libMesh A New User's Experience

Shayan Hoshyari

April, 2016



Outline

Getting Started

- Introduction
- Installing libMesh

2 Application

- A Sample Problem
- The Code





Major components of a mesh based numerical solution technique:

Read the mesh from file



- Read the mesh from file
- Initialize data structures



- Read the mesh from file
- Initialize data structures
- Onstruct a discrete representation of the governing equations



- Read the mesh from file
- Initialize data structures
- Onstruct a discrete representation of the governing equations
- Solve the discrete system



- Read the mesh from file
- Initialize data structures
- Onstruct a discrete representation of the governing equations
- Solve the discrete system
- Write out results



- Read the mesh from file
- Initialize data structures
- **③** Construct a discrete representation of the governing equations
- Solve the discrete system
- Write out results
- Optionally estimate error, refine the mesh, and repeat



Major components of a mesh based numerical solution technique:

- Read the mesh from file
- Initialize data structures
- **③** Construct a discrete representation of the governing equations
- Solve the discrete system
- Write out results
- Optionally estimate error, refine the mesh, and repeat

libMesh is a C++ library that offers functionality to handle the tasks above, with the exception of step 3.



Major components of a mesh based numerical solution technique:

- Read the mesh from file
- Initialize data structures
- **③** Construct a discrete representation of the governing equations
- Solve the discrete system
- Write out results
- Optionally estimate error, refine the mesh, and repeat

libMesh is a C++ library that offers functionality to handle the tasks above, with the exception of step 3.



Resources

- libMesh website: https://libmesh.github.io
- Stable Releases:

https://github.com/libMesh/libmesh/releases

- Development tree:
 - \$ git clone git://github.com/libMesh/libmesh.git



Environment Variables

```
# libMesh important directories
export LIBMESH_SRC="/path/to/libmesh/source/dir"
export LIBMESH_DIR="/path/to/libmesh/install/dir"
# Flavour to be used in runtime:
export METHOD="opt"
# If you wish to compile with PETSc
# MPI path is taken from PETSc configuration
export PETSC_ARCH="petsc-architecture"
export PETSC_DIR="/path/to/petsc"
```



Configure and Make

```
# Read through configure help first
./configure ---help
# Configure libMesh
./configure METHODS="dbg opt gprof" \
--disable-fortran \setminus
--with-metis=PETSc \setminus
--- disable -- strict -- lgpl \
--prefix=/home/hooshi/code/libmesh/mpich-petsc \
---enable-laspack \
---enable-unique-ptr
# Make and install
make - j 8
make install
```



Linking With libMesh

For small applications use the 'libmesh-config' executable found in the install directory.

For larger applications include Make.common in your Makefile. See Makefiles in the example folders.



Poisson Problem

- The equation: $\Delta u = f \qquad u \in \Omega$
- Penalty method for Dirichlet boundary condition: $\frac{1}{\epsilon}u(x) + u_n(x) = \frac{1}{\epsilon}u_0(x) \qquad x \in \partial\Omega$
- A mesh with appropriate boundary tags should be available in one of the many supported formats, e.g., gmsh, Triangle and Tetgen.



Supported Mesh Elements

Effect

- The mapping from the reference element to the computational element.
- Limits on the available finite element basis functions.
- 2, 3, and 4 noded edges (Edge2, Edge3, Edge4)
- 3 and 6 noded triangles (Tri3, Tri6)
- 4, 8, and 9 noded quadrilaterals (Quad4, Quad8, Quad9)
- 4 and 10 noded tetrahedrals (Tet4, Tet10)
- 8, 20, and 27 noded hexahedrals (Hex8, Hex20, Hex27)
- 6, 15, and 18 noded prisms (Prism6, Prism15, Prism18)
- 5, 13, and 14 noded pyramids (Pyramid5, Pyramid13, Pyramid14)



The main function

```
//Assembe Function to be introduced later
void assemble_poisson(EquationSystems& es, const string&);
int main (int argc, char** argv)
 // Initialize libraries.
  LibMeshInit init (argc, argv);
  // Create a mesh
  Mesh mesh(init.comm());
  // Read the mesh
 GmshIO gmsh(mesh);
  gmsh.read("../mesh/simple_box_5.msh");
  mesh.all_second_order(true);
  mesh.prepare_for_use();
```

// Create an equation systems object.
EquationSystems equation_systems (mesh);



The main function

```
// Add a system to be solved
equation_systems.
add_system<LinearImplicitSystem> ("Poisson");
```

```
// Add a variable
equation_systems.get_system("Poisson")
.add_variable("u", SECOND, HIERARCHIC);
```

```
// Attach the assembler function
equation_systems.get_system("Poisson")
.attach_assemble_function (assemble_poisson);
```



The main function

```
// Initialize the data structures.
equation_systems.init();
```

```
// Solve the system
equation_systems.get_system("Poisson").solve();
```

```
// write the results
VTKIO (mesh).write_equation_systems
("out.pvtu", equation_systems);
```

```
return 0;
}
```





Some useful ones

- ExplicitSystem
- LinearImplicitSystem
- TransientLinearImplicitSystem
- DifferentiableSystem
- FEMSystem



Finite Element Families

- Lagrange (Up to quadratic)
- High Order C0
 - Hierarchic
 - Bernstein
 - Szabo-Babuska
- C1 elements
 - Hermite
 - Clough-Tocher
- Discontinuous elements
 - Monomials
 - L2-Lagrange
 - L2-Hierarchic
- Vector-valued elements
 - Lagrange-Vec
 - Nedelec first type
 - No Raviart-Thomas as of now



Assemble Function

Nomenclature for the *i*th degree of freedom and *q*th quadrature point (volume or surface).

Code	Math	Description
JxW[q]	$ J(\xi_q) w_q$	Jacobian times weight
phi[i][q]	$\phi_i(\xi_q)$	value of i^{th} shape fn.
dphi[i][q]	$\nabla \phi_i(\xi_q)$	value of <i>i</i> th shape fn. gradient
d2phi[i][q]	$\nabla \nabla \phi_i(\xi_q)$	value of <i>i</i> th shape fn. Hessian
xyz [q]	$x(\xi_q)$	location of ξ_q in physical space
normals[q]	$\vec{n}(x(\xi_q))$	normal vector at x on a side



$$\begin{aligned} F_i^e &= \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q \\ K_{ij}^e &= \sum_{q=1}^{N_q} \nabla \phi_j(\xi_q) \cdot \nabla \phi_i(\xi_q) |J(\xi_q)| w_q \end{aligned}$$



```
for(q=0; q<Nq; ++q)
for (i=0; i<Ns; ++i)
{
    Fe(i) += JxW[q] * f(xyz[q])*phi[i][q];
    for (j=0; j<Ns; ++j)
      Ke(i,j) += JxW[q]*(dphi[j][q]*dphi[i][q]);
}</pre>
```

$$F_i^e = \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q$$

$$K_{ij}^{e} = \sum_{q=1}^{N_{q}} \nabla \phi_{j}(\xi_{q}) \cdot \nabla \phi_{i}(\xi_{q}) |J(\xi_{q})| w_{q}$$



$$F_i^e = \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q$$

$$K_{ij}^{e} = \sum_{q=1}^{N_{q}} \nabla \phi_{j}(\xi_{q}) \cdot \nabla \phi_{i}(\xi_{q}) |J(\xi_{q})| w_{q}$$



$$F_i^e = \sum_{q=1}^{N_q} f(\mathbf{x}(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q$$

$$K_{ij}^{e} = \sum_{q=1}^{N_{q}} \nabla \phi_{j}(\xi_{q}) \cdot \nabla \phi_{i}(\xi_{q}) |J(\xi_{q})| w_{q}$$



$$F_i^e = \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q$$

$$K_{ij}^{e} = \sum_{q=1}^{N_{q}} \nabla \phi_{j}(\xi_{q}) \cdot \nabla \phi_{i}(\xi_{q}) |J(\xi_{q})| w_{q}$$



$$\begin{aligned} F_i^e &= \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q \\ K_{ij}^e &= \sum_{q=1}^{N_q} \nabla \phi_j(\xi_q) \cdot \nabla \phi_i(\xi_q) |J(\xi_q)| w_q \end{aligned}$$



$$F_i^e = \sum_{q=1}^{N_q} f(x(\xi_q)) \phi_i(\xi_q) |J(\xi_q)| w_q$$

 $K_{ij}^e = \sum_{q=1}^{N_q} \nabla \phi_j(\xi_q) \cdot \nabla \phi_i(\xi_q) |J(\xi_q)| w_q$



Further Functionality

- Runtime selection of solver package: PETSc, Trillinos, Laspack
- Code can be parallelized with minor changes through threading or MPI
- Various error estimation algorithms
- Mesh adaptation and repartitioning in parallel
- Discontinuous Galerkin Methods





Roy Stogner, Derek Gaston libMesh Finite Element Library. http://users.ices.utexas.edu/~roystgnr/ libmeshpdfs/roystgnr/sandia_libmesh.pdf

Benjamin S. Kirk, John W. Peterson, Roy H. Stogner The libMesh Finite Element Library. http://www.training.prace-ri.eu/uploads/tx_ pracetmo/libmesh.pdf

