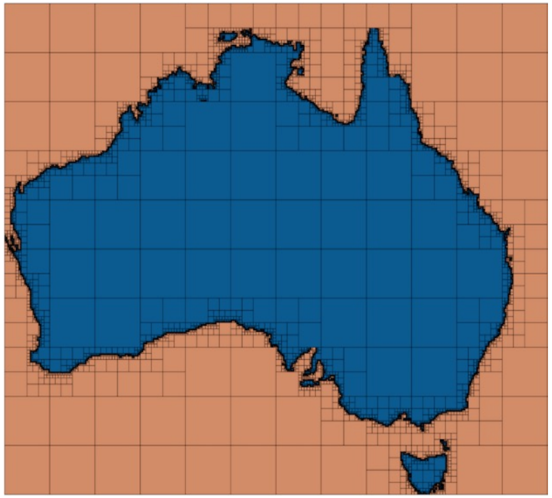
- Conforming local refinement on simplex meshes
- ***Non-conforming refinement for quad/hex meshes***
- h-refinement with fixed p

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)



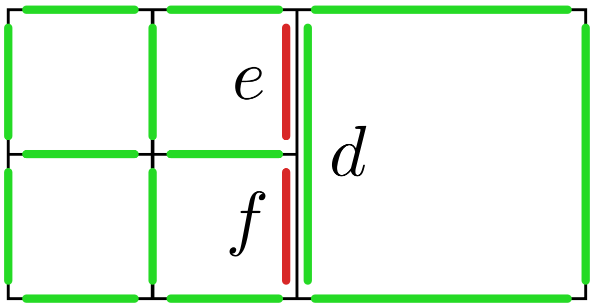
Example 15



Shaper miniapp

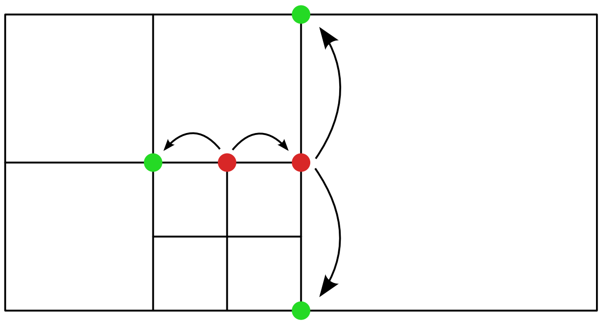
General nonconforming constraints

H(curl) elements



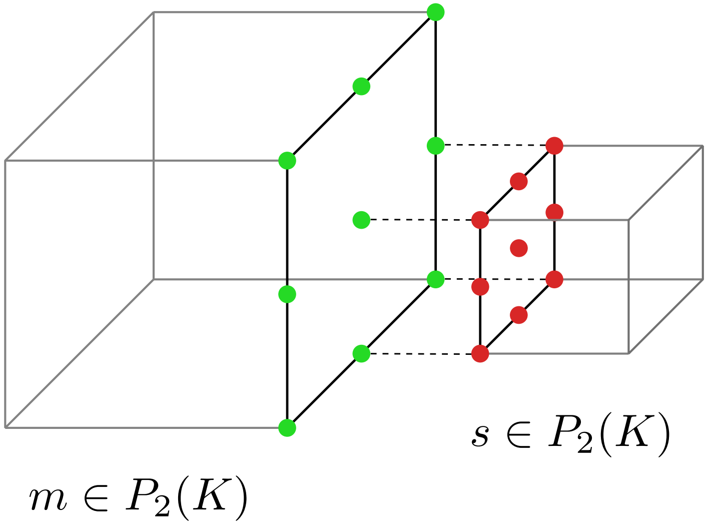
Constraint: $e = f = d/2$

Indirect constraints



More complicated in 3D…

High-order elements



Constraint: local interpolation matrix

$$s = Q \cdot m, \quad Q \in \mathbb{R}^{9\times 9}$$

Nonconforming variational restriction

- General constraint:

$$y = Px, \quad P = \begin{bmatrix} I \\ W \end{bmatrix}.$$

x – conforming space DOFs,
y – nonconforming space DOFs (unconstrained + slave),

$$\dim(x) \leq \dim(y)$$

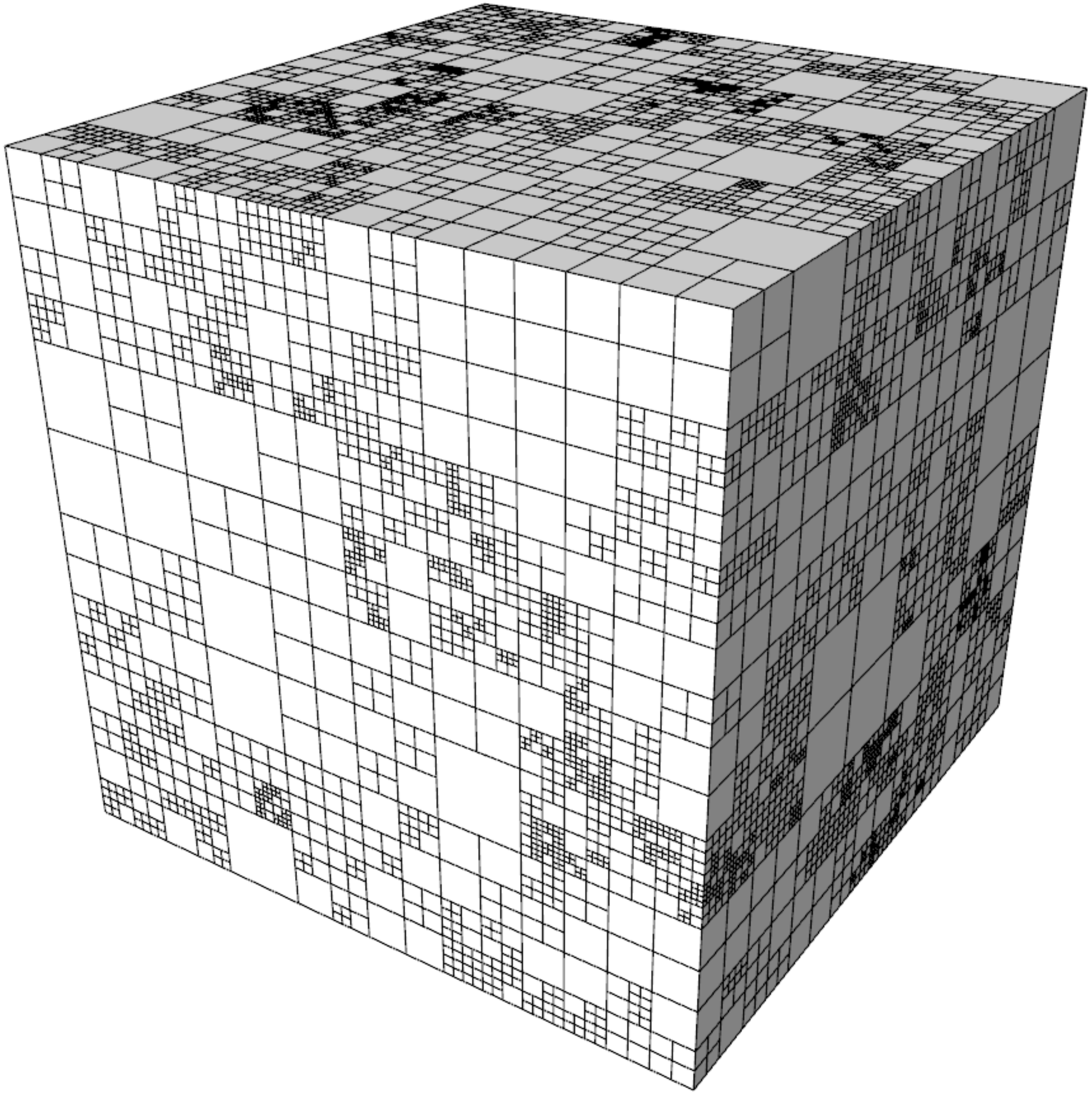
W – interpolation for slave DOFs

- Constrained problem:

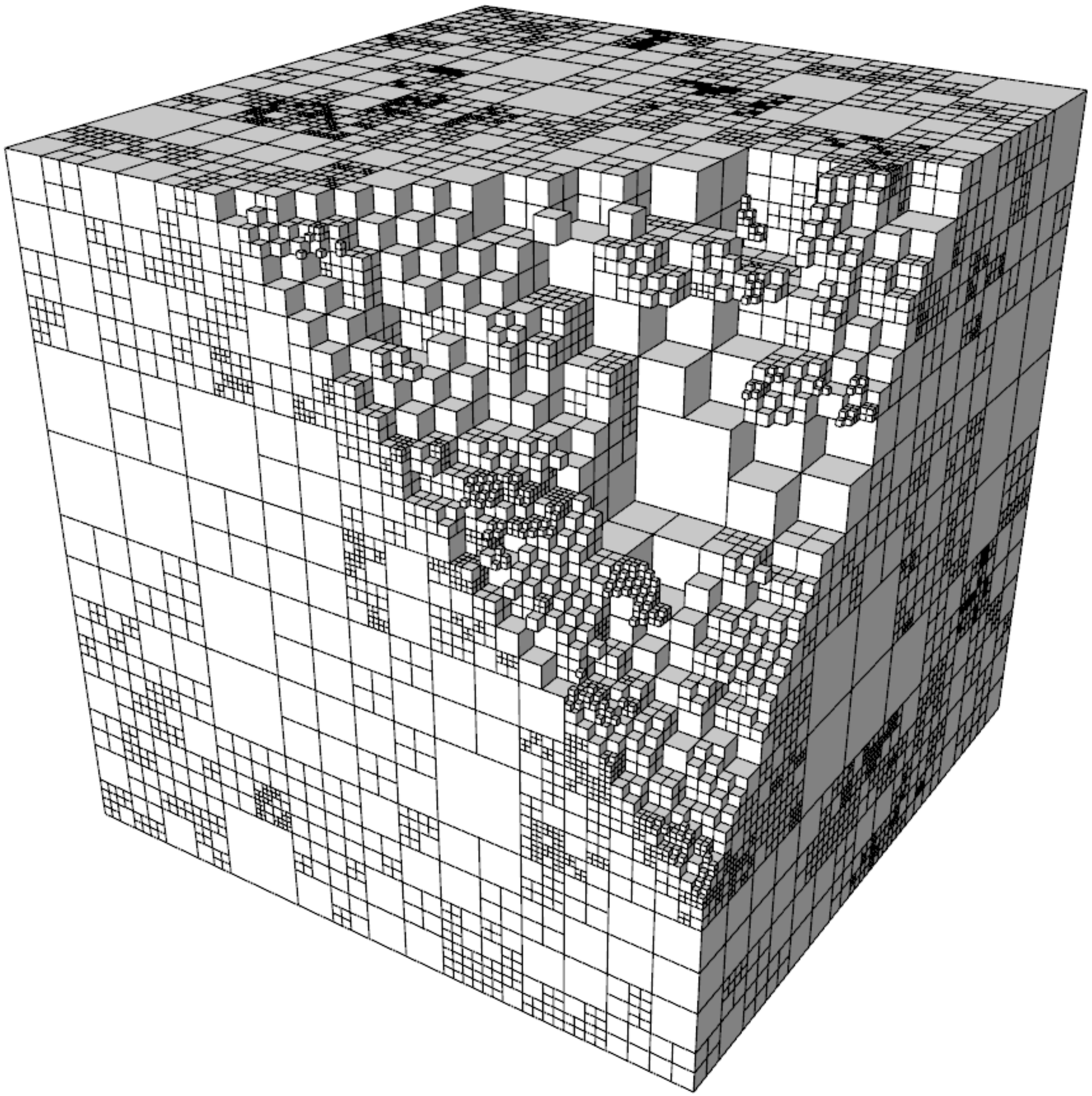
$$P^T A P x = P^T b,$$

$$y = Px.$$

Nonconforming variational restriction

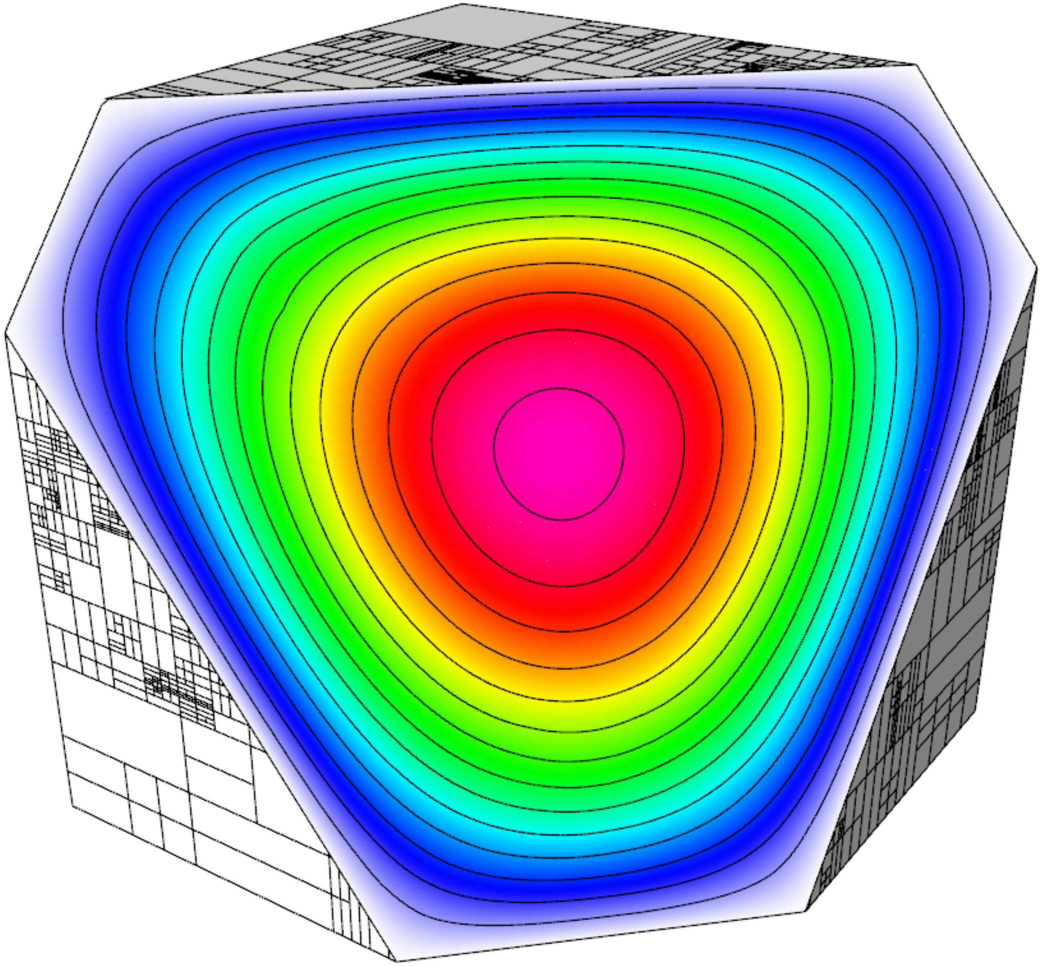


Nonconforming variational restriction



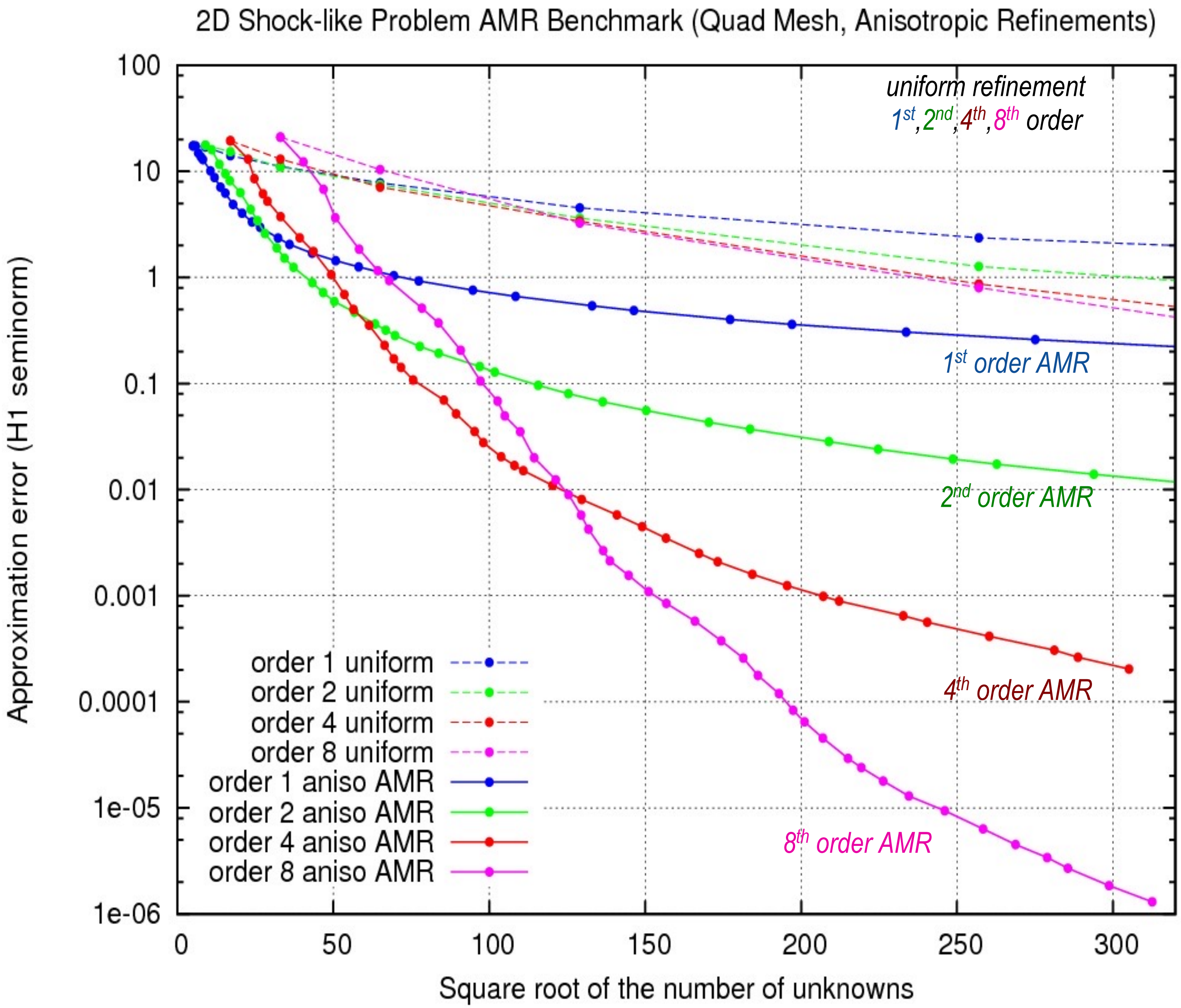
Regular assembly of A on the elements of the (cut) mesh

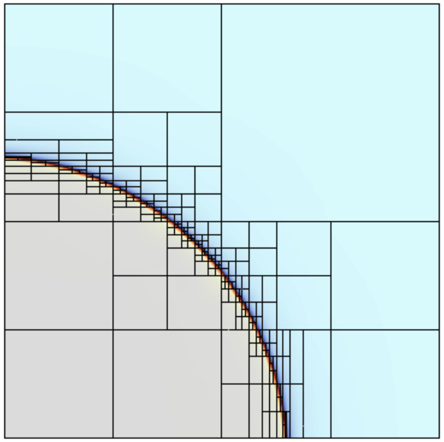
Nonconforming variational restriction

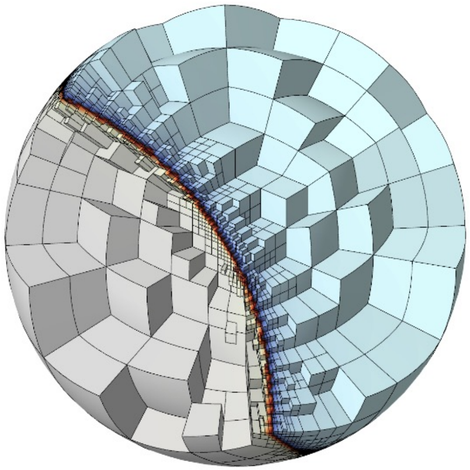


Conforming solution $y = P\,x$

AMR = smaller error for same number of unknowns

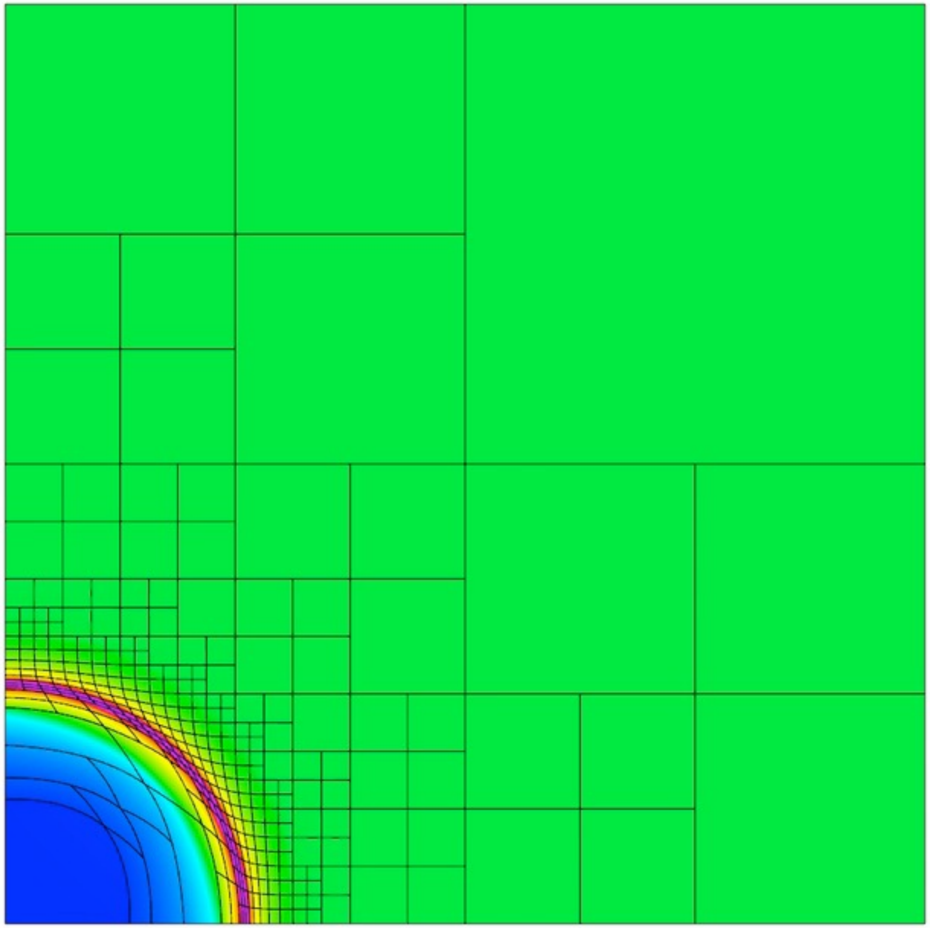




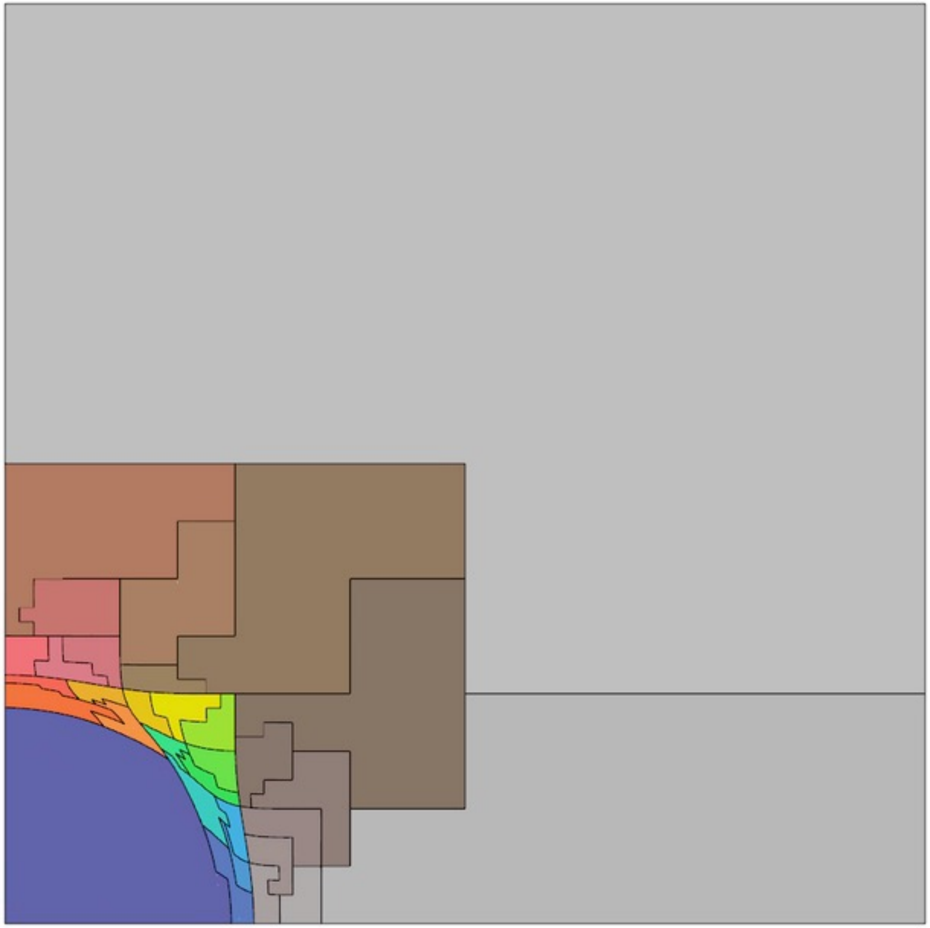


Anisotropic adaptation to shock-like fields in 2D & 3D

Parallel dynamic AMR, Lagrangian Sedov problem

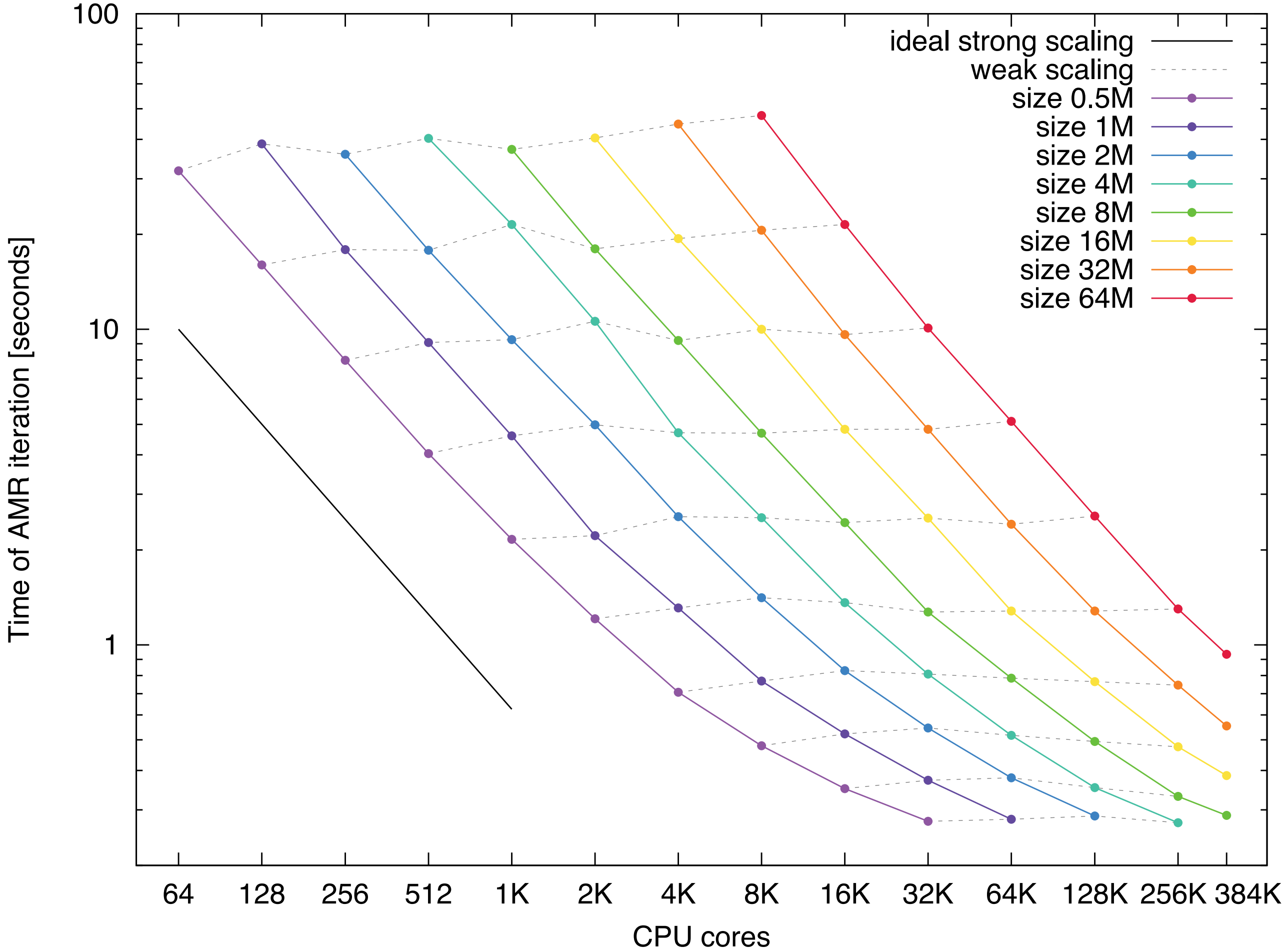


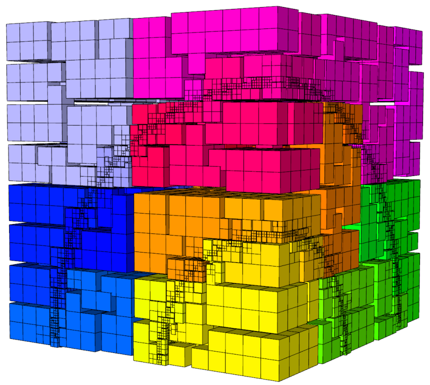
Adaptive, viscosity-based refinement and derefinement. 2nd order Lagrangian Sedov



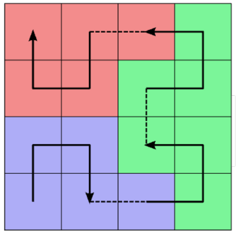
Parallel load balancing based on space-filling curve partitioning, 16 cores

Parallel AMR scaling to ~400K MPI tasks





Parallel decomposition (2048 domains shown)



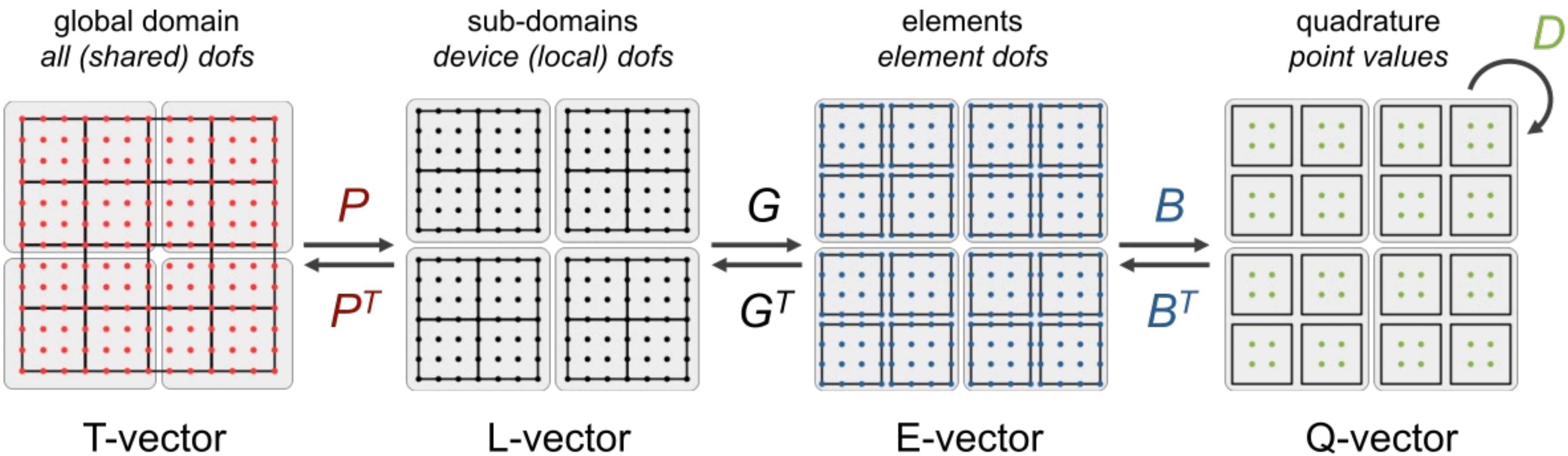
Parallel partitioning via Hilbert curve

- 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")

Fundamental finite element operator decomposition

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

$$A = P^T G^T B^T D B G P$$



- ✓ ***partial assembly*** = store only D, evaluate B (tensor-product structure)
- ✓ better representation than A: *optimal memory, near-optimal FLOPs*
- ✓ purely algebraic ✓ high-order *operator format* ✓ AD-friendly

* ***libCEED***, `github.com/ceed/libceed`

Example of a fast high-order operator

***Poisson problem** in variational form*

$$Find\ u \in Q_p \subset \mathcal{H}_0^1\ s.t.\ \forall v \in Q_p,$$

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f v$$

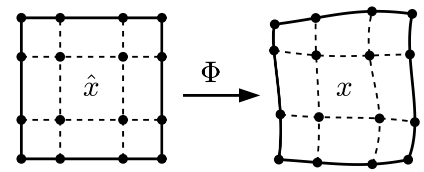
***Stiffness matrix** (unit coefficient)*

$$\underbrace{\int_\Omega \nabla\varphi_i \nabla\varphi_j}_{A_{ij}} = \sum_E \int_E \nabla\varphi_i \nabla\varphi_j$$

$$= \sum_E \sum_k \alpha_k\, J_E^{-1}(q_k)\hat{\nabla}\hat{\varphi}_i(q_k)\, J_E^{-1}(q_k)\hat{\nabla}\hat{\varphi}_j(q_k)\,|J_E(q_k)|$$

$$= \underbrace{\sum_E}_{G,G^T} \sum_k \underbrace{\hat{\nabla}\hat{\varphi}_i(q_k)}_{(B^T)_{ik}} \underbrace{\left(\alpha_k J_E^{-T}(q_k) J_E^{-1}(q_k) |J_E(q_k)|\right)}_{D_{kk}} \underbrace{\hat{\nabla}\hat{\varphi}_j(q_k)}_{B_{kj}}$$

- *J* is the Jacobian of the element mapping (geometric factors)

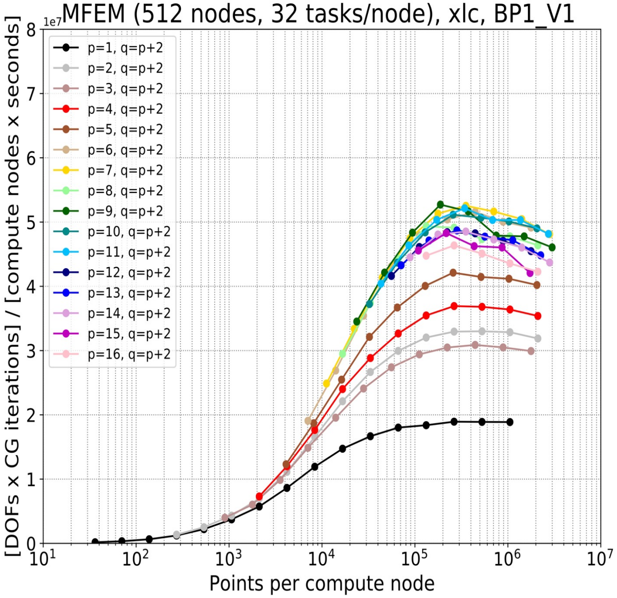


- *G* is usually Boolean (except AMR)
- Element matrices $A_E = B^T D B$, are full, account for bulk of the physics, can be applied in parallel

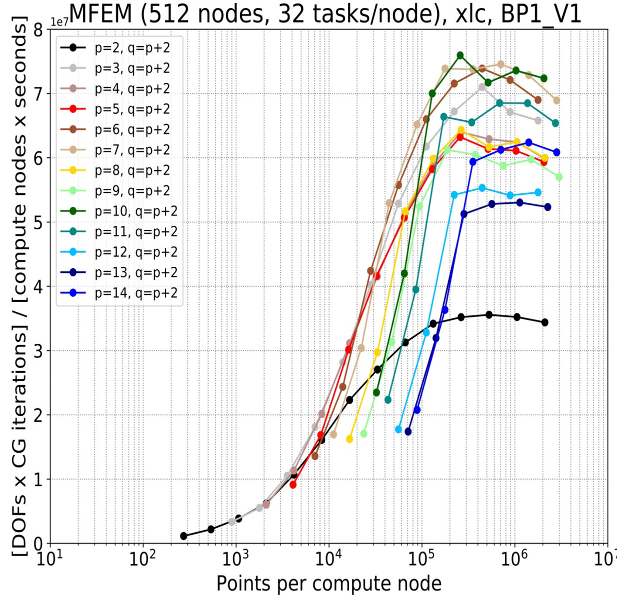
$$\begin{bmatrix} A^1 & & & \\ & A^2 & & \\ & & \ddots & \\ & & & A^4 \end{bmatrix}$$

- Never form A_E, just apply its action based on actions of B, B^T and D

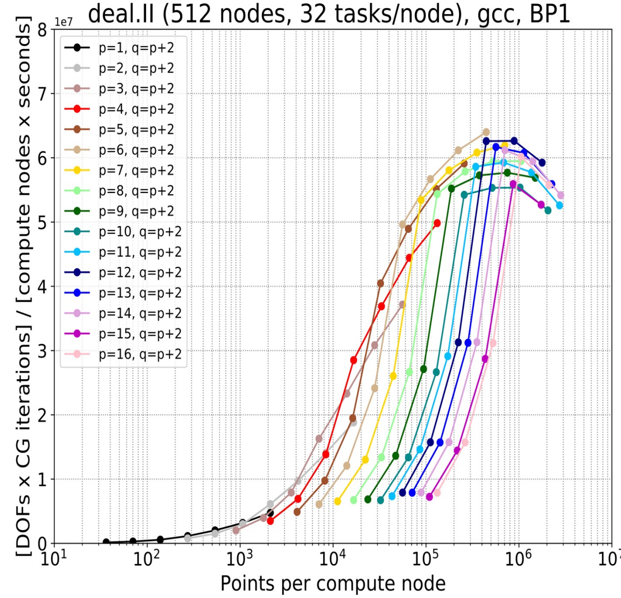
CEED BP1 bakeoff on BG/Q



Nek5000



MFEM-improved

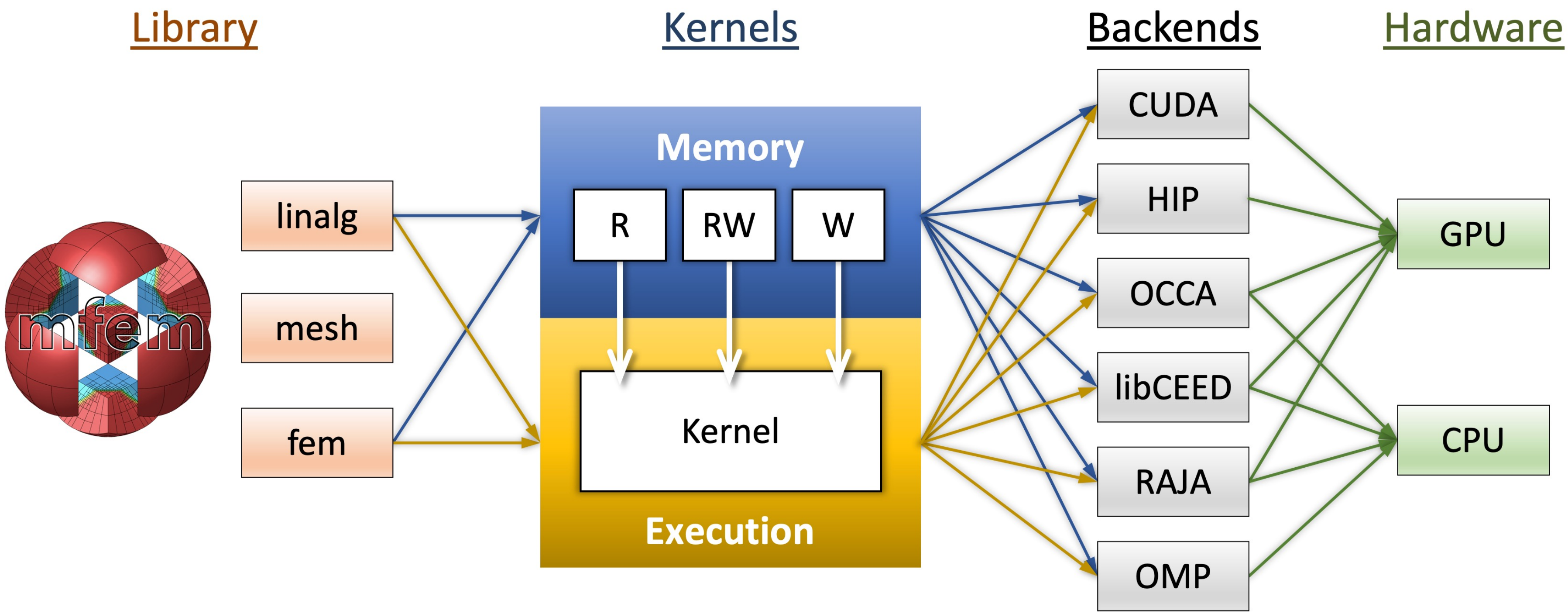


deal.ii

- ✔ All runs done on BG/Q (for repeatability), 16384 MPI ranks. Order p = 1, ...,16; quad. points q = p + 2.
- ✔ BP1 results of MFEM+xlc (left), MFEM+xlc+intrinsics (center), and deal.ii + gcc (right) on BG/Q.
- ✔ **Paper: "Scalability of High-Performance PDE Solvers", IJHPCA, 2020**
- ✔ Cooperation/collaboration is what makes the bake-offs rewarding.

Device support in MFEM

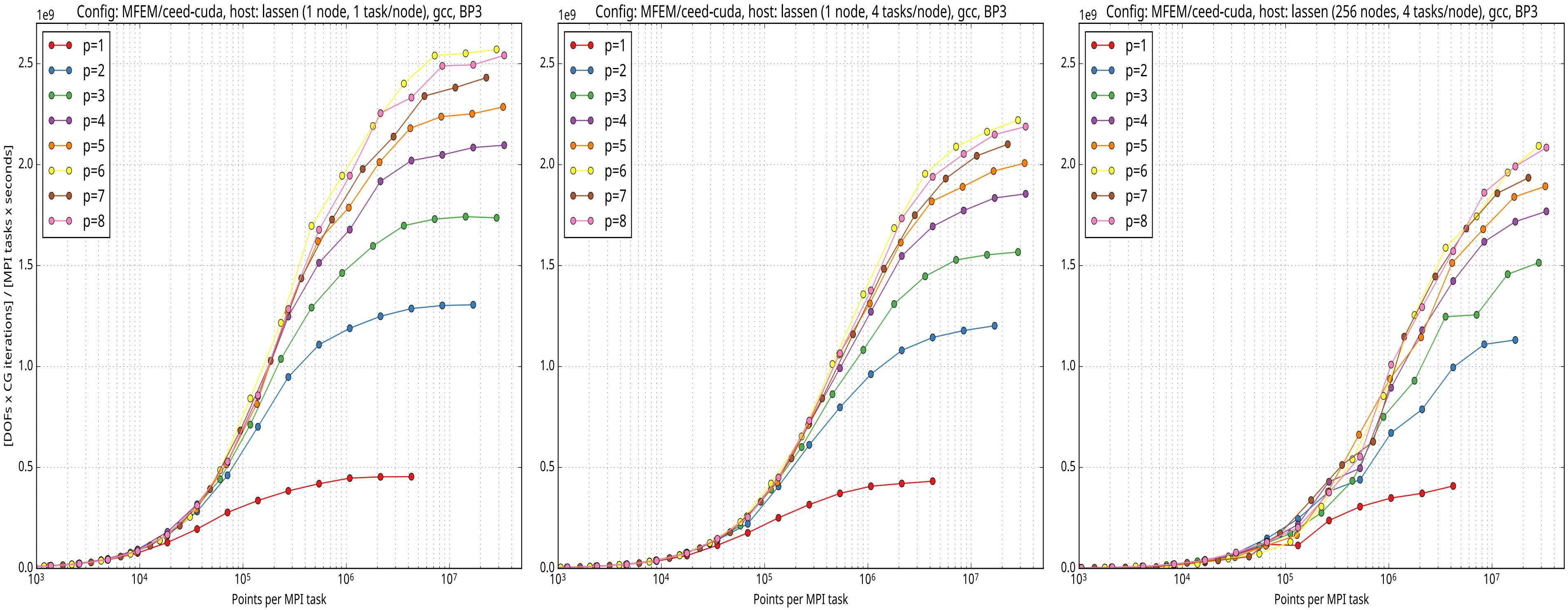
MFEM support GPU acceleration in many linear algebra and finite element operations



- Several MFEM examples + miniapps have been ported with small changes
- Many kernels have a single source for CUDA, RAJA and OpenMP backends
- Backends are runtime selectable, can be mixed
- Recent improvements in CUDA, HIP, RAJA, SYCL, …

"MFEM: A modular finite element methods library", CAMWA 2020

MFEM performance on multiple GPUs



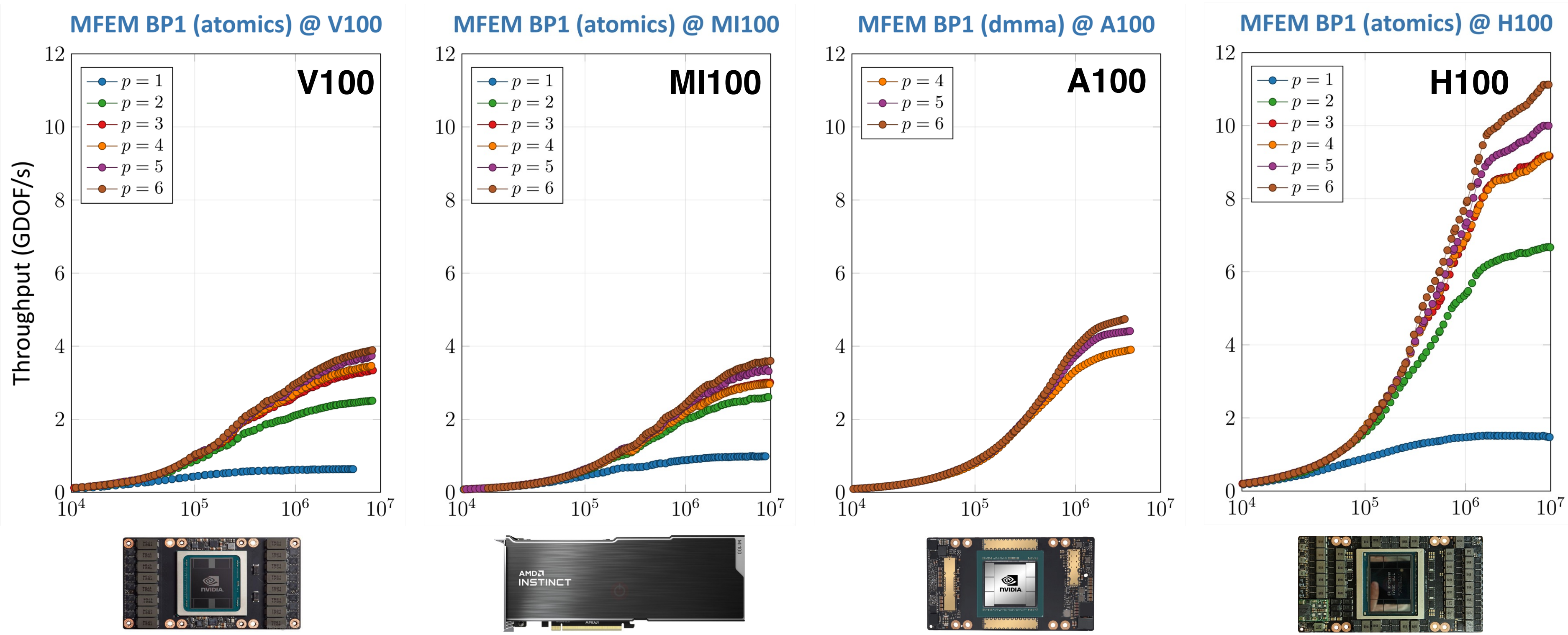
1 GPU *4 GPUs* *1024 GPUs*

Single GPU performance: **2.6 GDOF/s**
Problem size: 10+ million

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

Optimized kernels for MPI buffer packing/unpacking on the GPU

Recent improvements on NVIDIA and AMD GPUs

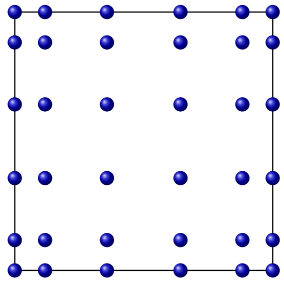


New MFEM GPU kernels: perform on both V100 + MI100,
have better strong scaling,
can utilize tensor cores on A100
achieve 10+ GDOFs on H100

MI250X results in the CEED-MS39 report: `ceed.exascaleproject.org/pubs`

Matrix-free preconditioning

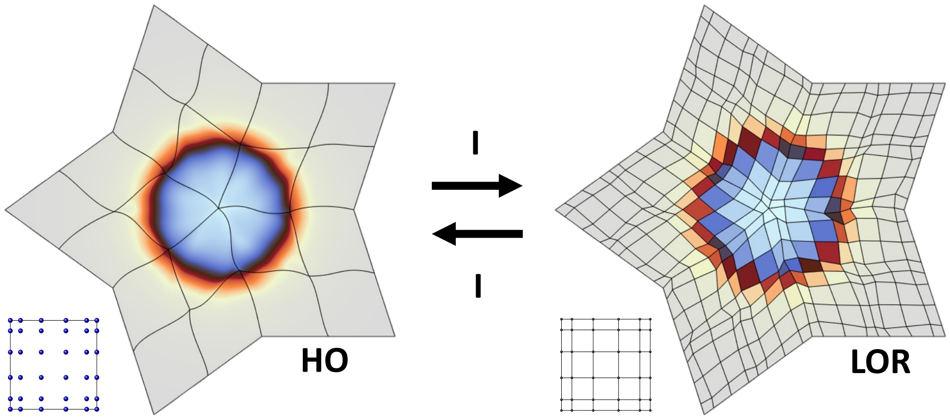
- ***Explicit matrix assembly impractical at high order:***
  - Polynomial degree p, spatial dimension d
  - Matrix assembly + sparse matvecs:
    - $\mathcal{O}(p^{2d})$ memory transfers
    - $\mathcal{O}(p^{3d})$ computations
    - can be reduced to $\mathcal{O}(p^{2d+1})$ computations by sum factorization
  - Matrix-free action of the operator (partial assembly):
    - $\mathcal{O}(p^{d})$ memory transfers – *optimal*
    - $\mathcal{O}(p^{d+1})$ computations – *nearly-optimal*
    - efficient iterative solvers ***if combined with effective preconditioners***



- ***Challenges:***
  - Traditional matrix-based preconditioners (e.g. AMG) not available
  - Condition number of diffusion systems grows like $\mathcal{O}(p^3/h^2)$

Low-Order-Refined (LOR) preconditioning

Efficient LOR-based preconditioning of H1, H(curl), H(div) and L2 high-order operators

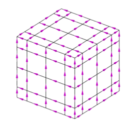


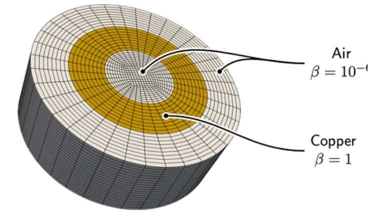
- Pick LOR space and HO basis so **P=R=I** (Gerritsma, Dohrmann)
- $\mathbf{A}_{\mathbf{LOR}}$ is sparse and spectrally equivalent to $\mathbf{A}_{\mathbf{HO}}$

Theorem 2. *Let $M_\star$ and $K_\star$ denote the mass and stiffness matrices, respectively, where $\star$ represents one of the above-defined finite element spaces with basis as in Section 4.3. Then we have the following spectral equivalences, independent of mesh size h and polynomial degree p.*

$$\begin{aligned} M_{V_h} &\sim M_{V_p}, & K_{V_h} &\sim K_{V_p}, \\ M_{\boldsymbol{W}_h} &\sim M_{\boldsymbol{W}_p}, & K_{\boldsymbol{W}_h} &\sim K_{\boldsymbol{W}_p}, \\ M_{\boldsymbol{X}_h} &\sim M_{\boldsymbol{X}_p}, & K_{\boldsymbol{X}_h} &\sim K_{\boldsymbol{X}_p}, \\ M_{Y_h} &\sim M_{Y_{p-1}}, & & \\ M_{Z_h} &\sim M_{Z_p}, & K_{Z_h} &\sim K_{Z_p}. \end{aligned}$$

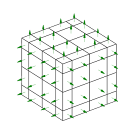
- $(\mathbf{A}_{\mathbf{HO}})^{-1} \approx (\mathbf{A}_{\mathbf{LOR}})^{-1} \approx \mathbf{B}_{\mathbf{LOR}}$ - can use BoomerAMG, AMS, ADS

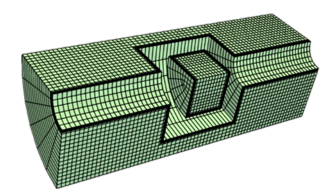




$\nabla \times \nabla \times \boldsymbol{u} + \beta \boldsymbol{u} = \boldsymbol{f}$

p	Its.	Assembly (s)	AMG Setup (s)	Solve (s)	# DOFs	# NNZ
LOR–AMS						
2	41	0.082	0.277	0.768	516,820	1.65×10^7
3	63	0.251	0.512	2.754	1,731,408	5.64×10^7
4	75	0.679	1.133	7.304	4,088,888	1.34×10^8
5	62	1.574	2.185	11.783	7,968,340	2.61×10^8
6	89	3.336	4.024	30.702	13,748,844	4.51×10^8
Matrix-Based AMS						
2	39	0.140	0.385	1.423	516,820	5.24×10^7
3	44	1.368	1.572	9.723	1,731,408	4.01×10^8
4	49	9.668	5.824	45.277	4,088,888	1.80×10^9
5	53	61.726	15.695	148.757	7,968,340	5.92×10^9
6	56	502.607	40.128	424.100	13,748,844	1.59×10^{10}





$\nabla(\alpha \nabla \cdot \boldsymbol{u}) - \beta \boldsymbol{u} = \boldsymbol{f}$

	LOR–ADS		Matrix-Based ADS		
p	Runtime (s)	Memory (GB)	Runtime (s)	Memory (GB)	Speedup
2	2.11	0.04	2.98	0.20	1.41×
3	6.64	0.15	22.58	1.84	3.40×
4	17.40	0.35	114.35	9.13	6.57×
5	43.70	0.68	422.74	32.21	9.67×
6	92.76	1.18	1324.94	91.09	14.28×

"Low-order preconditioning for the high-order de Rham complex", Pazner, Kolev, Dohrmann, 2022

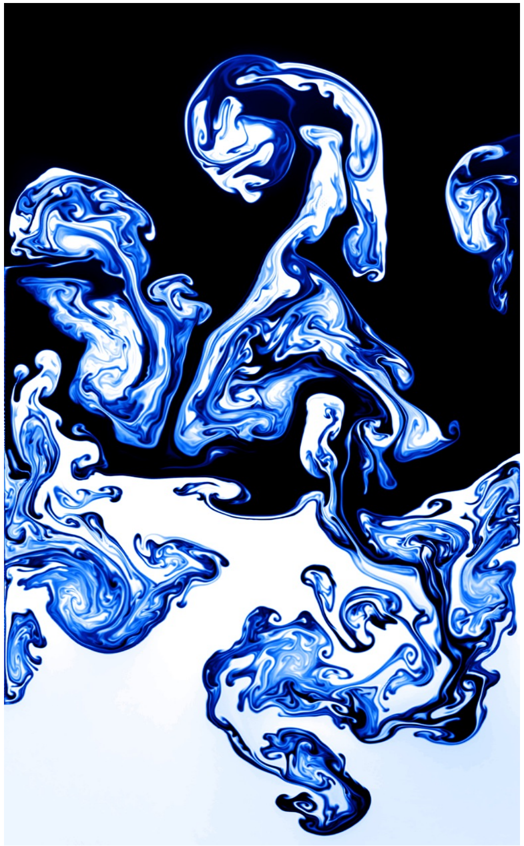
High-order FE methods show promise for high-quality & performance simulations on exascale platforms

- **More information and publications**
  - MFEM – **mfem.org**
  - BLAST – **computation.llnl.gov/projects/blast**
  - CEED – **ceed.exascaleproject.org**

- **Open-source software**

mfem CEED EXASCALE DISCRETIZATIONS

- **Ongoing R&D**
  - GPU-oriented algorithms for Frontier, Aurora, El Capitan
  - Matrix-free scalable preconditioners
  - Automatic differentiation, design optimization
  - Deterministic transport, multi-physics coupling

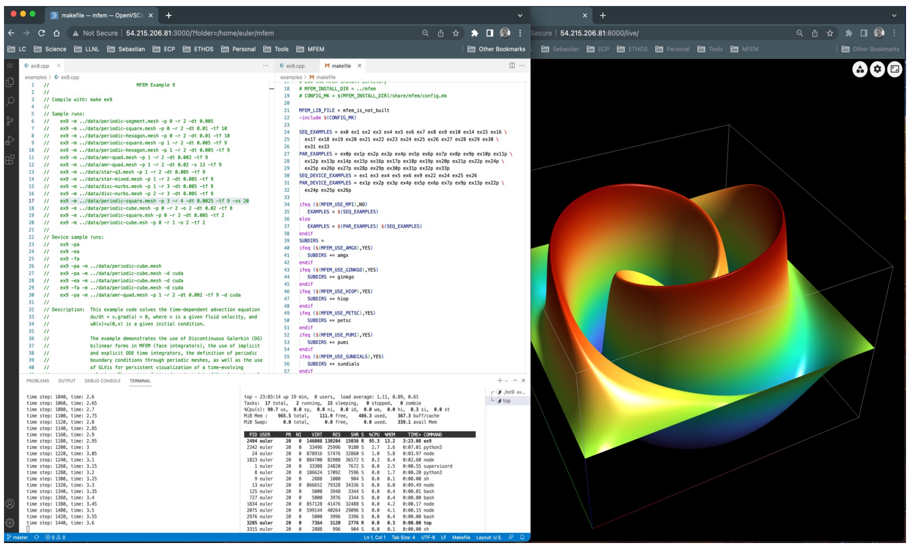


Q4 Rayleigh-Taylor single-material ALE on 256 processors

Upcoming MFEM Events

MFEM in the Cloud Tutorial

August 22, 2024



https://mfem.org/tutorial

MFEM Community Workshop

October 22-24, 2024

https://mfem.org/workshop

FEM@LLNL **Seminar series:** https://mfem.org/seminar

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