Introdution to LifeV

Davide Baroli LifeV-admin: Luca Paglieri

Politecnico di Milano Laboratory for Modeling and Scientific Computing

29-01-2015





LifeV in Action

- ≥ Why LifeV?
- Distribuite Communication
- Mesh
- Linear Algebra Matrix, Vector, distributor of elements
- Finite Element Space
- ETA: Expression Template Assembler
- Linear Solver
- Post-Processing: Exporter/Importer



LifeV is a open source Finite Element Library for the solution of PDEs developed at MOX, CMCS (EPFL), E(CM)² (Emory) and Estime (INRIA).

- Object oriented, c++ code.
- Trilinos Epetra backend for distribuite parallel computation.
- Research code oriented to the development novel numerical methods and algorithms.
- Aim: Solve large-scale, complex multi-physics engineering and scientific problems.
- Scalable library on HPC.
- Licensed under the GNU PBS.
- Release Versions are hosted at public repository https://github.com/lifev/lifev
- Google groups for mailing lists (lifev-user and lifev-dev)



Original features of LifeV:

- Type of Mesh: Hexaedra, Tetraedra (3D), Quad and Triangle (2D), Line (1D)
- Internal mesh generator for structured hypercube of dimension 1,2,3.
- Supporting external mesh format: .mesh (MEDIT), .msh (GMSH), .vol (NETGEN), m++
- Different Mesh Partitioner: Parmetis, Zoltan (Trilinos' package);
 offline-online partitioner to speed up the computation on HPC.
- Parallel I/O based on hdf5 format: internal wrapper of HDF5 library and EpetraExt Trilinos' HDF5 interface.
- Parser: GetPot for datafile and Teuchos (Trilinos) for XML.

4 / 42

- Construction of finite element assembly based on Epetra_FECrsMatrix, Epetra_FEVector and Epetra_Map
- Assembly of Finite Element based on DSEL principle: ETA Expression Template Assembly
- Internal Extension of Epetra Linear Algebra to assembly block matrix and block vector: "MatrixEpetraStructured" and "VectorEpetraStructured"
- Matrix-free methods are derived from Epetra_Operator
 - 1. LinearOperator
 - 2. SolverOperator(interface of an Invertible Linear Operator)
 - ConfinedOperator (interface for restriction to a block part of Linear Block Operator)
- Preconditioner and Linear Solver:
 - Internal interface for block preconditioner and multiplicative composition of preconditioner: SIMPLE,PCD and Yoshida.
 - Wrapper of Ifpack (one-level Additive Schwarz Preconditioner), ML (Algebraic Multigrid), Teko (Block Preconditioner- LSC),
 - 3. Wrapper of Aztec00 (GMRES, CG,BICGSTAB) and Belos (Block GMRES) (Iterative solver)
 - 4. Wrapper of Anasazi (Eigenvalue) and Amesos (direct linear solver).



Algorithms and Modelling:

- 1. Geometric Multiscale Method
- 2. Level-Set
- 3. Monolithic and segregated algorithms for Fluid-Structure Interaction
- 4. Elettrophysiology for cardiovascular system
- 5. Structure: Linear and NonLinear Elasticity
- 6. Fluid: Navier-Stokes
- 7. Porous Media: Darcy, Non-Darcy and Hyperbolic Problem

Ongoing Research about novel discretizations, methods and models hosted at https://cmcsforge.epfl.ch/projects/lifev

- 1. Variational MultiScale
- 2. eXtended Finite Element Method
- IsoGeometric Analysis on Surface (interface LifeV-LibIGA) and Structural problem (interface FEAP-LifeV)
- 4. Hierarchical Model reduction
- 5. Data Assimilation
- 6. Turbolence Models



Firstly in a own user/developed code in LifeV library, we need to include in header

```
#include <lifev/core/LifeV.hpp>
```

"LifeV.hpp" defines a number of types that are used in the library. The most used (in the tutorial) are

```
//uint32_type a 32 bit unsigned integer
typedef uint32_type UInt;
//! IDs
typedef uint32_type ID;
typedef double Real;
```

Epetra Communicator Objects

The Epetra Communicator Objects which encapsulates the general information and services needed to run on serial or parallel our computation.

```
#include <Epetra_ConfigDefs.h>
#ifdef EPETRA_MPI

#include <mpi.h>
#include <Epetra_MpiComm.h>
#else
#include <Epetra_SerialComm.h>
#endif
```

Listing 1: Header

```
int main ( int argc, char** argv )
3 #ifdef HAVE MPI
      MPI Init (&argc, &argv);
5 //For MPI distributed memory executions
      boost::shared ptr<Epetra Comm> Comm (new Epetra MpiComm
      (MPI COMM WORLD) );
7 #else
  //For serial executions
      boost::shared ptr < Epetra Comm > Comm (new
      Epetra SerialComm);
  #endif
  Int NumProc = Comm -> NumProc();
   Int MyPID = Comm -> MyPID();
13 // ... other code follows ...
  #ifdef HAVE MPI
   MPI Finalize();
  #endif
17 return 0:
```

2

Create Structured Mesh

```
#include < lifev / core / mesh / Region Mesh 1 D Structured . hpp>
typedef Region Mesh < Linear Line > mesh _ Type;
mesh Ptr _ Type Full Mesh Ptr (new mesh _ Type (Comm));
// Marker ID = 0; Domain = [-1,2] with 10 Elements along x
regular Mesh 1 D (*Full Mesh Ptr, 0, 10, 3, -1);
```

Create Structured Mesh

```
#include <|ifev/core/mesh/RegionMesh2DStructured.hpp>
typedef RegionMesh<br/>
typedef RegionMesh<br/>
| Type | Typ
```

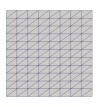
Create Structured Mesh

```
#include <lifev/core/mesh/RegionMesh3DStructured.hpp>
typedef RegionMesh<LinearTetra> mesh_Type;
meshPtr_Type FullMeshPtr ( new mesh_Type ( Comm ) );
// MarkerID=0; Domain=[-1,1]x[-1,1]x[-1,1] with 10 Elements
along x; 11 Elements along y; 12 Elements along y
regularMesh3D ( *FullMeshPtr, 0, 10, 11,12, 1.,1.,1.,
-1.,-1.,-1 );
```

Declaration of the Method

```
template <typename GeoShape, typename MC >
  void regularMesh3D ( RegionMesh < GeoShape, MC > &
      mesh, markerID Type regionFlag,
                        const UInt& m x.
                         const UInt& m y,
                         const UInt& m z,
                         bool verbose = false.
                        const Real& | x = 1.0,
                        const Real& | y = 1.0,
                        const Real& | z = 1.0,
9
                        const Real& t^- x = 0.0,
                         const Real& t y = 0.0,
                         const Real& t z = 0.0
13
```

Geoshape: LinearTriangle, LinearTetra (see ElementShape.hpp) MC define the policy for the entityFlag treatment



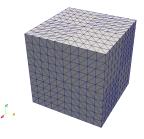


Figure: Triangular Mesh (left) and Tetrahedra Mesh (right)

For 2d Mesh, the Marker(Label) are

- for Edge are: 1 (BOTTOM), 2(LEFT), 3(TOP),4(RIGHT)
- for Corner are: 5(BOTTOM_RIGHT), 6(TOP_RIGHT),7(TOP_LEFT), 8(BOTTOM_LEFT)

For 3d Mesh, see "RegionMesh3DStructured.hpp".

The mesh is build up over the following base properties:

- Markers: label associated to any entity and has a partial order relation. The markers are: point marker,edge marker,face marker,volume marker.
- Geometric Entities (GeoShape): Line, Triangle, Quad; their properties (member) are S_dimension, S_numFaces,S_numEdges,S_numVertices,S_shape, S_geometry
- Geometric Entities to define Finite Element: LinearTriangle, QuadTriangle whose properties are: S_numPoints (number of DOF),S_numPointsPerVertex . . .
- Basic Entities of Mesh ("MeshEntity.hpp"), whose properties are: identifiers (localld and globalld) and flags to specify geometrical properties (PHYSICAL_BOUNDARY, SUBDOMAIN_INTERFACE, INTERNAL_INTERFACE)

In addition it is provided operation over the Mesh ("meshElementBare.hpp"), mesh Utility ("MeshUtility.hpp") and MeshCheck.hpp, which it is useful when we read external mesh. Finally it also defined the Container ("MeshEntityContainer.hpp") for mesh entity.



Change Marker ID according to a function.

```
1 #include < lifev / core/mesh/MeshUtility.hpp>
 #include <lifev/core/array/VectorSmall.hpp>
3 // Defining a function (outside main)
 UInt colour fun ( const VectorSmall < 3> & barycentre )
5
     if (barycentre [0] < 0.5 & barycentre [1] < 0.5)
     return 2;
     return 3:
 MeshUtility::assignRegionMarkerID (*FullMeshPtr,
     colour fun );
 // How many element have markerID =2?
 const UInt ElementID2=
     FullMeshPtr->elementList().countElementsWithMarkerID (
     2, std::equal to<markerID Type>());
```

Extract Extract elements and facets from a mesh based on a functor.

```
#include <lifev/core/mesh/MeshEntityContainer.hpp>
```

We need to define the "Predicates" (functors) whose templates are:

- 1. Mesh Entity
- Comparison Policy which must be a function able to compare two flag_Type.

The main method of Predicate is

```
bool operator()(const MeshEntity & entity)const
```

Example is provided in core/testsuite/mesh "entity selection.cpp".

The format supported by LifeV are: Mesh++, INRIA mesh, GMSH (.mesh), NETGEN (.vol) and MEDIT (.msh).

```
#include fev / core/filter / GetPot.hpp>
#include <lifev / core/mesh/MeshData.hpp>

// Read From dataFile
   GetPot command_line (argc, argv);
   const std::string data_file_name =
      command_line.follow ("data", 2, "-f", "--file");
   GetPot dataFile (data_file_name);
   const std::string discretization_section = "mesh";

MeshData meshData (dataFile,
   (discretization_section).c_str());
   readMesh (*fullMeshPtr, meshData);
```

```
7
```

Using HDF5IO.hpp and MeshPartitionerTool.hpp it is possible to divide-et-impera the partitioning in offline(rootprocessor-writer)-online(parallel-read). It is possible to choose:

- MeshPartioner
- Parmetis
- Zoltan

Detail TestCase can be found in "core/testsuite/offline_partition_io".

Repeated is used during assembly, while Unique structured is used for post-processing

Operations: Addition, Assign and Juxtaposition for MapVector



EpetraMatrix manage the Matrix (wrapper of Epetra_FECrsMatrix)

Operations: Addition, Subtraction, vector-matrix multiplication Spy (open in matlab),save in hdf5
To fill-in matrix:setCoefficient, addToCoefficients and sumIntoCoefficients Close and re-open matrix:openCrsMatrix(), globalAssemble()



EpetraVector manage the Matrix (wrapper of Epetra_FEVector)

Operations: Addition, Subtraction, division, comparison To fill-in vector: setCoefficient, add, replace, sumIntoGlobalValues Close vector, globalAssemble(), and calculating norm norm1(),...

7

ETFESpace defines a templete version of Finite Element Space.

```
template < typename MeshType, typename MapType, UInt
SpaceDim, UInt FieldDim >
ETFESpace < MeshType, MapType, SpaceDim, FieldDim >
(const meshPtr_Type& mesh, const ReferenceFE* refFE, const
GeometricMap* geoMap, commPtr_Type& commptr)
```

If GeometricMap is guessed in the constructor, it is used the shape of the element of the mesh. Any information about the quadrature can be recover using QuadratureRuleProvider.hpp or "FESpace.hpp" (using method "qr()")

```
QuadratureRuleProvider::provideExactness (TETRA, 0)
```

Finite Element Space: Scalar and Vector Field

```
#include <lifev/eta/fem/ETFESpace.hpp>
```

```
boost::shared_ptr<ETFESpace< mesh_Type, MapEpetra, 3, 1 >>
ETuSpace
( new ETFESpace< mesh_Type, MapEpetra, 3, 1 >
 (|oca|MeshPtr, &feTetraP1, Comm) );
```

```
boost::shared_ptr<ETFESpace< mesh_Type, MapEpetra, 3, 3 >>
ETuSpace
( new ETFESpace< mesh_Type, MapEpetra, 3,3 >
  (localMeshPtr, &feTetraP1, Comm) );
```

Defining before an FESpace:

Diffusion-Reaction Equation

Let a domain Ω with a partion of $\partial \Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$.

$$-\nabla \cdot (K\nabla u) + a_R u = f \text{ in } \Omega$$

$$u = g_D \text{ on } \Gamma_D$$

$$\frac{\partial u}{\partial n} = g_N \text{ on } \Gamma_N$$

$$\alpha u + \frac{\partial u}{\partial n} = g_R \text{ on } \Gamma_R$$
(1)

Find $u \in H^1_{\Gamma_n}(\Omega)$ such that

$$\int_{\Omega} K \nabla u \nabla v + \int_{\Omega} a_{R} u + \alpha \int_{\Gamma_{R}} u v = \int_{\Omega} f v + \int_{\Gamma_{N}} g_{N} v + \int_{\Gamma_{R}} g_{R} v \quad \forall v \in H_{0}^{1}(\Omega)$$
(2)

28 / 42

See "lifev/eta/examples/diffusionReaction/main.cpp"

```
V
```

```
Real scalardiffusion ( const Real& /*t*/, const Real& x , const Real& y , const Real& z , const ID& /*i*/)

{
    return 1.; // std::sin (2* pi / y ) * std::cos ( 2*pi / x ) * std::exp ( z ) ;

4
```

```
class scalar Diffusion Functor
  public:
      typedef Real return Type;
      return Type operator() ( const VectorSmall <3>
6
      spaceCoordinates )
           return scalardiffusion (0, spaceCoordinates[0],
8
      spaceCoordinates[1], spaceCoordinates[2], 0 );
10
      scalarDiffusionFunctor() {}
      scalarDiffusionFunctor (const scalarDiffusionFunctor&)
12
      {}
      ~scalarDiffusionFunctor() {}
14
```

```
boost::shared ptr<scalarDiffusionFunctor>
       scalarDiffusionFct ( new scalarDiffusionFunctor );
    {using namespace ExpressionAssembly;
   integrate ( elements (ETuFESpace->mesh() ),
                         quadRuleTetra4pt,
                         ETuFESpace,
                         ETuFESpace,
6
                         eval ( scalarDiffusionFct , X) * dot (
      grad (phi j) , grad (phi i) )
                         - eval \overline{(} scalarReactionFct , X) *
      phi j * phi i
10
                   >> *SvstemMatrix:
12
```

```
{ using namespace ExpressionAssembly;
integrate ( elements (ETuFESpace->mesh() ), // Mesh

uFESpace->qr(), // QR

ETuFESpace,

eval ( ScalarFctRhs, X ) * phi_i

)
>> uRhs;
}
```

```
4
```

```
QuadratureBoundary myBDQR (buildTetraBDQR (quadRuleTria4pt));
integrate ( boundary (ETuFESpace—>mesh(),
BCFlags::BOTTOMWALL),
myBDQR,
ETuFESpace,
ETuFESpace,
value (alpha) * phi_j * phi_i

)
>> *SystemMatrix;
```

```
Y
```

```
Y
```

```
BCHandler bcHandler:
BCFunctionBase dirichletBCFct ( dirichlet );
 bcHandler addBC ("Left", BCFlags::LEFTWALL, Essential,
 Full, dirichlet BCFct, 1);
 bcHandler.addBC ("Right", BCFlags::RIGHTWALL,
Essential, Full, dirichlet BCFct, 1);
 bcHandler.addBC ("Back", BCFlags::BACKWALL, Essential,
Full, dirichlet BCFct, 1);
 bcHandler.bcUpdate ( *meshPtr, uFESpace—>feBd(),
uFESpace—>dof());
bcManage (*SystemMatrix, *uRhsUnique,
           *uFESpace->mesh(), uFESpace->dof(),
           bcHandler, uFESpace—>feBd(), 1.0, Real (0.0)
);
```



Setting the Algebraic System Solver

```
prec Type* precRawPtr;
basePrecPtr Type precPtr;
precRawPtr = new prec Type;
precRawPtr->setDataFromGetPot ( dataFile , "prec" );
precPtr reset ( precRawPtr );
Teuchos::RCP< Teuchos::ParameterList > solverList =
Teuchos::rcp ( new Teuchos::ParameterList );
const std::string solverParam = dataFile
("solver/listName", "SolverParamListBelos.xml");
solverList = Teuchos::getParametersFromXm|File
(solverParam);
LinearSolver linearSolver:
linearSolver.setCommunicator ( Comm );
linearSolver setParameters ( *solverList );
linearSolver setPreconditioner ( precPtr );
```



Solving the Algebraic System

```
vectorPtr_Type uSolution ( new vector_Type (
ETuFESpace—>map() , Unique) );
linearSolver.setOperator ( SystemMatrix );
linearSolver.setRightHandSide ( uRhsUnique );
linearSolver.solve ( uSolution );
```

```
2
```

```
std::string const exporterFileName = dataFile (
"exporter/filename", "cube");
ExporterHDF5<mesh_Type> exporter ( dataFile, meshPtr,
exporterFileName, Comm—>MyPID() );
exporter.setMultimesh (false);
boost::shared_ptr<vector_Type> uExported ( new
vector_Type (ETuFESpace—>map(), exporter.mapType() ));
exporter.addVariable (
ExporterData<mesh_Type>::ScalarField, "u", uFESpace,
uSolution, UInt (0));
exporter.postProcess ( 1.0 );
exporter.closeFile();
```

```
7
```

```
#include #include fev / core/fem/TimeAdvanceBDF.hpp>
const Real initialTime = 0.0;
const Real endTime = 100.0;
const Real timestep = 1e-1;
Ulnt BDFOrder = 2;
TimeAdvanceBDF<vector_Type> bdf;
bdf.setup (BDFOrder);
Real currentTime = initialTime - timestep * BDFOrder;
bdf.setInitialCondition (*usolution);
```

```
bdf_updateRHSContribution ( timestep );
   *uRhsUnique = *MassMatrix *
     bdf.rhsContributionFirstDerivative();
   SystemMatrix reset (new matrix Type ( ETuFESpace—>map() )
   double alpha Time = bdf.coefficient First Derivative (0) /
     timestep;
   *SystemMatrix += *MassMatrix * alphaTime;
   *SystemMatrix += *BaseMatrix;
   bcManage (*SystemMatrix, *uRhsUnique,
            *uFESpace->mesh(), uFESpace->dof(),
8
                bcHandler, uFESpace—>feBd(), 1.0, Real (0.0)
  SystemMatrix—>globalAssemble();
```

Tutorial Hand-on

Tutorial is hosted at Github Portal:

https://github.com/DavideBaroli/LifeVTutorial in the folder "/lifev/eta/example"

- Laplacian with Convergence Test
- Diffusion-Reaction Scalar and Vectorial
- Time-Dependent Diffusion Reaction Scalar
- Darcy Problem in Mixed Formulation
- Stokes
- Complex Coupled Problem: vortex and bi-phasic with different stabilization: VMS,PSPG, SUPG and Mesh Transformation.

Advance examples:

- Structure
- Pseudo-FSI





Efficient and Fast Expression Template Assembler for PDEs discretization

Purpose: Educational Use of LifeV, programming Expression Template, c++11 standard.

Use LifeV Assembler: ETA

- Mixed-Hybrid and low-Raviart-Thomas formulation for Darcy Problem .
- 2. Hyperbolic discretization by Godunov Flux for Saturation Equation .
- 3. Laplace-Beltrami problem applied to porous media flow .
- **4.** Multigrid Space-Time preconditioner for solving Navier-Stokes system.