The libMesh Finite Element Library

a case for Object-Oriented High-Performance Computing

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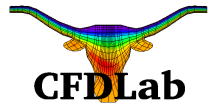
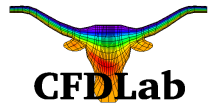
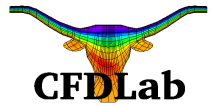




CFDLab

Background

- Modern simulation software is complex:
  - Implicit numerical methods
  - Massively parallel computers
  - Adaptive methods
  - Multiple, coupled physical processes
- There are a host of existing software libraries that excel at treating various aspects of this complexity.
- Leveraging existing software whenever possible is the most efficient way to manage this complexity.



Background

- Modern simulation software is multidisciplinary:
  - Physical Sciences
  - Engineering
  - Computer Science
  - Applied Mathematics
  - ...
- It is not reasonable to expect a single person to have all the necessary skills for developing & implementing high-performance numerical algorithms on modern computing architectures.
- Teaming is a prerequisite for success.

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Background

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- Consider some of the major components such a simulation:

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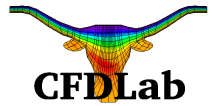
  1. Read the mesh from file
  2. Initialize data structures
  3. Construct a discrete representation of the governing equations
  4. Solve the discrete system
  5. Write out results
  6. Optionally estimate error, refine the mesh, and repeat



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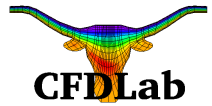

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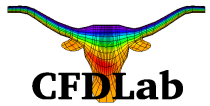
- This allows the major components of such a simulation to be abstracted & implemented in a reusable software library.



The libMesh Software Library

- In 2002, the libMesh library began with these ideas in mind.
- Primary goal is to provide data structures and algorithms that can be shared by disparate physical applications, that may need some combination of
  - Implicit numerical methods
  - Adaptive mesh refinement techniques
  - Parallel computing
- Unifying theme: mesh-based simulation of partial differential equations (PDEs).

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The libMesh Software Library

Key Point

- The libMesh library is designed to be used by studendts, researchers, scientists, and engineers as a tool for developing simulation codes or as a tool for rapidily implementing a numerical method.
- libMesh is not an application code.
- It does not "solve problem XYZ."
  - It can be used to help you develop an application to solve problem XYZ, and to do so quickly with advanced numerical algorithms on high-performance computing platforms.

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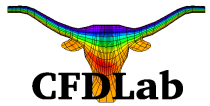
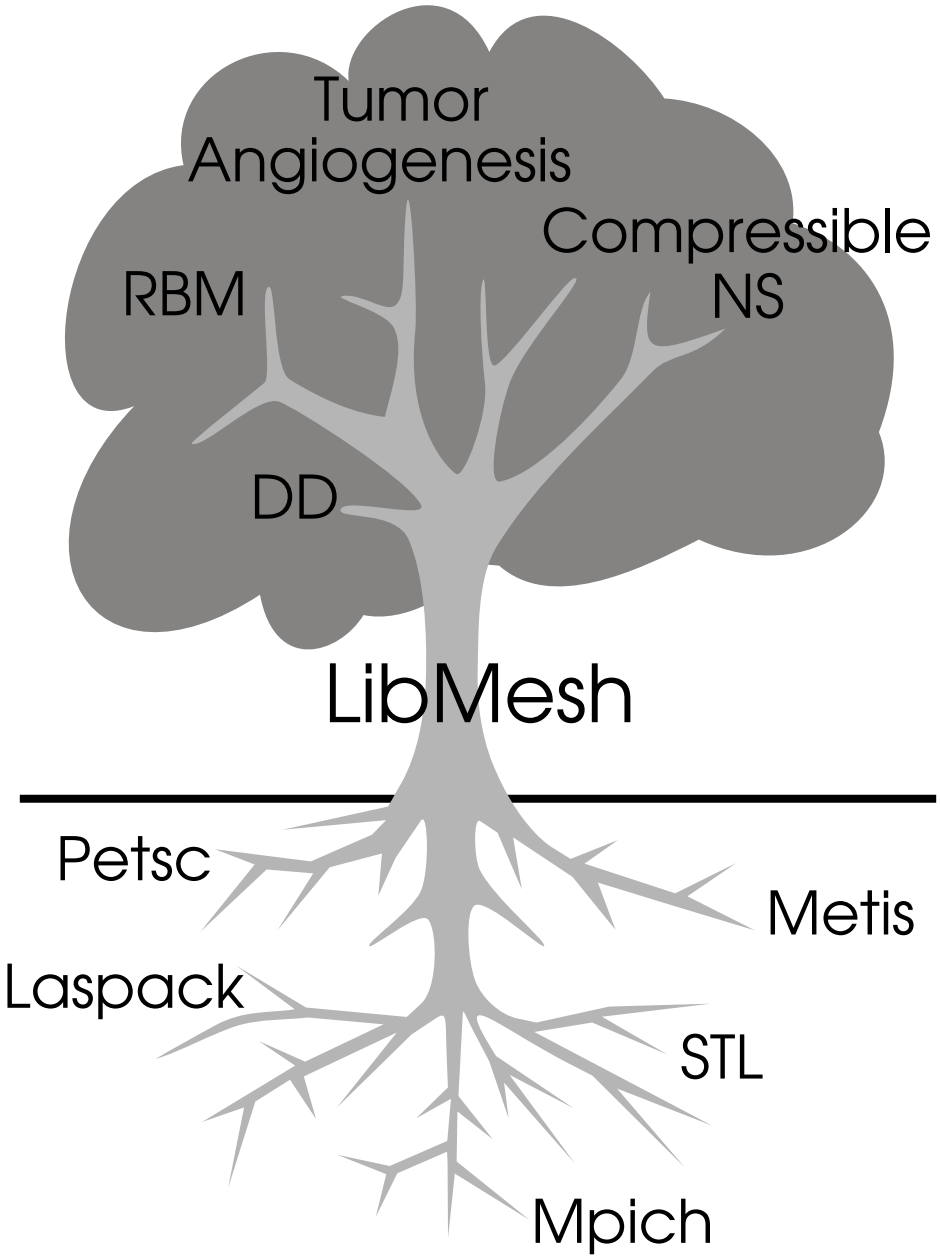
Software Reusability

- At the inception of `libMesh` in 2002, there were many high-quality software libraries that implemented some aspect of the end-to-end PDE simulation process:
  - Parallel linear algebra
  - Partitioning algorithms for domain decomposition
  - Visualization formats
  - ...
- A design goal of `libMesh` has always been to provide flexibile & extensible interfaces to existing software whenever possible.
- We implement the "glue" to these pieces, as well as what we viewed as the missing infrastructure:
  - Flexibile data structures for the discretization of spatial domains and systems of PDEs posed on these domains.





Library Structure

- Basic libraries are `libMesh`'s "roots"
- Application "branches" built off the library "trunk"

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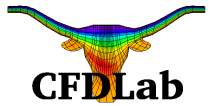
The “Glue”

- The C++ programming language provides a powerful abstraction mechanism for separating a software interface from its implementation.
- The notion of Base Classes defining an abstract interface and Derived Classes implementing the interface is key to this programming model.



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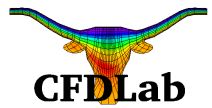
- The notion of Base Classes defining an abstract interface and Derived Classes implementing the interface is key to this programming model.
- The classic C++ example: Shapes.

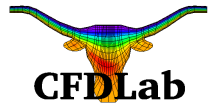
```
int main ()
{
  /* using shapes polymorphically */
  Shape * shapes[2];
  shapes[0] = new Rectangle (10, 20, 5, 6);
  shapes[1] = new Circle (15, 25, 8);

  for (int i=0; i<2; ++i)
    shapes[i]->Draw();
  ...
}
```



Abstract Shape

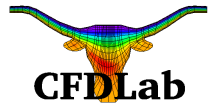
```
/* abstract interface declaration */
class Shape
{
public:
  virtual void Draw () = 0;
  virtual void MoveTo (int newx, int newy) = 0;
  virtual void RMoveTo (int dx, int dy) = 0;
};
```



Specific Shape: Rectangle

```
/* Class Rectangle */
class Rectangle : public Shape
{
public:
  Rectangle (int x, int y, int w, int h);
  virtual void Draw ();
  virtual void MoveTo (int newx, int newy);
  virtual void RMoveTo (int dx, int dy);
  virtual void SetWidth (int newWidth);
  virtual void SetHeight (int newHeight);

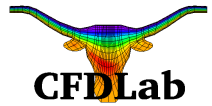
private:
  int x, y;
  int width;
  int height;
};
```



Specific Shape: Circle

```
/* Class Circle */
class Circle : public Shape
{
public:
  Circle (int initx, int inity, int initr);
  virtual void Draw ();
  virtual void MoveTo (int newx, int newy);
  virtual void RMoveTo (int dx, int dy);
  virtual void SetRadius (int newRadius);

private:
  int x, y;
  int radius;
};
```

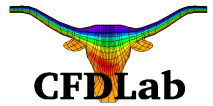


Object Polymorphism

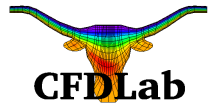
```
int main ()
{
  /* using shapes polymorphically */
  Shape * shapes[2];
  shapes[0] = new Rectangle (10, 20, 5, 6);
  shapes[1] = new Circle (15, 25, 8);

  for (int i=0; i<2; ++i)
    {
      shapes[i]->Draw();
      DoSomethingWithShape (shapes[i]);
    }

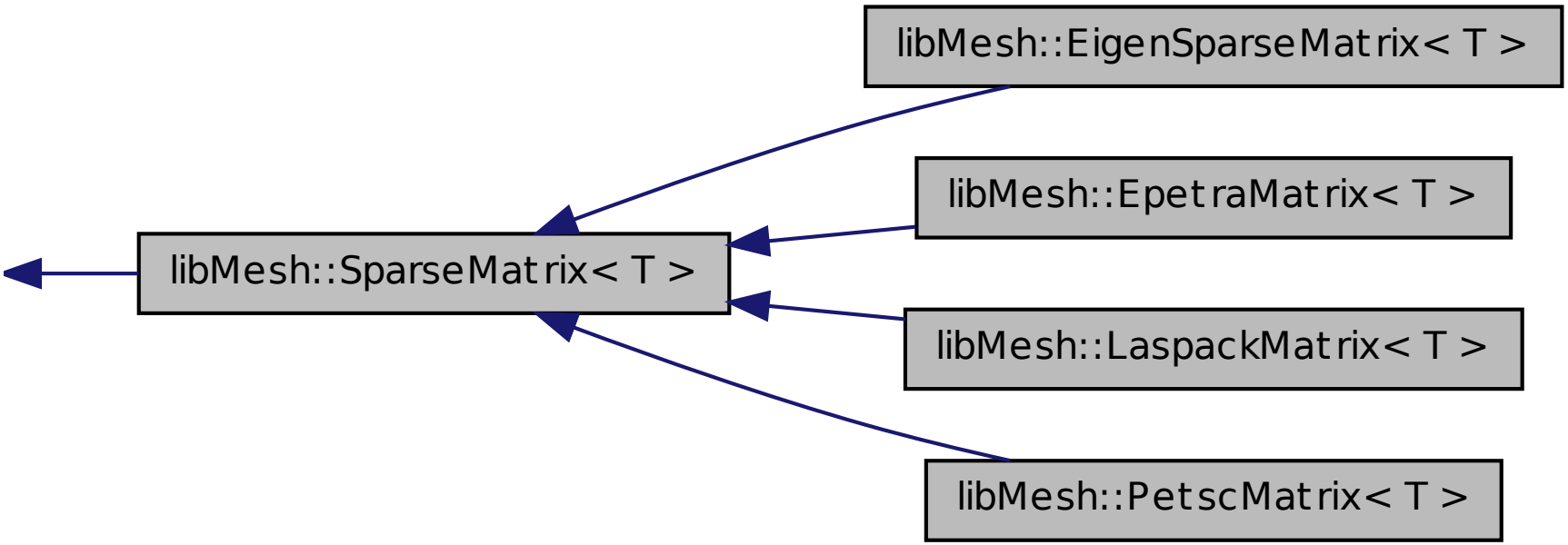
  /* access a rectangle specific function */
  Rectangle rect(0, 0, 15, 15);
  rect.SetWidth (30);
  rect.Draw ();
  ...
}
```



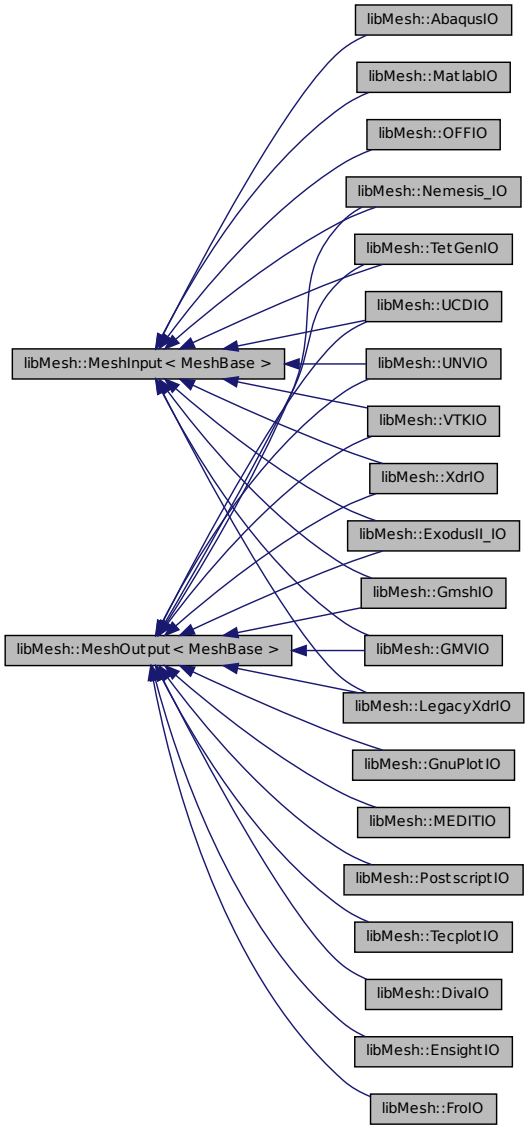
Examples of Polymorphism in `libMesh`



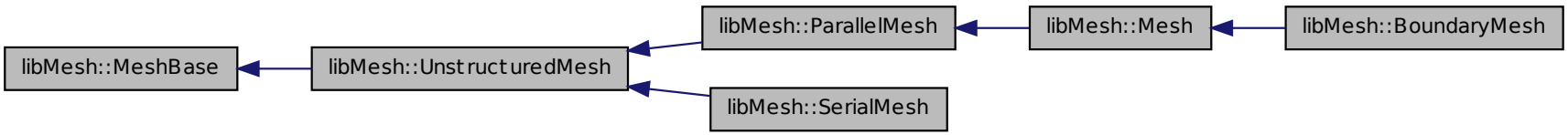
The “Glue:” Linear Algebra



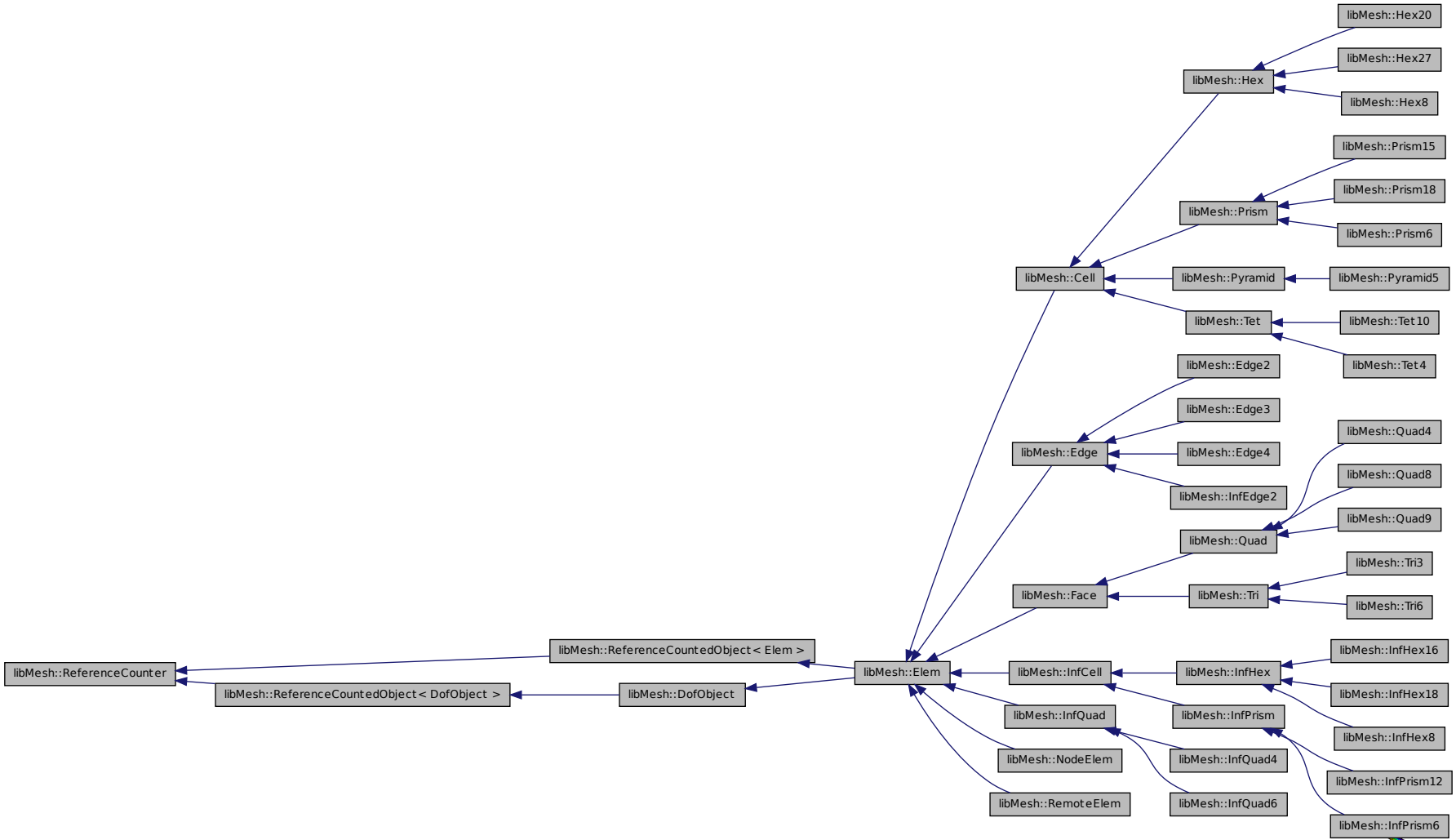
The “Glue:” I/O formats



Disretization: The Mesh



Disretization: Geometric Elements



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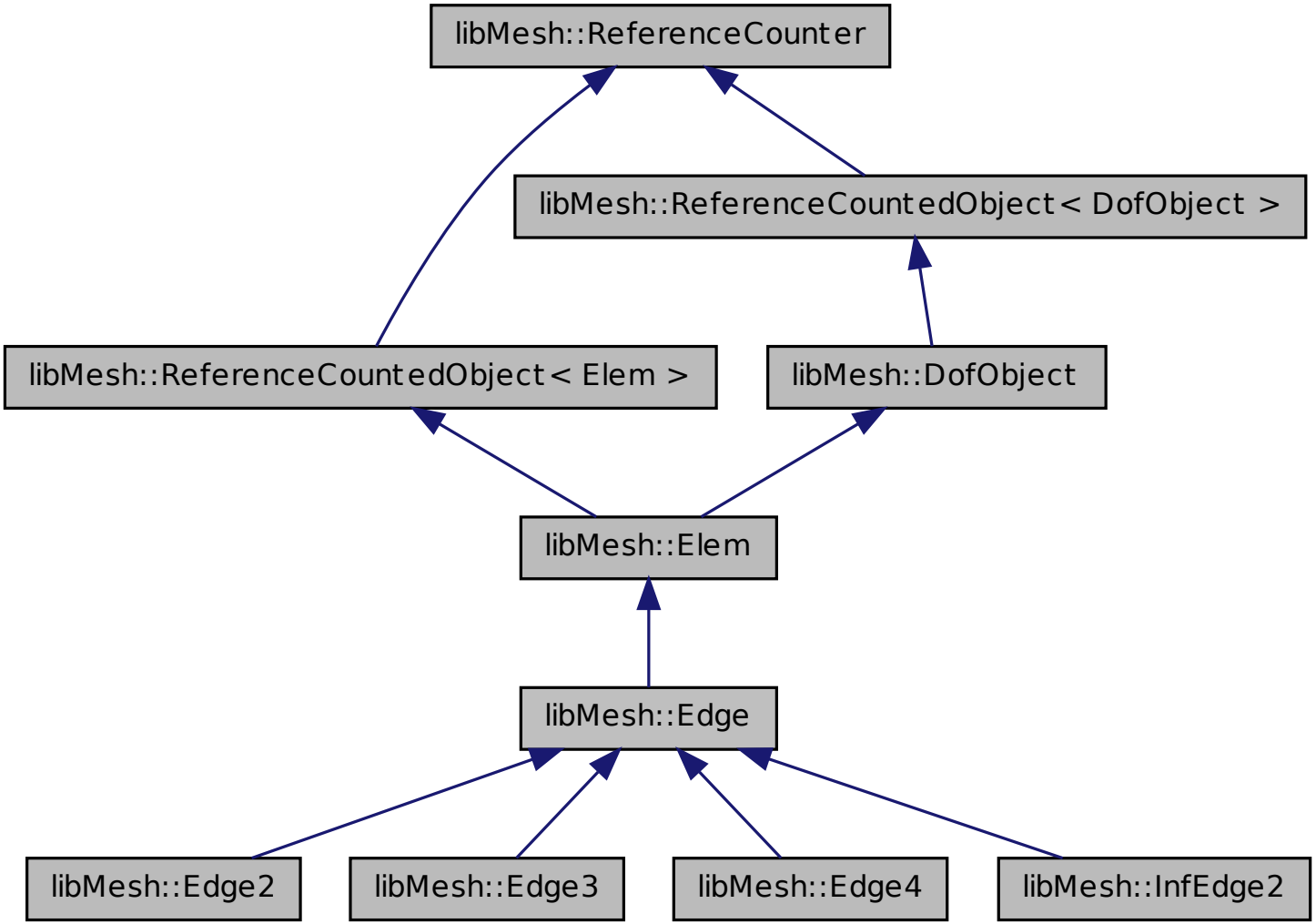

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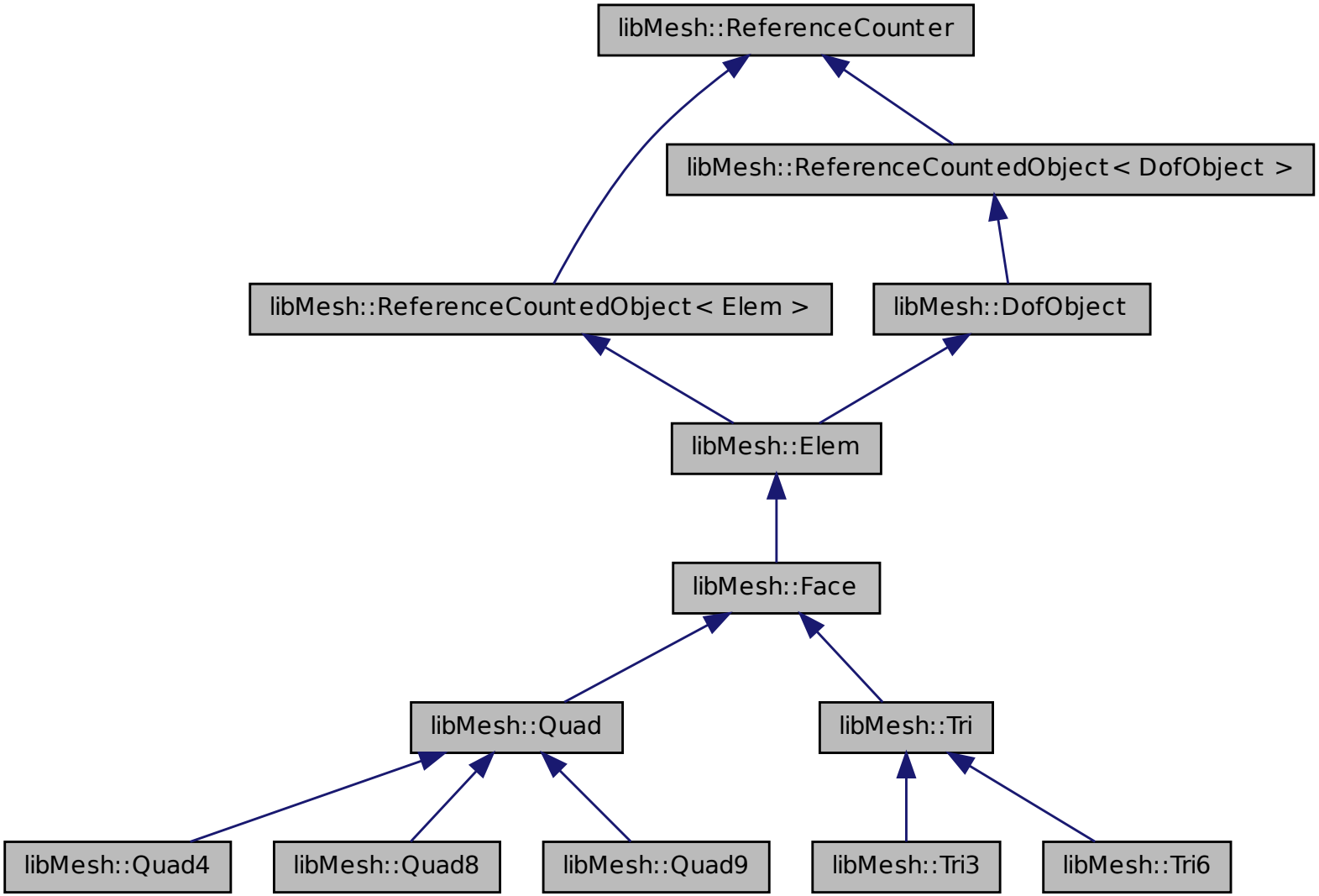

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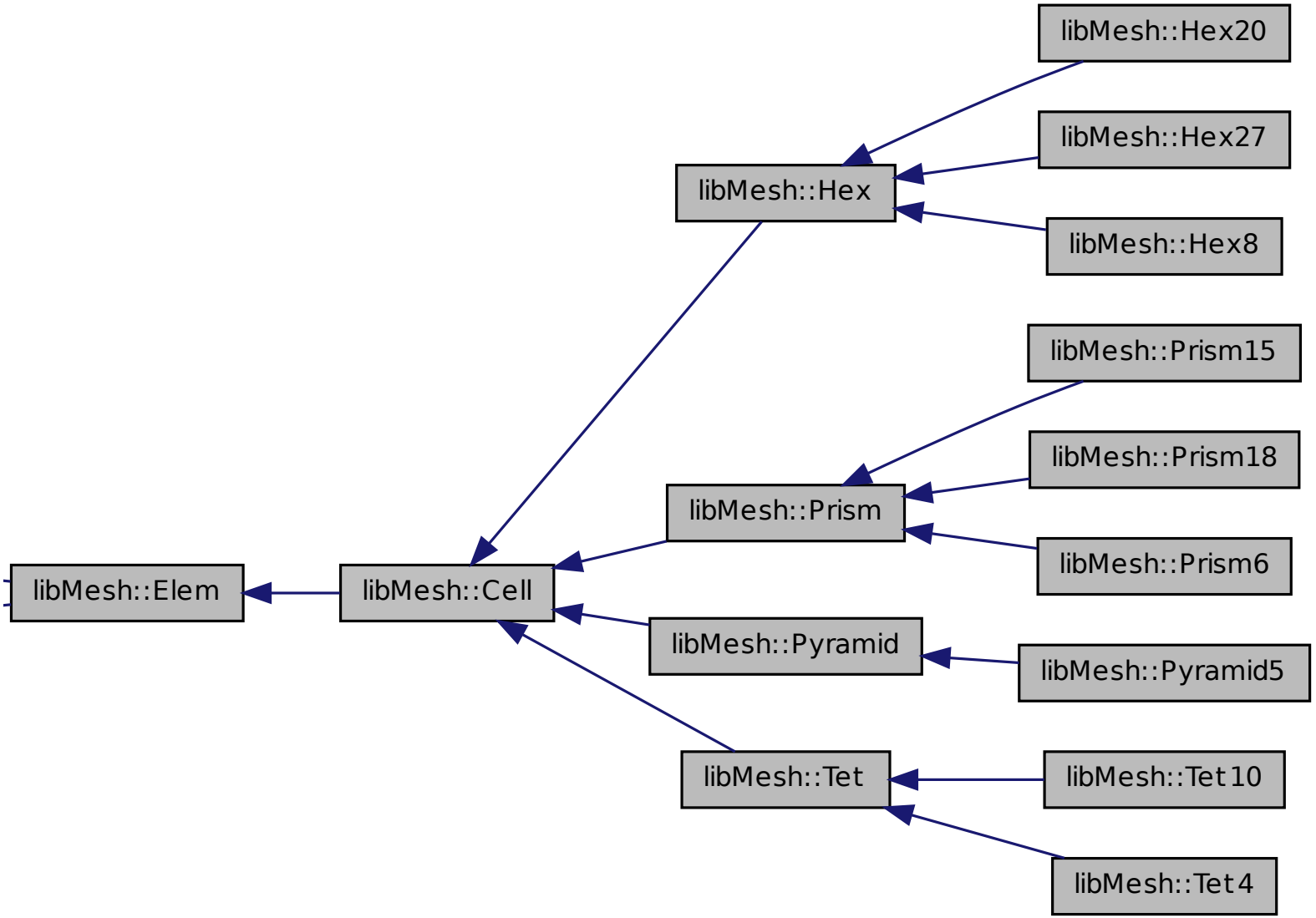

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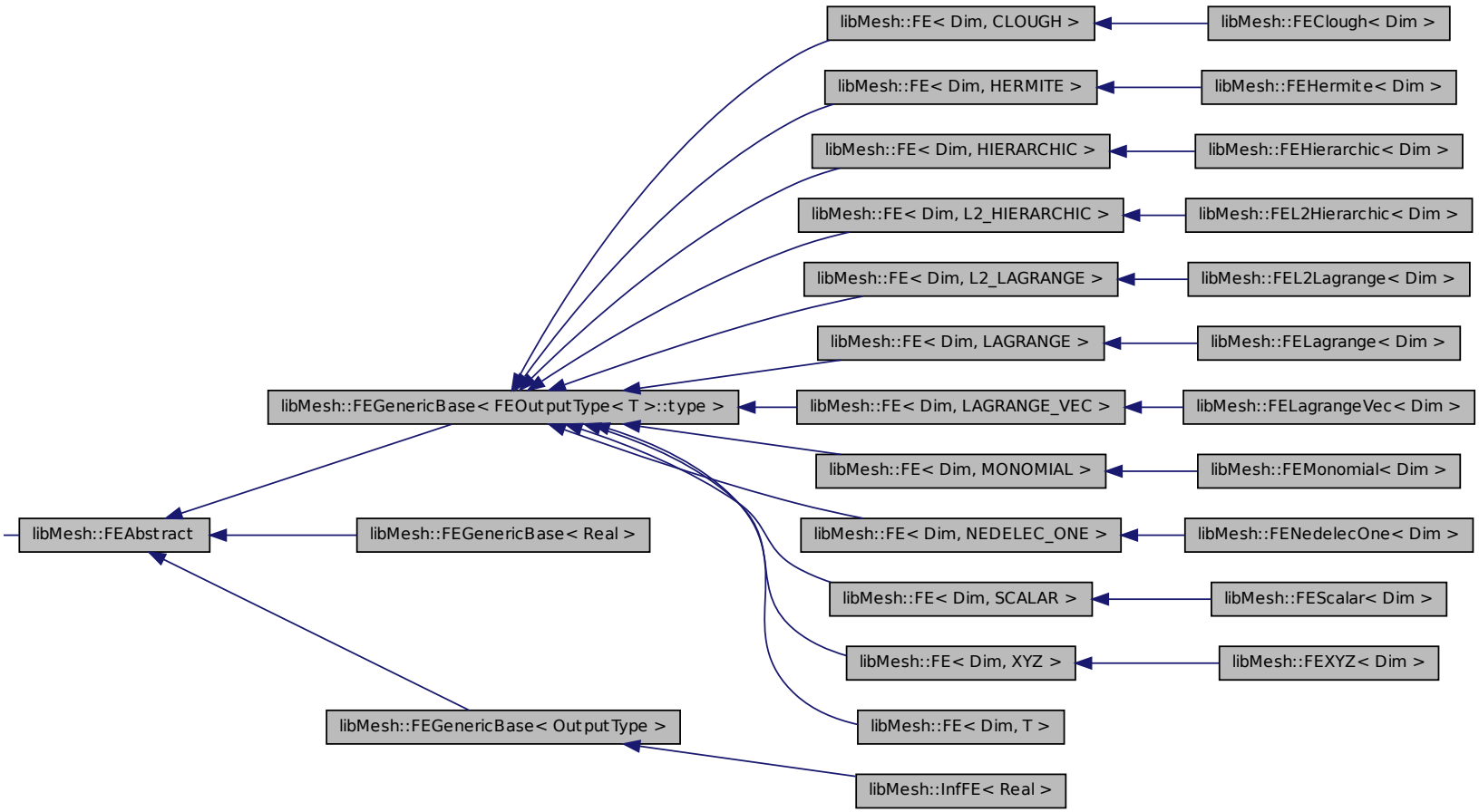
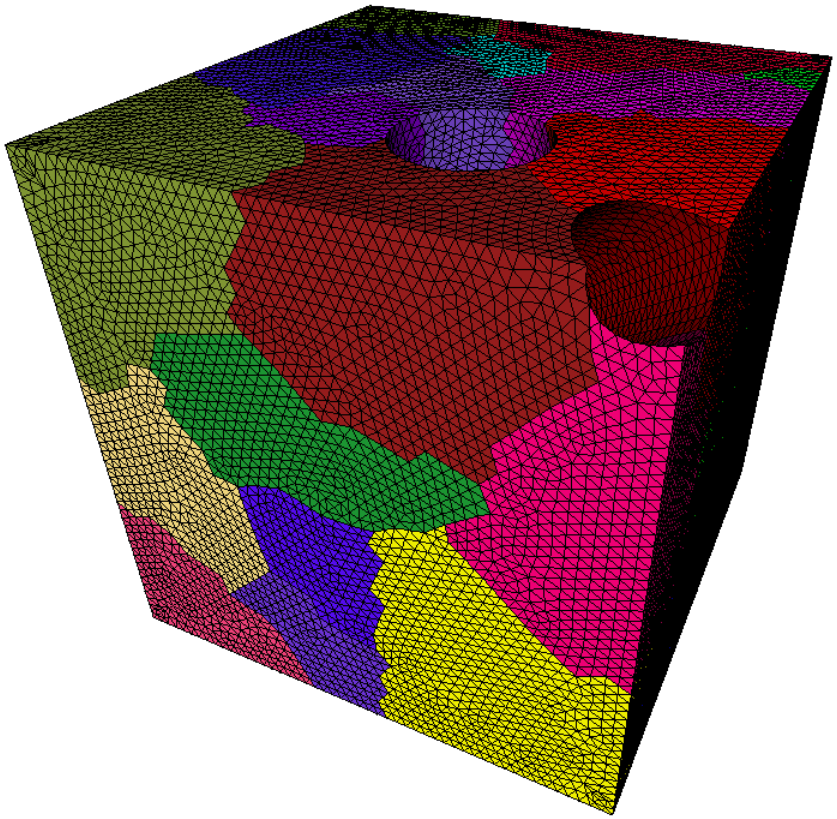
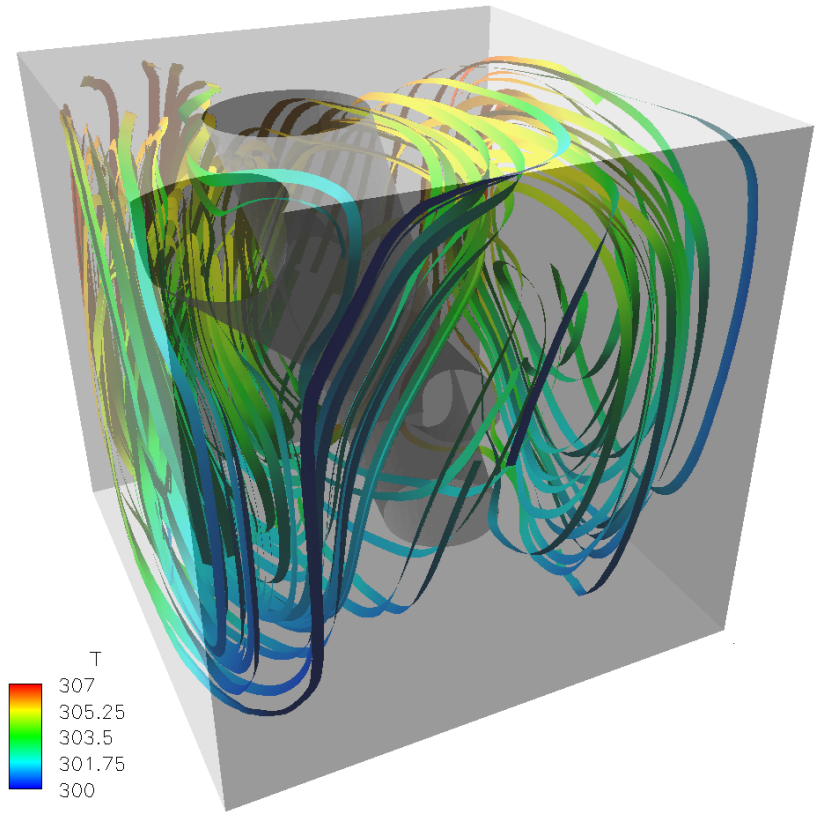
Disretization: Finite Elements



Algorithms: Domain Partitioning





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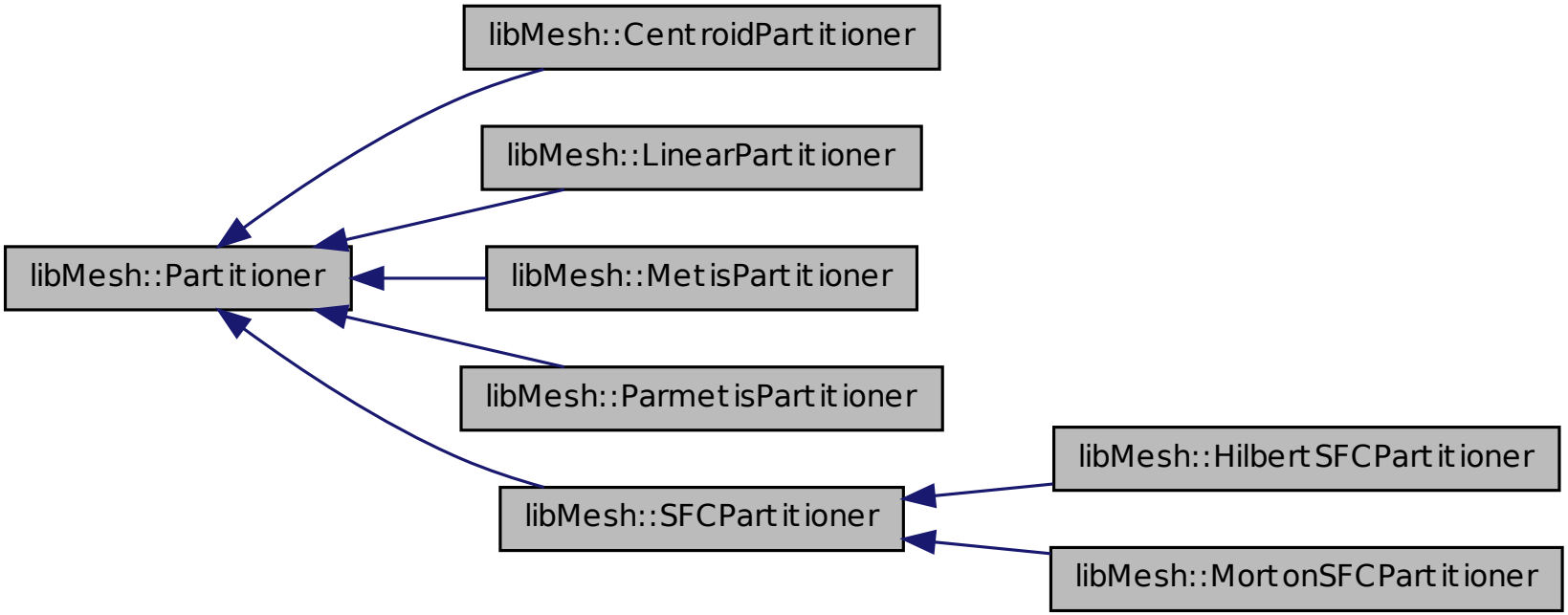

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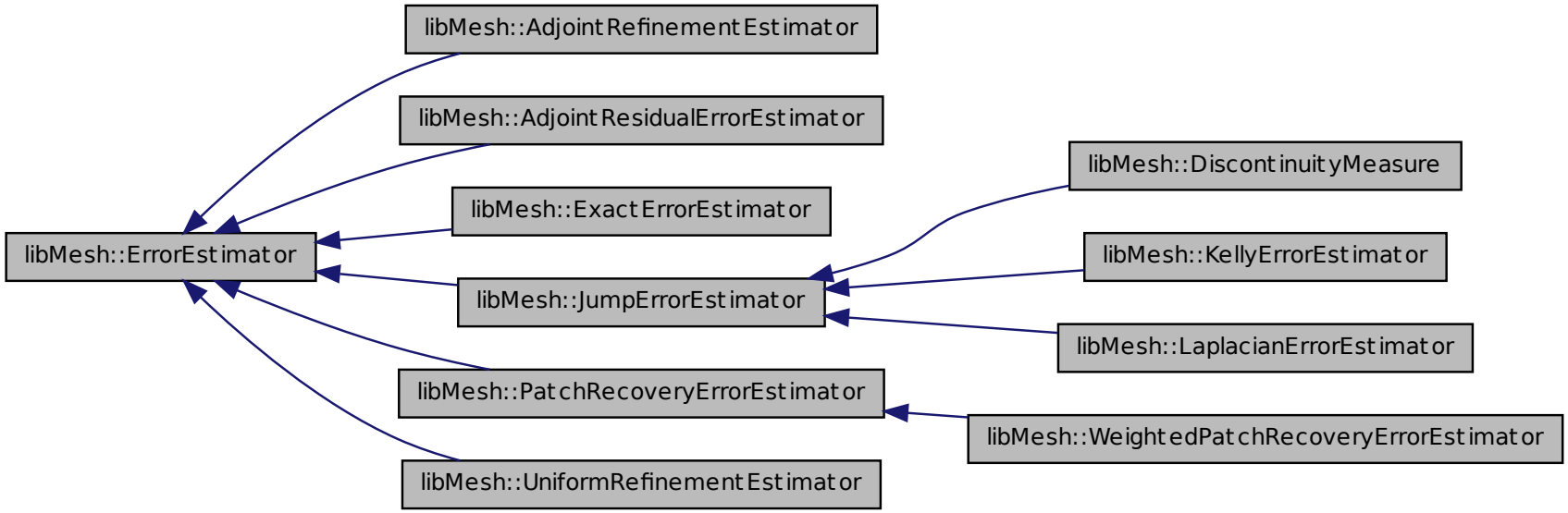
Algorithms: Error Estimation



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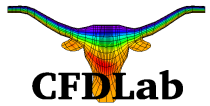
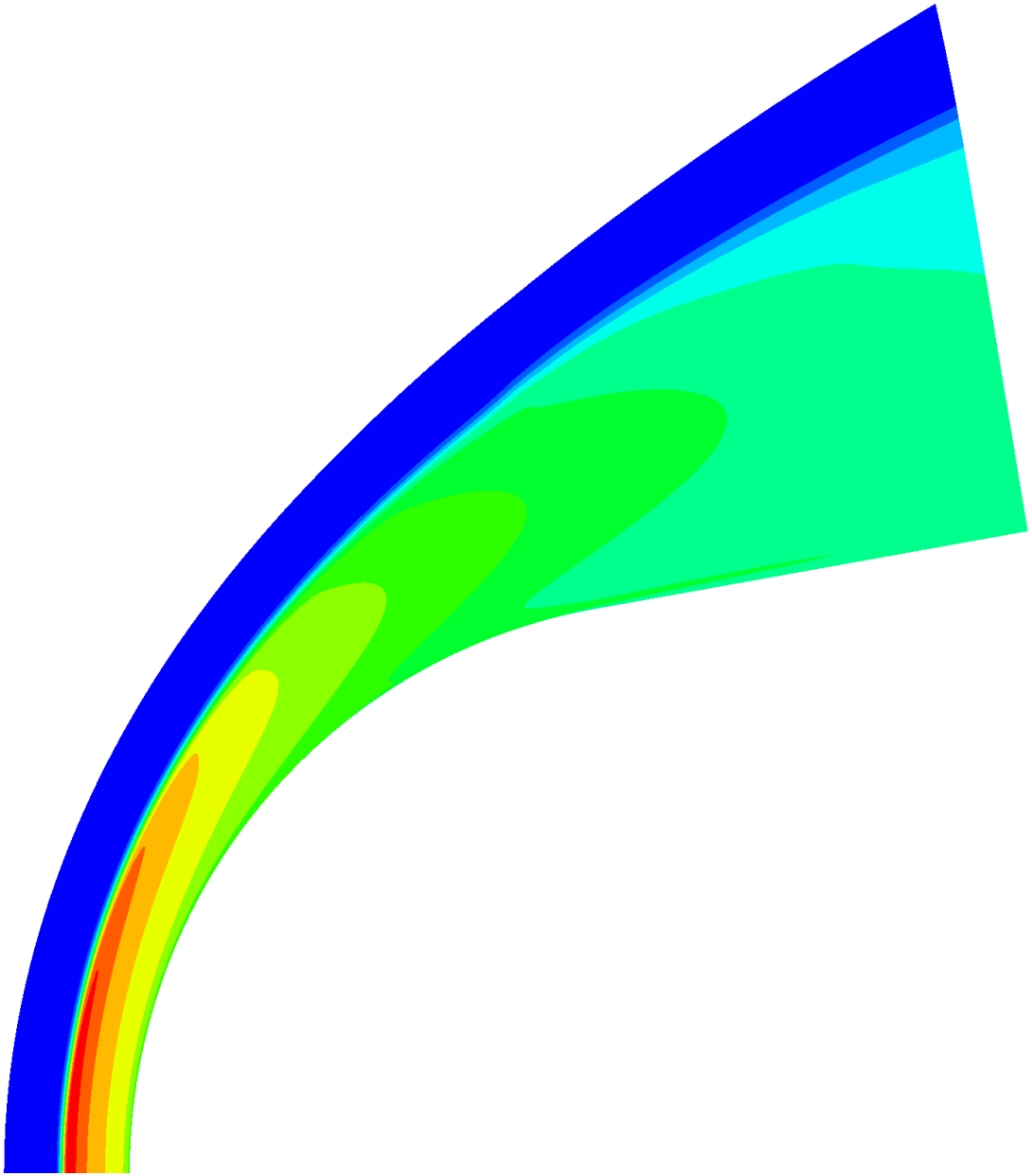
Results from Physics Applications built on top of **libMesh**



Compressible Navier-Stokes



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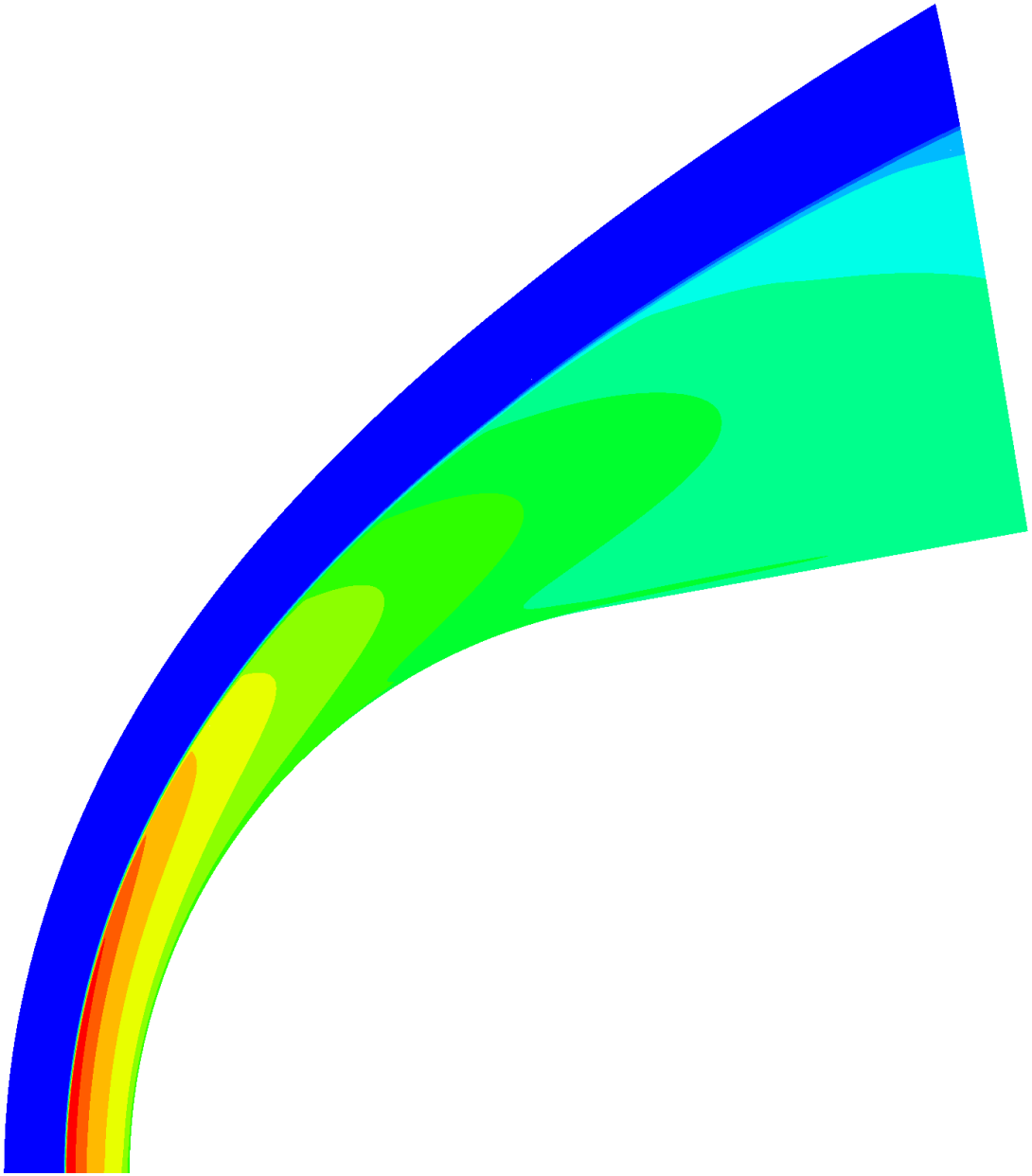

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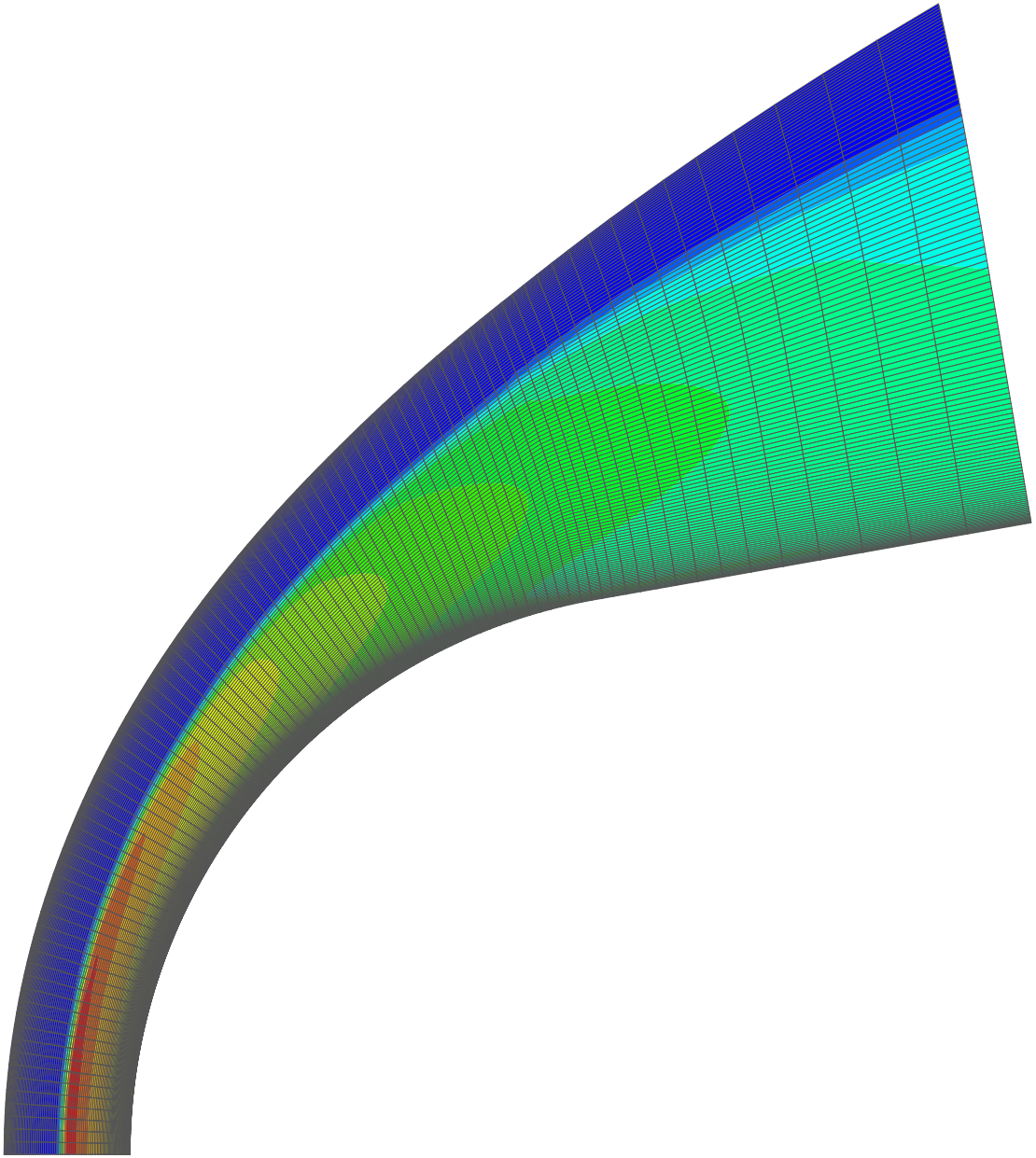

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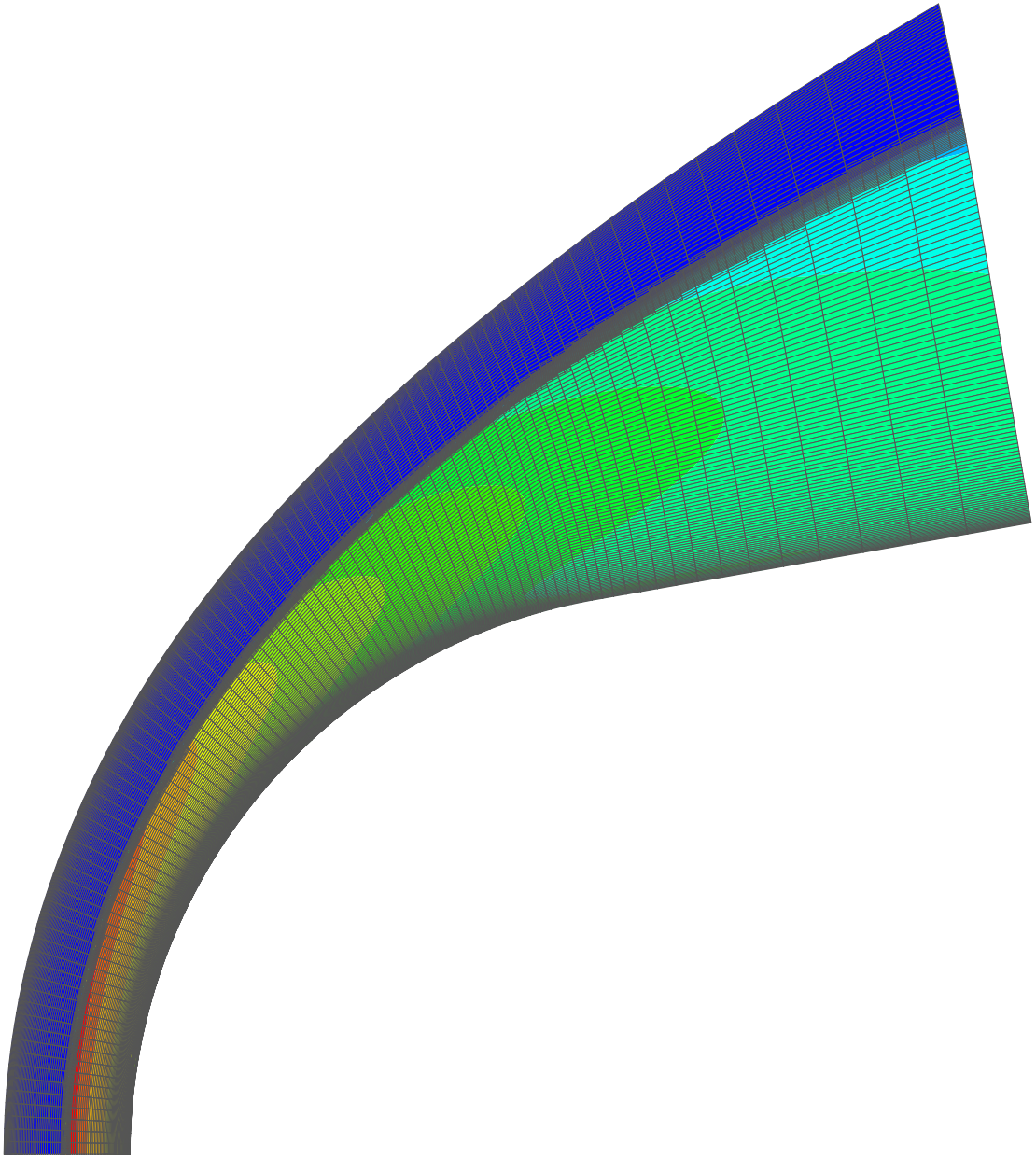
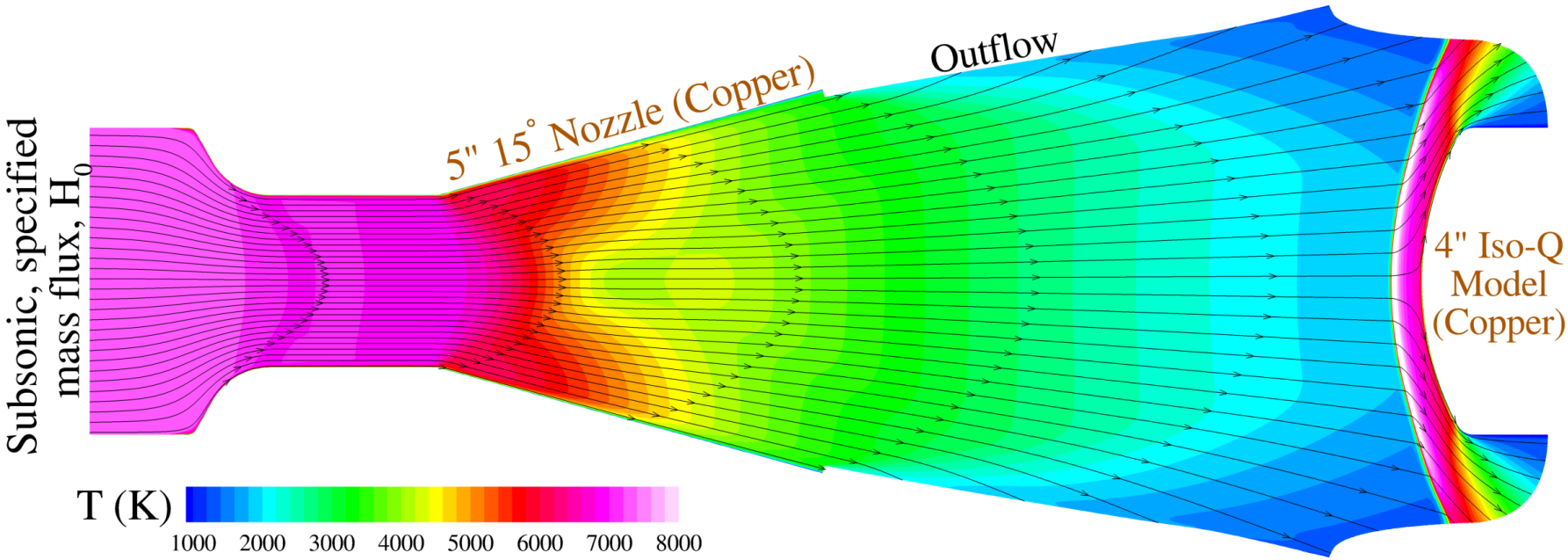


Arcjet Nozzle Calculation



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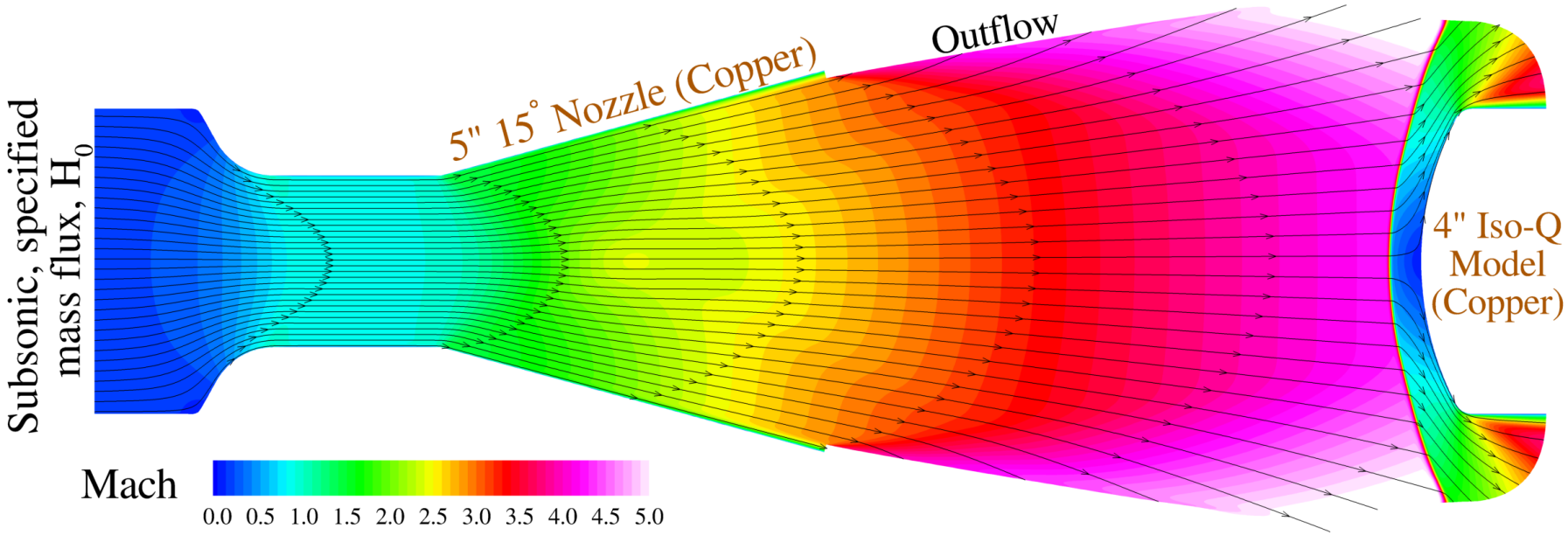

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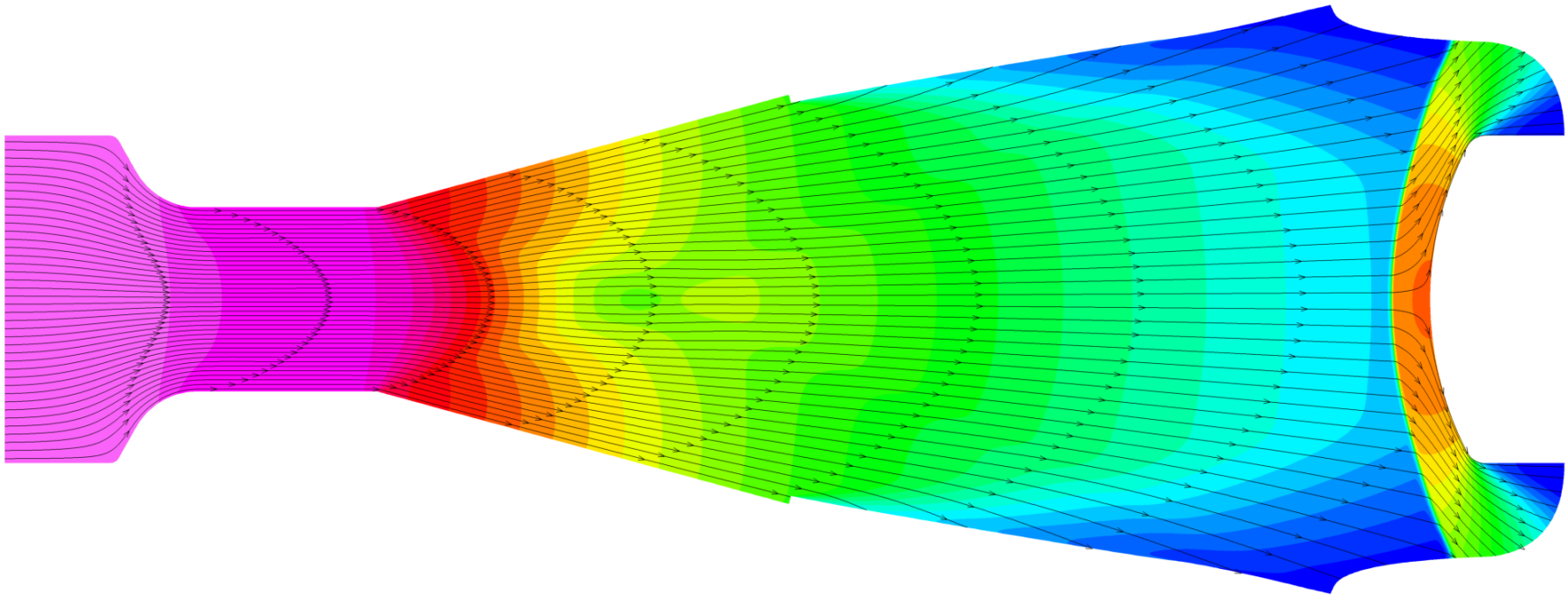

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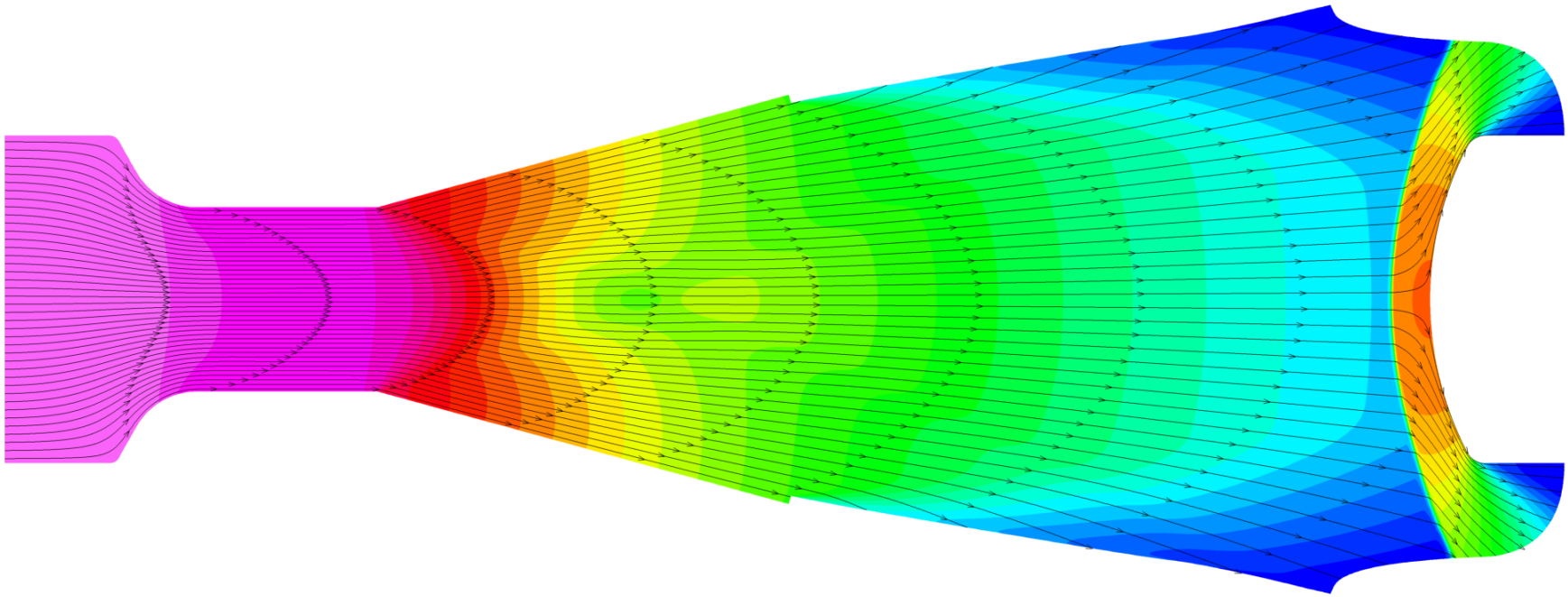

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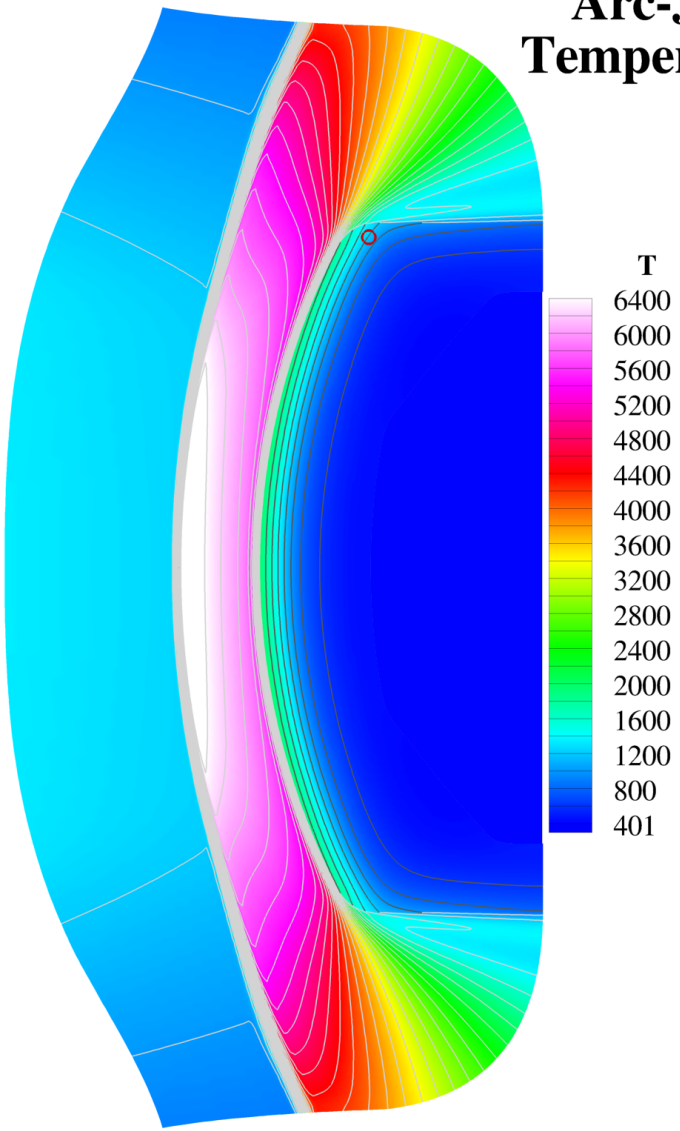
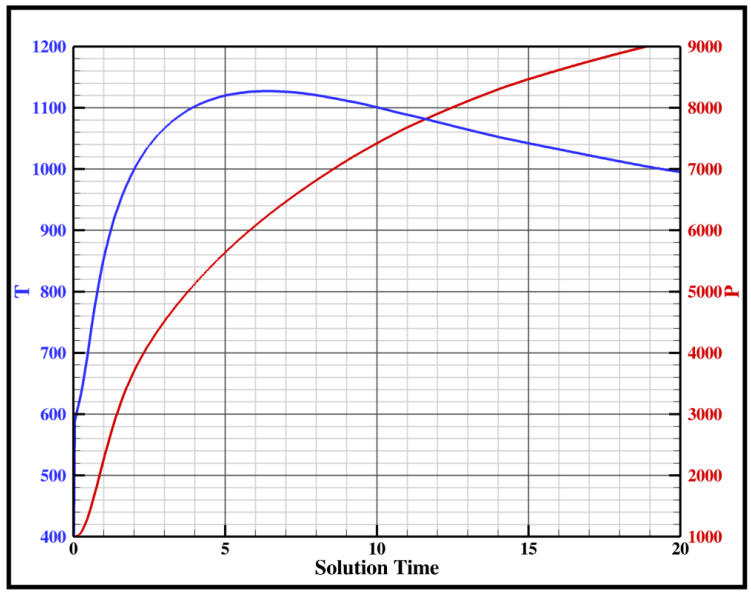
Coupled Pyrolysis, Temperature





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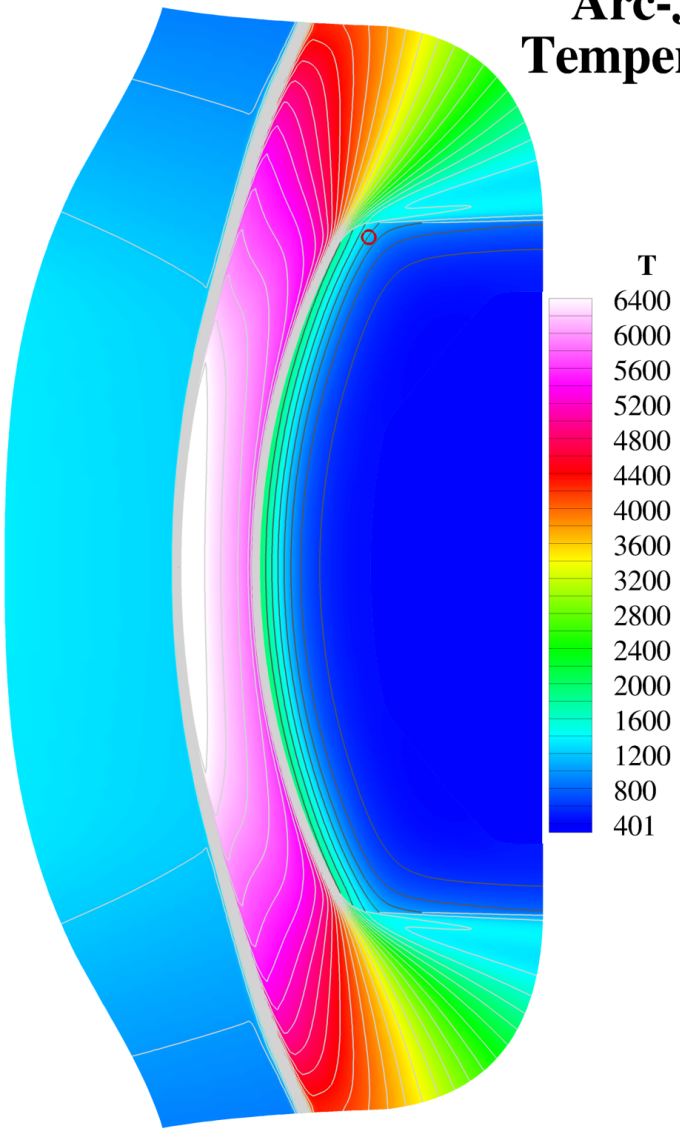

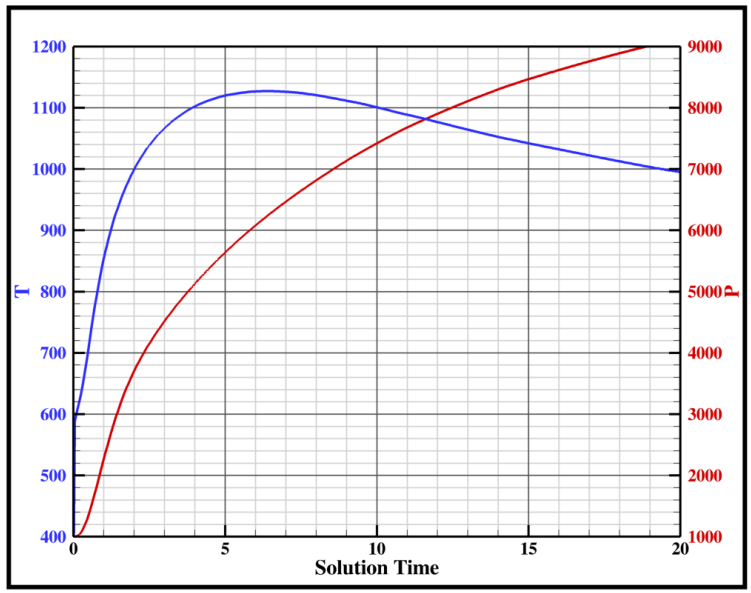

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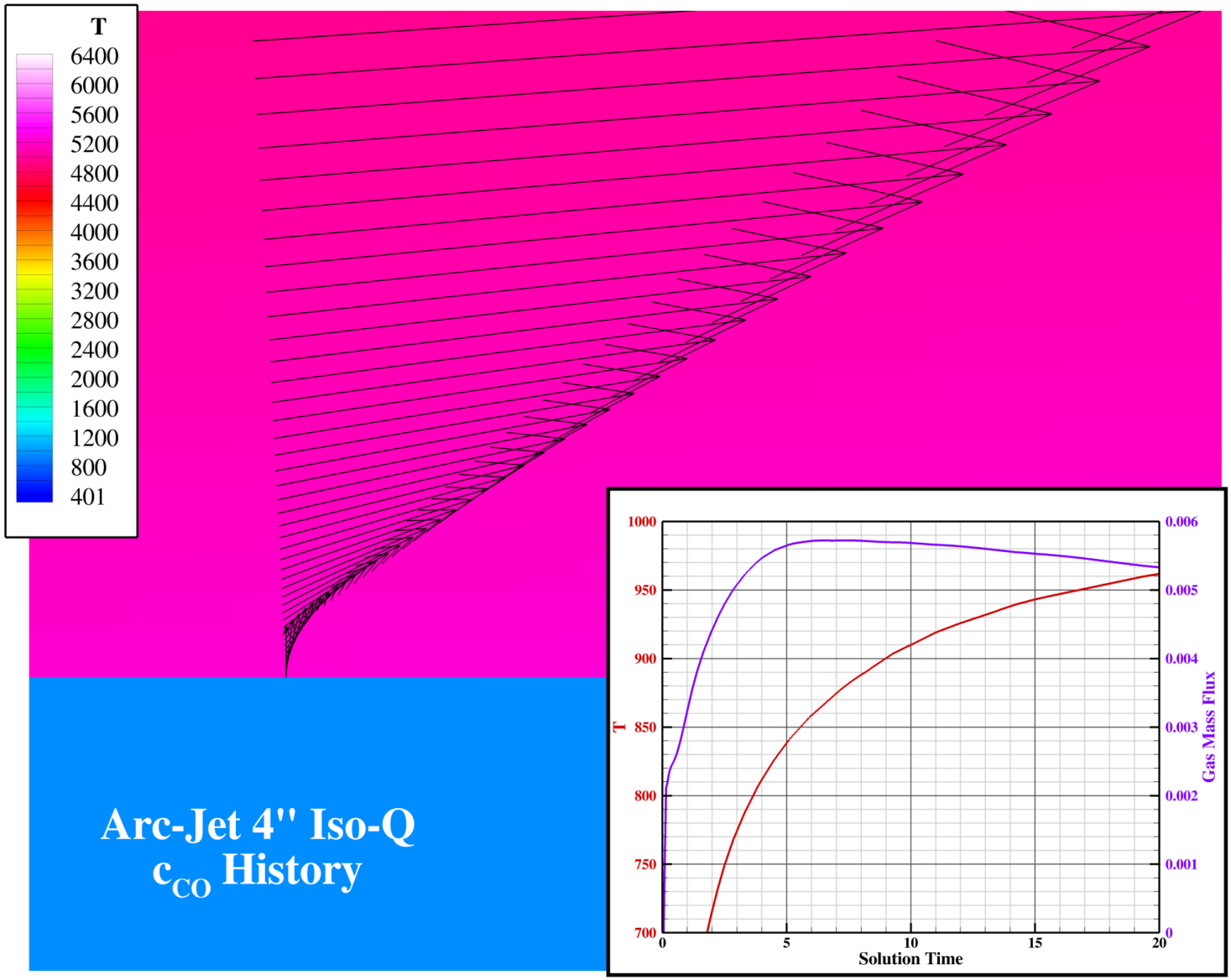
Coupled Pyrolysis, Pyrolysis gas mass flux, $\dot{m}$



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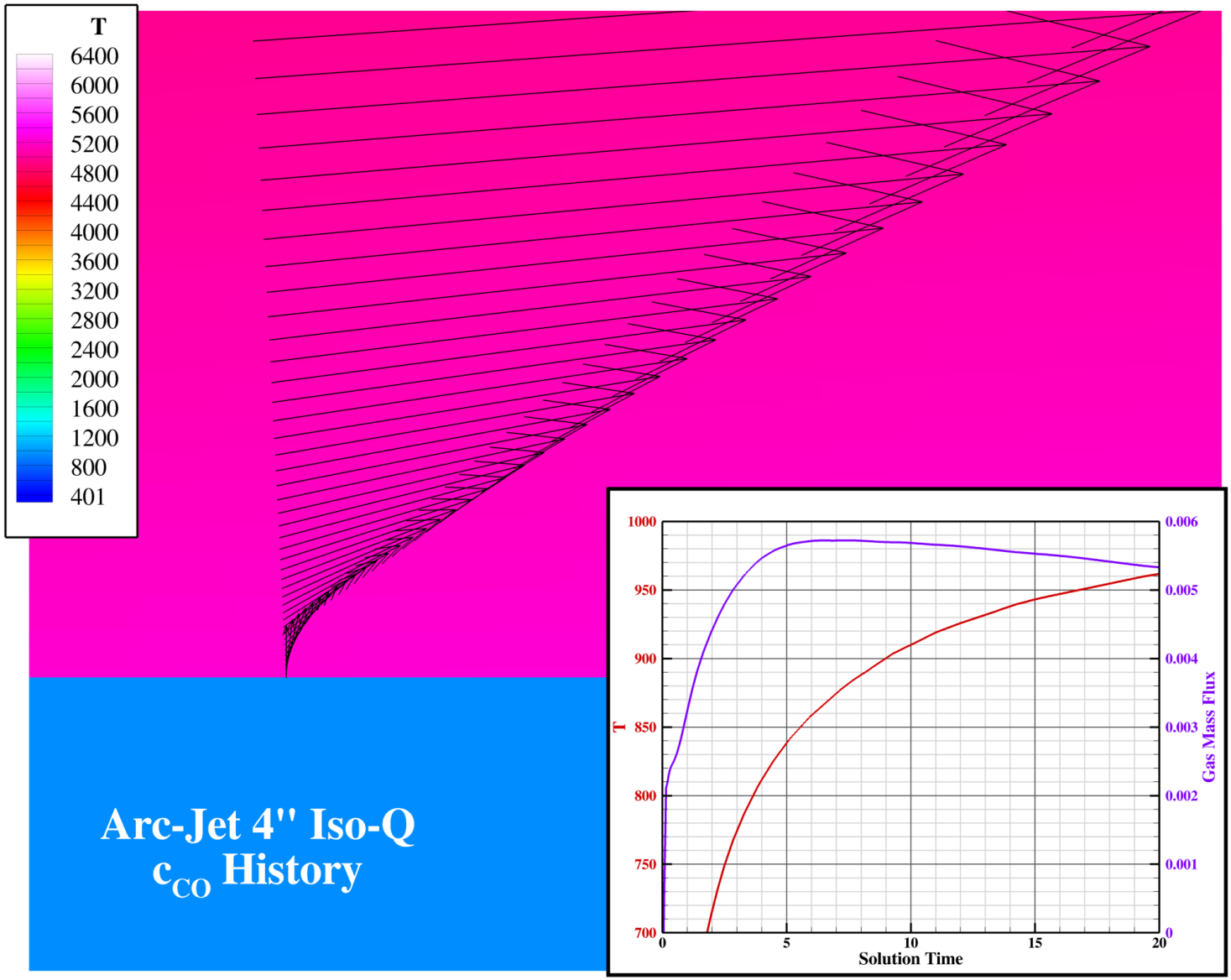

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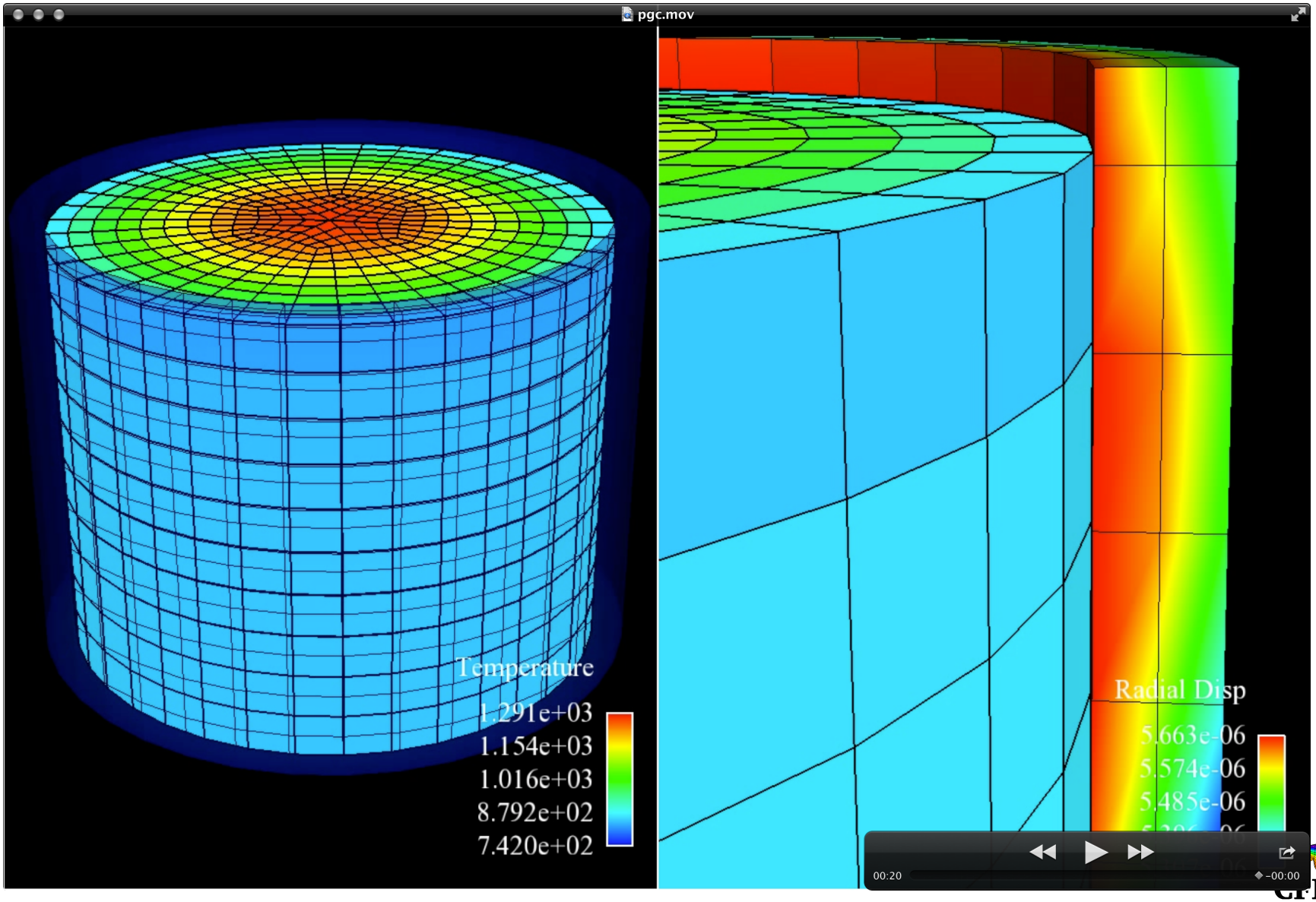
Coupled Thermal/Solid Mechanics



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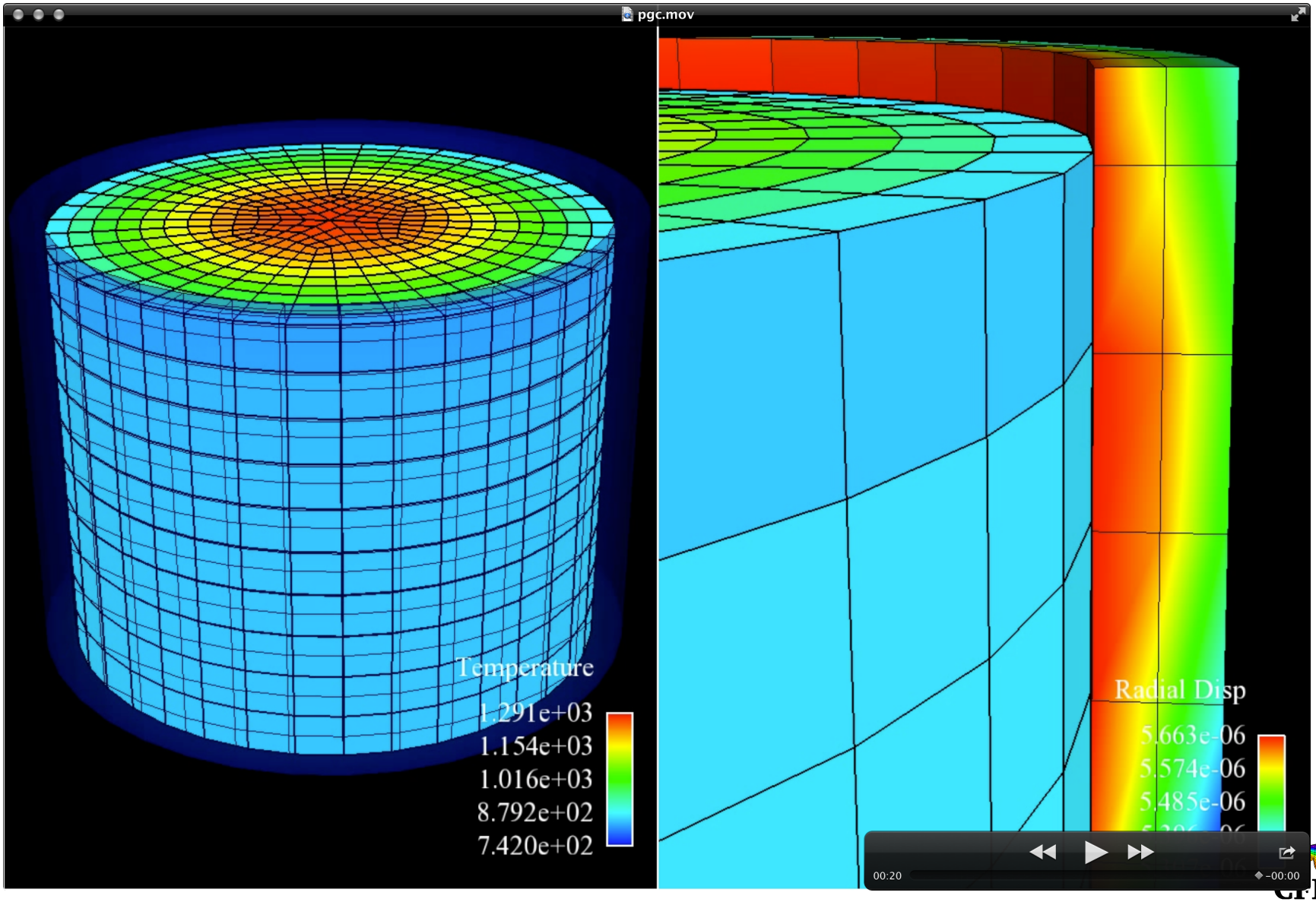

The MOOSE Framework - Gaston et al., INL

MOOSE

Derek Gaston, Idaho National Laboratory

Collaborators:
Dana Knoll, LANL
Glen Hansen, INL
Chris Newman, LANL
Ryosuke Park, INL
Cody Permann, INL
David Andrs, INL
Hai Huang, INL
Michael Tonks, INL
Robert Podgorney, INL

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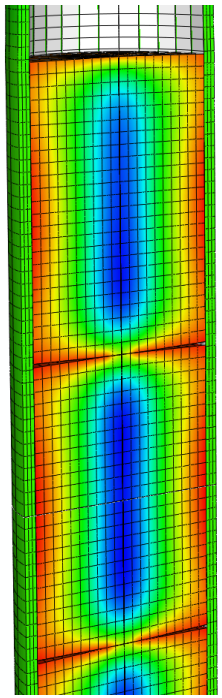
The MOOSE Framework - Gaston et al., INL

Idaho National Laboratory

MOOSE – Multiphysics Object Oriented Simulation Environment

- A framework for solving computational nuclear engineering problems in a well planned, managed, and coordinated way
  - *Leveraged across multiple programs*
- Designed to significantly reduce the expense and time required to develop new applications
- Designed to develop analysis tools
  - *Uses very robust solution methods*
  - *Designed to be easily extended and maintained*
  - *Efficient on both a few and many processors*
- Currently supports ~7 applications which are developed and used by ~20 scientists.



CFDLab

The MOOSE Framework - Gaston et al., INL

MOOSE Ecosystem

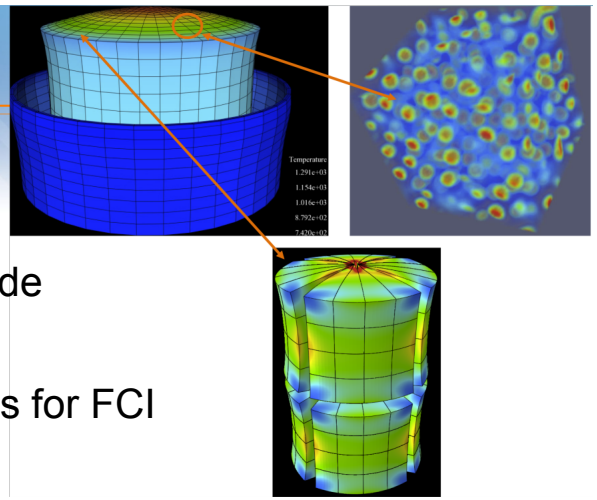
INL Idaho National Laboratory

Application	Physics	Start	Time To Results	Lines of Code
BISON	Thermo-mechanics, Chemical Diffusion, coupled mesoscale	June 2008	4 Months	931
PRONGHORN	Neutronics, Porous Flow, Eigenvalue	September 2008	3 Months	2,883
SALMON	Multiphase Porous Flow	June 2009	3 Months	800
MARMOT	4^{th} Order Phasefield Mesoscale	August 2009	1 Month	838
RAT	Porous ReActive Transport	August 2009	1 Month	439
FALCON	Geo-mechanics, coupled mesoscale	September 2009	3 Months	810

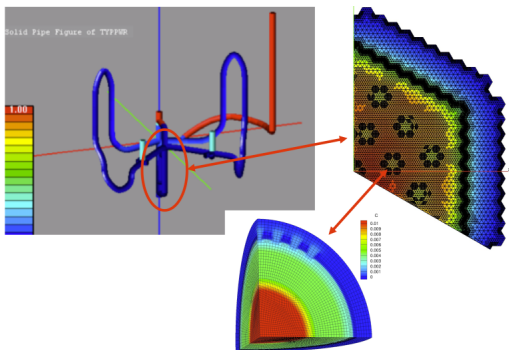
CFDLab

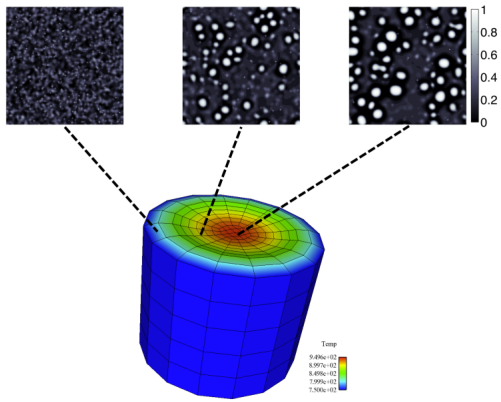
The MOOSE Framework - Gaston et al., INL

BISON fuel performance



- LWR, Triso, and TRU fuel performance code
- Parallel 1D-3D thermomechanics code
- Thermal, mechanical, and chemical models for FCI
- Constituent redistribution
- Material, fission product swelling, fission gas release models
- Mesoscale-informed material models





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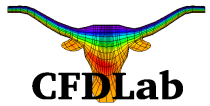
Sidebar:

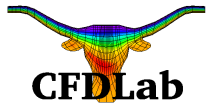
Revision Control & Collaboration with GitHub

Continuous Integration with Buildbot



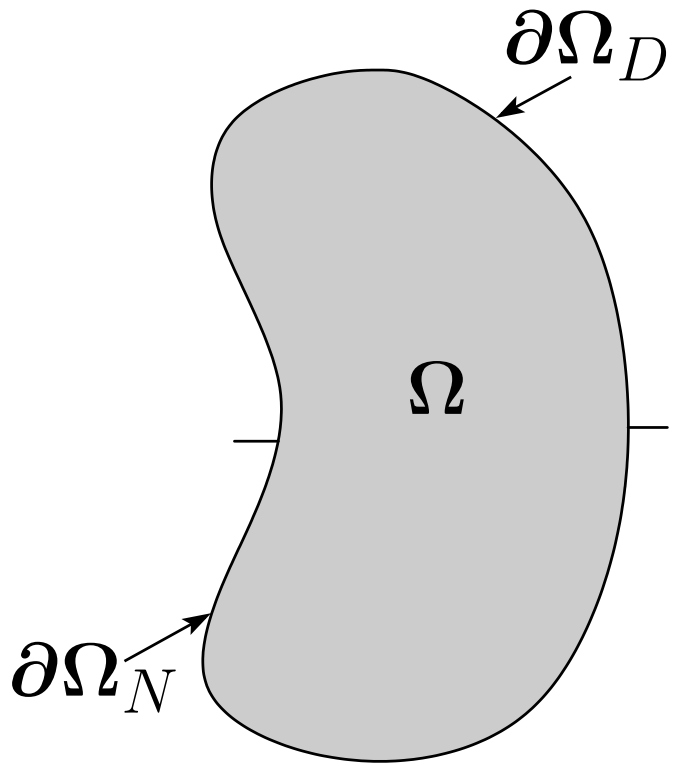
Solving Problems the **libMesh** way

Discretizing a Generic Boundary Value Problem



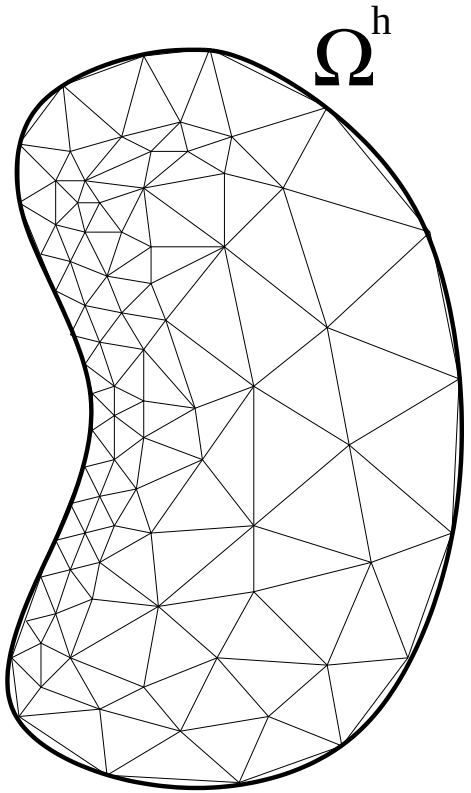
- We assume there is a Boundary Value Problem of the form

$$
\begin{aligned}
M\frac{\partial u}{\partial t} &= F(u) && \in \Omega \\
G(u) &= 0 && \in \Omega \\
u &= u_D && \in \partial\Omega_D \\
N(u) &= 0 && \in \partial\Omega_N \\
u(\boldsymbol{x},0) &= u_0(\boldsymbol{x})
\end{aligned}
$$



- Associated to the problem domain Ω is a `libMesh` data structure called a `Mesh`
- A `Mesh` is essentially a collection of finite elements

$$\Omega^h := \bigcup_e \Omega_e$$



CFDLab

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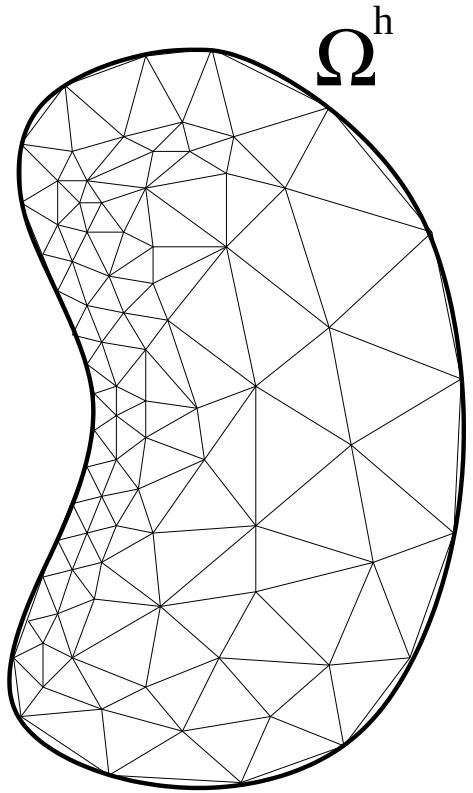


- `libMesh` provides some simple structured mesh generation routines, file inputs, and interfaces to Triangle and TetGen.

CFDLab

The Mesh

```
int main (int argc, char** argv)
{
  // Initialize the library.  This is necessary because the library
  // may depend on a number of other libraries (i.e. MPI and PETSc)
  // that require initialization before use.  When the LibMeshInit
  // object goes out of scope, other libraries and resources are
  // finalized.
  LibMeshInit init (argc, argv);

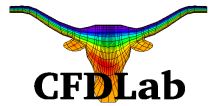
  // Create a mesh
  Mesh mesh;

  // Read the input mesh.
  mesh.read ("in.exo");

  // Print information about the mesh to the screen.
  mesh.print_info();

  // Write the output mesh
  mesh.write ("out.dat");

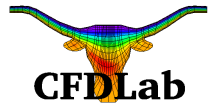
  ...
}
```



The Mesh

```
************************************************************
* Running Example introduction_ex1:
*   example-opt -d 3 reference_elements/3D/one_hex27.xda -o output.xda
************************************************************

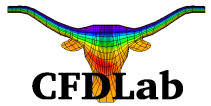
 Mesh Information:
  mesh_dimension()=3
  spatial_dimension()=3
  n_nodes()=27
    n_local_nodes()=27
  n_elem()=1
    n_local_elem()=1
    n_active_elem()=1
  n_subdomains()=1
  n_partitions()=1
  n_processors()=1
  n_threads()=1
  processor_id()=0
```



Mesh Iterators

```
void foo (const MeshBase &mesh)
{
  // Now we will loop over all the elements in the mesh that
  // live on the local processor. We will compute the element
  // matrix and right-hand-side contribution.  Since the mesh
  // may be refined we want to only consider the ACTIVE elements,
  // hence we use a variant of the \p active_elem_iterator.
  MeshBase::const_element_iterator
    el     = mesh.active_local_elements_begin();
  const MeshBase::const_element_iterator
    end_el = mesh.active_local_elements_end();

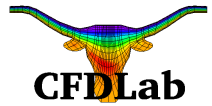
  for ( ; el != end_el; ++el)
    {
      // Store a pointer to the element we are currently
      // working on.  This allows for nicer syntax later.
      const Elem* elem = *el;
      ...
    }
  ...
}
```



Mesh Iterators

```
void foo (const MeshBase &mesh)
{
  // We will now loop over all nodes.
  MeshBase::const_node_iterator       node_it  = mesh.nodes_begin();
  const MeshBase::const_node_iterator node_end = mesh.nodes_end();

  for ( ; node_it != node_end; ++node_it)
    {
      // the current node pointer
      const Node* node = *node_it;
      ...
    }
  ...
}
```



```
...
// Create a mesh.
Mesh mesh;

// Create a uniform 5x5 mesh on the unit square.
MeshTools::Generation::build_square (mesh, 5, 5);
mesh.print_info();

// Create an equation systems object. This object can contain
// multiple systems of different flavors for solving loosely coupled
// physics.  Each system can contain multiple variables of different
// approximation orders. The EquationSystems object needs a
// reference to the mesh object, so the order of construction here
// is important.
EquationSystems equation_systems (mesh);

// Now we declare the system and its variables.  We begin by adding
// a "TransientLinearImplicitSystem" to the EquationSystems object,
// and we give it the name "Simple System".
equation_systems.add_system<TransientLinearImplicitSystem> ("Simple System");

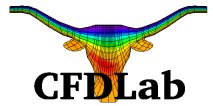
// Adds the variable "u" to "Simple System".  "u" will be
// approximated using first-order approximation.
equation_systems.get_system("Simple System").add_variable("u", FIRST);

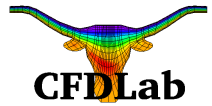
// Next we'll by add an "ExplicitSystem" to the EquationSystems
// object, and we give it the name "Complex System".
equation_systems.add_system<ExplicitSystem> ("Complex System");

// Give "Complex System" three variables -- each with a different
// approximation order.  Variables "c" and "T" will use first-order
// Lagrange approximation, while variable "dv" will use a
// second-order discontinuous approximation space.
equation_systems.get_system("Complex System").add_variable("c", FIRST);
equation_systems.get_system("Complex System").add_variable("T", FIRST);
equation_systems.get_system("Complex System").add_variable("dv", SECOND, MONOMIAL);

// Initialize the data structures for the equation system.
equation_systems.init();

// Prints information about the system to the screen.
equation_systems.print_info();
...
```





- The point of departure in any FE analysis which uses `libMesh` is the weighted residual statement

$$(F(u), v) = 0 \qquad \forall v \in \mathcal{V}$$

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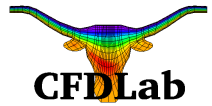
$$(F(u), v) = 0 \qquad \forall v \in \mathcal{V}$$

- Or, more precisely, the weighted residual statement associated with the finite-dimensional space $\mathcal{V}^h \subset \mathcal{V}$

$$(F(u^h), v^h) = 0 \qquad \forall v^h \in \mathcal{V}^h$$



Poisson Equation

$$-\Delta u = f \qquad \in \quad \Omega$$

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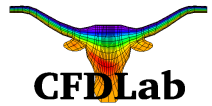
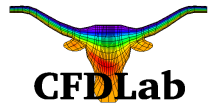
Weighted Residual Statement

$$(F(u), v) := \int_\Omega \left[\nabla u \cdot \nabla v - fv\right] dx + \int_{\partial\Omega_N} (\nabla u \cdot \boldsymbol{n})\, v \, ds$$



Linear Convection-Diffusion

$$-k\Delta u + \boldsymbol{b} \cdot \nabla u = f \qquad \in \quad \Omega$$



Linear Convection-Diffusion

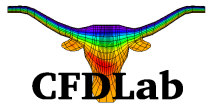
$$-k\Delta u + \boldsymbol{b} \cdot \nabla u = f \qquad \in \quad \Omega$$

Weighted Residual Statement

$$(F(u), v) := \int_{\Omega} \left[k\nabla u \cdot \nabla v + (\boldsymbol{b} \cdot \nabla u)v - fv \right] dx + \int_{\partial\Omega_N} k \left(\nabla u \cdot \boldsymbol{n} \right) v \, ds$$

Stokes Flow

$$\begin{aligned} \nabla p - \nu \Delta \boldsymbol{u} &= \boldsymbol{f} \\ \nabla \cdot \boldsymbol{u} &= 0 \end{aligned} \qquad \in \quad \Omega$$



Stokes Flow

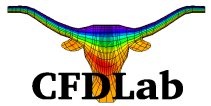
$$\begin{aligned} \nabla p - \nu \Delta \boldsymbol{u} &= \boldsymbol{f} \\ \nabla \cdot \boldsymbol{u} &= 0 \end{aligned} \qquad \in \quad \Omega$$

Weighted Residual Statement

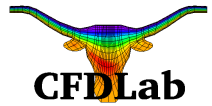
$$u := [\boldsymbol{u}, p] \quad , \quad v := [\boldsymbol{v}, q]$$

$$(F(u), v) := \int_{\Omega} \left[-p \left(\nabla \cdot \boldsymbol{v} \right) + \nu \nabla \boldsymbol{u} : \nabla \boldsymbol{v} - \boldsymbol{f} \cdot \boldsymbol{v} \right.$$

$$\left. + \left(\nabla \cdot \boldsymbol{u} \right) q \right] dx + \int_{\partial \Omega_N} \left(\nu \nabla \boldsymbol{u} - p \boldsymbol{I} \right) \boldsymbol{n} \cdot \boldsymbol{v} \, ds$$



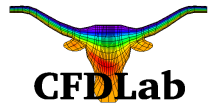
- To obtain the approximate problem, we simply replace $u \leftarrow u^h$, $v \leftarrow v^h$, and $\Omega \leftarrow \Omega^h$ in the weighted residual statement.



CFDLab

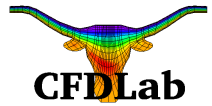
- For simplicity we start with the weighted residual statement arising from the Poisson equation, with $\partial\Omega_N = \emptyset$,

$$(F(u^h), v^h) := \int_{\Omega^h} \left[\nabla u^h \cdot \nabla v^h - f v^h\right] dx = 0 \qquad \forall v^h \in \mathcal{V}^h$$



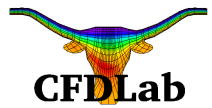
- The integral over Ω^h ...

$$0 = \int_{\Omega^h} \left[\nabla u^h \cdot \nabla v^h - f v^h \right] dx \qquad \forall v^h \in \mathcal{V}^h$$



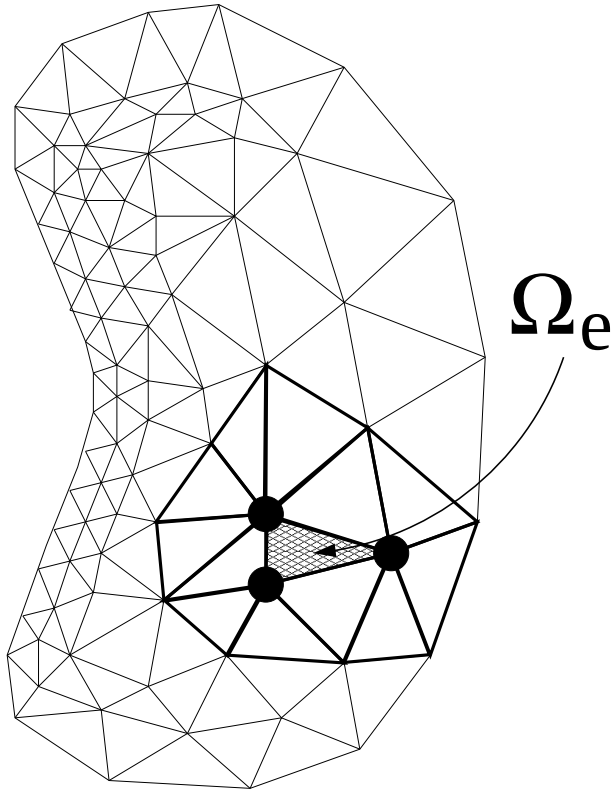
- The integral over Ω^h ... is written as a sum of integrals over the N_e finite elements:

$$
\begin{aligned}
0 &= \int_{\Omega^h} \left[\nabla u^h \cdot \nabla v^h - f v^h\right] dx \qquad \forall v^h \in \mathcal{V}^h \\
&= \sum_{e=1}^{N_e} \int_{\Omega_e} \left[\nabla u^h \cdot \nabla v^h - f v^h\right] dx \qquad \forall v^h \in \mathcal{V}^h
\end{aligned}
$$



- An element integral will have contributions only from the global basis functions corresponding to its nodes.
- We call these local basis functions ϕ_i, $0 \leq i \leq N_s$.

$$v^h\big|_{\Omega_e} = \sum_{i=1}^{N_s} c_i \phi_i$$



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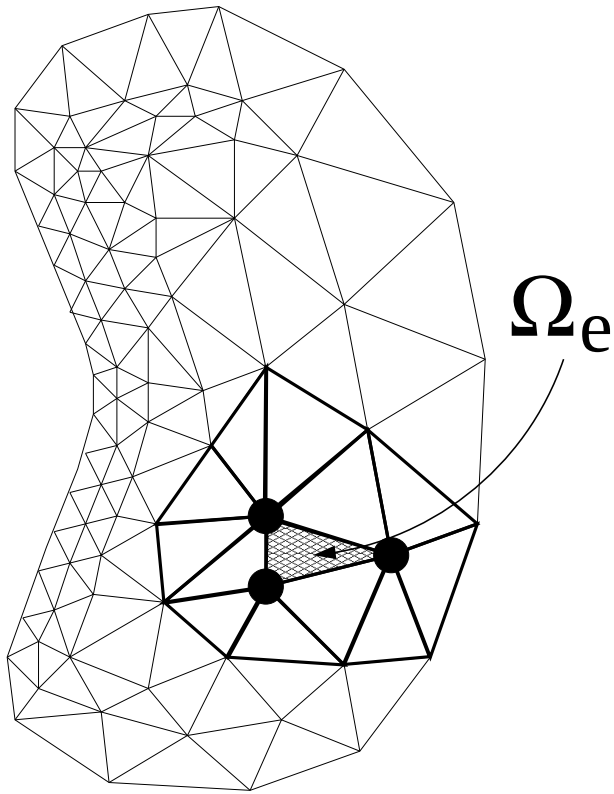

$$v^h\big|_{\Omega_e} = \sum_{i=1}^{N_s} c_i \phi_i$$

$$\int_{\Omega_e} v^h \, dx = \sum_{i=1}^{N_s} c_i \int_{\Omega_e} \phi_i \, dx$$

- The element integrals . . .

$$\int_{\Omega_e} \left[\nabla u^h \cdot \nabla v^h - f v^h \right] dx$$

- The element integrals . . .

$$\int_{\Omega_e} \left[\nabla u^h \cdot \nabla v^h - f v^h \right] dx$$

- are written in terms of the local "ϕ_i" basis functions

$$\sum_{j=1}^{N_s} u_j \int_{\Omega_e} \nabla \phi_j \cdot \nabla \phi_i \, dx - \int_{\Omega_e} f \phi_i \, dx \quad , \quad i = 1, \ldots, N_s$$

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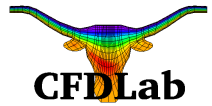
$$\sum_{j=1}^{N_s} u_j \int_{\Omega_e} \nabla \phi_j \cdot \nabla \phi_i \, dx - \int_{\Omega_e} f \phi_i \, dx \quad , \quad i = 1, \ldots, N_s$$

- This can be expressed naturally in matrix notation as

$$\boldsymbol{K}^e \boldsymbol{U}^e - \boldsymbol{F}^e$$



- The entries of the element stiffness matrix are the integrals

$$\boldsymbol{K}_{ij}^{e} := \int_{\Omega_e} \nabla\phi_j \cdot \nabla\phi_i \, dx$$

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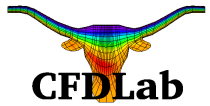
$$\boldsymbol{K}_{ij}^{e} := \int_{\Omega_e} \nabla \phi_j \cdot \nabla \phi_i \, dx$$

- While for the element right-hand side we have

$$\boldsymbol{F}_{i}^{e} := \int_{\Omega_e} f \phi_i \, dx$$



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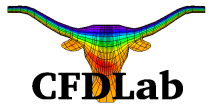
$$\boldsymbol{K}_{ij}^{e} := \int_{\Omega_e} \nabla \phi_j \cdot \nabla \phi_i \, dx$$

- While for the element right-hand side we have

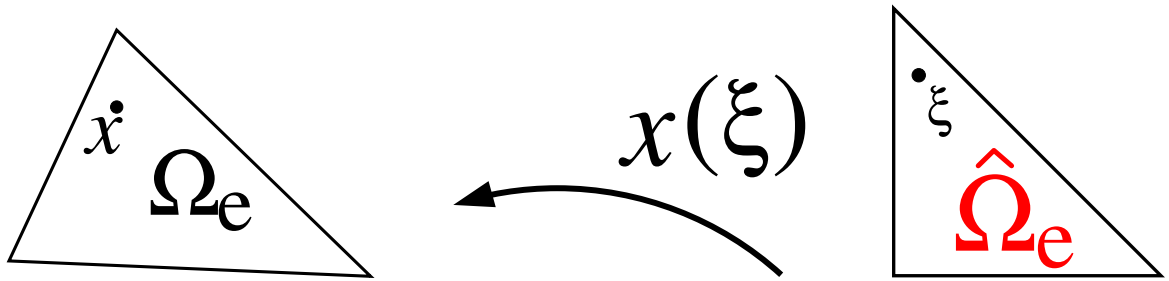
$$\boldsymbol{F}_{i}^{e} := \int_{\Omega_e} f \phi_i \, dx$$

- The element stiffness matrices and right-hand sides can be "assembled" to obtain the global system of equations

$$\boldsymbol{K}\boldsymbol{U} = \boldsymbol{F}$$



- The integrals are performed on a “reference” element $\hat{\Omega}_e$



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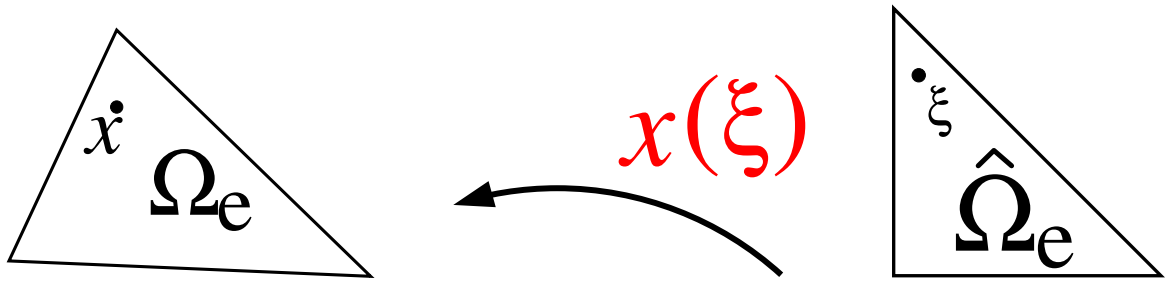
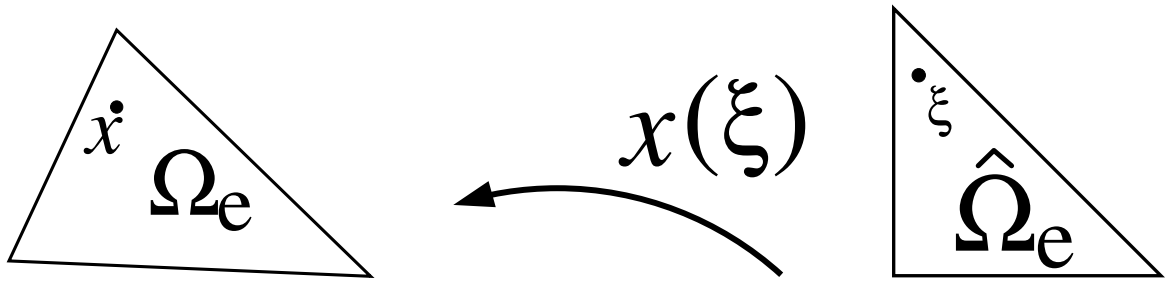


- The Jacobian of the map $x(\xi)$ is J.

$$\boldsymbol{F}_i^e = \int_{\Omega_e} f\phi_i dx = \int_{\hat{\Omega}_e} f(x(\xi))\phi_i |\boldsymbol{J}| d\xi$$

- The integrals are performed on a "reference" element $\hat{\Omega}_e$



- Chain rule: $\nabla = J^{-1}\nabla_\xi := \hat{\nabla}_\xi$

$$\boldsymbol{K}_{ij}^e = \int_{\Omega_e} \nabla\phi_j \cdot \nabla\phi_i \, dx = \int_{\hat{\Omega}_e} \hat{\nabla}_\xi\phi_j \cdot \hat{\nabla}_\xi\phi_i \, |J| d\xi$$

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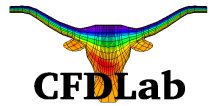

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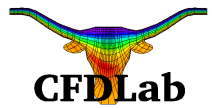

- libMesh provides the following variables at each quadrature point q

Code	Math	Description
JxW[q]	$\lvert J(\xi_q)\rvert w_q$	Jacobian times weight
phi[i][q]	$\phi_i(\xi_q)$	value of i^{th} shape fn.
dphi[i][q]	$\hat{\nabla}_\xi \phi_i(\xi_q)$	value of i^{th} shape fn. gradient
xyz[q]	$x(\xi_q)$	location of ξ_q in physical space

- The `libMesh` representation of the matrix and rhs assembly is similar to the mathematical statements.

```
for (q=0; q<Nq; ++q)
  for (i=0; i<Ns; ++i) {
    Fe(i)   += JxW[q]*f(xyz[q])*phi[i][q];

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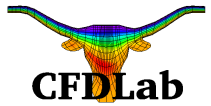

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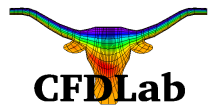

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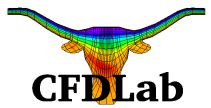

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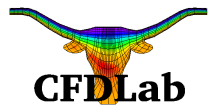

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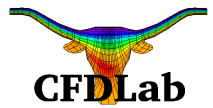

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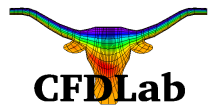


```
// We now define the matrix assembly function for the Poisson system
// by computing the element matrices and right-hand sides.  We are
// omitting BCs for brevity.
void assemble_poisson(EquationSystems& es,
                      const std::string& system_name)
{
  // Get a constant reference to the mesh object.
  const MeshBase& mesh = es.get_mesh();

  // The dimension that we are running
  const unsigned int dim = mesh.mesh_dimension();

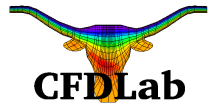
  // Get a reference to the LinearImplicitSystem we are solving
  LinearImplicitSystem& system = es.get_system<LinearImplicitSystem>("Poisson");

  // A reference to the DofMap object for this system.  The DofMap
  // object handles the index translation from node and element
  // numbers to degree of freedom numbers.  We will talk more about
  // the DofMap in future examples.
  const DofMap& dof_map = system.get_dof_map();

  // Get a constant reference to the Finite Element type for the first
  // (and only) variable in the system.
  FEType fe_type = dof_map.variable_type(0);

  // Build a Finite Element object of the specified type.  Since the
  // FEBase::build() member dynamically creates memory we will store
  // the object as an AutoPtr<FEBase>.  This can be thought of as a
  // pointer that will clean up after itself.
  AutoPtr<FEBase> fe (FEBase::build(dim, fe_type));

  // A 5th order Gauss quadrature rule for numerical integration.
  QGauss qrule (dim, FIFTH);
```



```
// Tell the finite element object to use our quadrature rule.
fe->attach_quadrature_rule (&qrule);

// Here we define some references to cell-specific data that will be
// used to assemble the linear system.  We begin with the element
// Jacobian * quadrature weight at each integration point.
const std::vector<Real>& JxW = fe->get_JxW();

// The physical XY locations of the quadrature points on the
// element.  These might be useful for evaluating spatially varying
// material properties at the quadrature points.
const std::vector<Point>& q_point = fe->get_xyz();

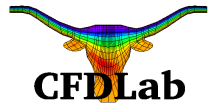
// The element shape functions evaluated at the quadrature points.
const std::vector<std::vector<Real> >& phi = fe->get_phi();

// The element shape function gradients evaluated at the quadrature
// points.
const std::vector<std::vector<RealGradient> >& dphi = fe->get_dphi();

// Define data structures to contain the element matrix and
// right-hand-side vector contribution.  Following basic finite
// element terminology we will denote these "Ke" and "Fe".
DenseMatrix<Number> Ke;
DenseVector<Number> Fe;

// This vector will hold the degree of freedom indices for the
// element.  These define where in the global system the element
// degrees of freedom get mapped.
std::vector<dof_id_type> dof_indices;

// Now we will loop over all the elements in the mesh.  We will
```



```
// compute the element matrix and right-hand-side contribution.  See
// example 3 for a discussion of the element iterators.
MeshBase::const_element_iterator       el     = mesh.active_local_elements_begin();
const MeshBase::const_element_iterator end_el = mesh.active_local_elements_end();

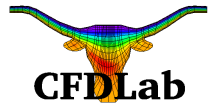
for ( ; el != end_el; ++el)
  {
    // Store a pointer to the element we are currently working on.
    // This allows for nicer syntax later.
    const Elem* elem = *el;

    // Get the degree of freedom indices for the current element.
    // These define where in the global matrix and right-hand-side
    // this element will contribute to.
    dof_map.dof_indices (elem, dof_indices);

    // Compute the element-specific data for the current element.
    // This involves computing the location of the quadrature points
    // (q_point) and the shape functions (phi, dphi) for the current
    // element.
    fe->reinit (elem);

    // Zero the element matrix and right-hand side before summing
    // them.  We use the resize member here because the number of
    // degrees of freedom might have changed from the last element.
    // Note that this will be the case if the element type is
    // different (i.e. the last element was a triangle, now we are
    // on a quadrilateral).
    Ke.resize (dof_indices.size(),
               dof_indices.size());

    Fe.resize (dof_indices.size());
```

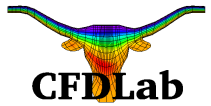


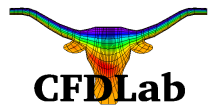
```
      // Now we will build the element matrix.  This involves a double
      // loop to integrate the test funcions (i) against the trial
      // functions (j).
      for (unsigned int qp=0; qp<qrule.n_points(); qp++)
        for (unsigned int i=0; i<phi.size(); i++)
          for (unsigned int j=0; j<phi.size(); j++)
            Ke(i,j) += JxW[qp]*(dphi[i][qp]*dphi[j][qp]);

      // Now we build the element right-hand-side contribution.  This
      // involves a single loop in which we integrate the "forcing
      // function" in the PDE against the test functions.
      for (unsigned int qp=0; qp<qrule.n_points(); qp++)
        for (unsigned int i=0; i<phi.size(); i++)
          Fe(i) += JxW[qp]*10.*phi[i][qp];

      // If we are using an adaptive mesh this will apply any hanging
      // node constraint equations
      dof_map.heterogenously_constrain_element_matrix_and_vector (Ke, Fe, dof_indices);

      // The element matrix and right-hand-side are now built for this
      // element.  Add them to the global matrix and right-hand-side
      // vector.  The SparseMatrix::add_matrix() and
      // NumericVector::add_vector() members do this for us.
      system.matrix->add_matrix (Ke, dof_indices);
      system.rhs->add_vector    (Fe, dof_indices);
    }
}
```





- The matrix assembly routine for the linear convection-diffusion equation,

$$-k\Delta u + \boldsymbol{b} \cdot \nabla u = f$$

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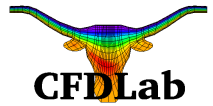

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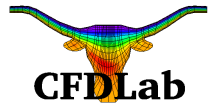

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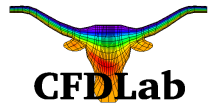

- For multi-variable systems like Stokes flow,

$$\begin{aligned} \nabla p - \nu \Delta \boldsymbol{u} &= \boldsymbol{f} \\ \nabla \cdot \boldsymbol{u} &= 0 \end{aligned} \qquad \in \quad \Omega \subset \mathbb{R}^2$$

- The element stiffness matrix concept can extended to include sub-matrices

$$\left[\begin{array}{cc|c} K^e_{u_1u_1} & K^e_{u_1u_2} & K^e_{u_1p} \\ K^e_{u_2u_1} & K^e_{u_2u_2} & K^e_{u_2p} \\ \hline K^e_{pu_1} & K^e_{pu_2} & K^e_{pp} \end{array}\right] \left[\begin{array}{c} U^e_{u_1} \\ U^e_{u_2} \\ \hline U^e_p \end{array}\right] - \left[\begin{array}{c} F^e_{u_1} \\ F^e_{u_2} \\ \hline F^e_p \end{array}\right]$$

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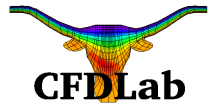

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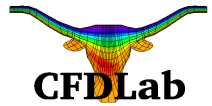

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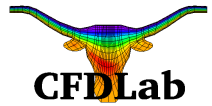
- We have an array of submatrices: `Ke[1][1]`



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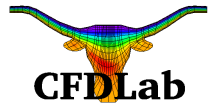
- We have an array of submatrices: `Ke[2][1]`



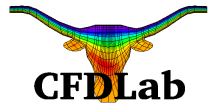
- For multi-variable systems like Stokes flow,

$$\begin{aligned} \nabla p - \nu \Delta \boldsymbol{u} &= \boldsymbol{f} \\ \nabla \cdot \boldsymbol{u} &= 0 \end{aligned} \qquad \in \quad \Omega \subset \mathbb{R}^2$$

- The element stiffness matrix concept can extended to include sub-matrices

$$\left[\begin{array}{cc|c} K^e_{u_1u_1} & K^e_{u_1u_2} & K^e_{u_1p} \\ K^e_{u_2u_1} & K^e_{u_2u_2} & K^e_{u_2p} \\ \hline K^e_{pu_1} & K^e_{pu_2} & K^e_{pp} \end{array}\right] \left[\begin{array}{c} U^e_{u_1} \\ U^e_{u_2} \\ \hline U^e_p \end{array}\right] - \left[\begin{array}{c} F^e_{u_1} \\ F^e_{u_2} \\ \hline F^e_p \end{array}\right]$$

- And an array of right-hand sides: `Fe[]`.



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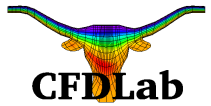
- And an array of right-hand sides: `Fe[0]`.



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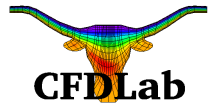
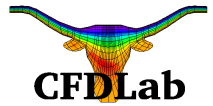
- And an array of right-hand sides: `Fe[1]`.



- The matrix assembly can proceed in essentially the same way.
- For the momentum equations:

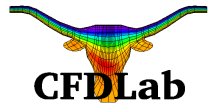
```
for (q=0; q<Nq; ++q)
  for (d=0; d<2; ++d)
    for (i=0; i<Ns; ++i) {
      Fe[d](i) += JxW[q]*f(xyz[q],d)*phi[i][q];

      for (j=0; j<Ns; ++j)
        Ke[d][d](i,j) +=
            JxW[q]*nu*(dphi[j][q]*dphi[i][q]);
    }
```



- For linear problems, we have already seen how the weighted residual statement leads directly to a sparse linear system of equations

$$\boldsymbol{KU} = \boldsymbol{F}$$



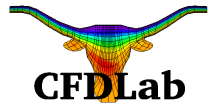
- For time-dependent problems,

$$\frac{\partial u}{\partial t} = F(u)$$

- we also need a way to advance the solution in time, e.g. a θ-method

$$\begin{aligned} \left(\frac{u^{n+1} - u^n}{\Delta t}, v^h \right) &= \left(F(u_\theta), v^h \right) \quad \forall v^h \in \mathcal{V}^h \\ u_\theta &:= \theta u^{n+1} + (1-\theta) u^n \end{aligned}$$

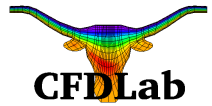
- Leads to $\boldsymbol{KU} = \boldsymbol{F}$ at *each timestep*.



- For nonlinear problems, typically a sequence of linear problems must be solved, e.g. for Newton's method

$$(F'(u^k)\delta u^{k+1}, v) = -(F(u^k), v)$$

  where $F'(u^k)$ is the linearized (Jacobian) operator associated with the PDE.
- Must solve $\boldsymbol{KU} = \boldsymbol{F}$ (Inexact Newton method) at *each iteration step*.



- B. Kirk, J. Peterson, R. Stogner and G. Carey, “libMesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations”, *Engineering with Computers*, vol. 22, no. 3–4, p. 237–254, 2006.

- Public site, mailing lists, SVN tree, examples, etc.: `http://libmesh.sf.net/`

CFDLab