Emory Updates

LifeV Workshop 2013

The Emory team

- 1 supervisor (AV)
- 2 senior developers (TP, LB)
- 1 junior developer (Huanhuan Yang)
- 2 trainees (Boyi Yang, Jim Munch)
- Several users (mostly grads/undergrads)

- External collaborators (UV, Adrien Lefieux, Annalisa Quaini…)

Projects

- CFD for blood flow problems (TP, AV, BY)
  - Pre-processing (mesh)
  - Post-processing (export, "secondary" computations)
  - **Validation**
  - Software usability, portability…
- Inverse problems / parameter estimation (LB, HY)
  - Verification
  - Efficiency

Objectives (related to LifeV)

- Use LifeV in teaching labs (summer 2013)
  - Additional documentation
  - Website
  - Solved exercises
- Software distribution (2013)
  - Through cmcsforge
  - Through personal web pages? Github? …
- Inject LifeV in the Biomed community
  - Workshop on software tools for Biomed Engineering

How to market LifeV?

- algorithms and data structures for the solution of PDE (with FEM)
  - Freely available! (www.lifev.org)
  - strongly related to Trilinos (LifeV = "assembly" package for Trilinos-based FEM solvers)
  - "open" laboratory for **new ideas/methods**
  - **HPC technologies**

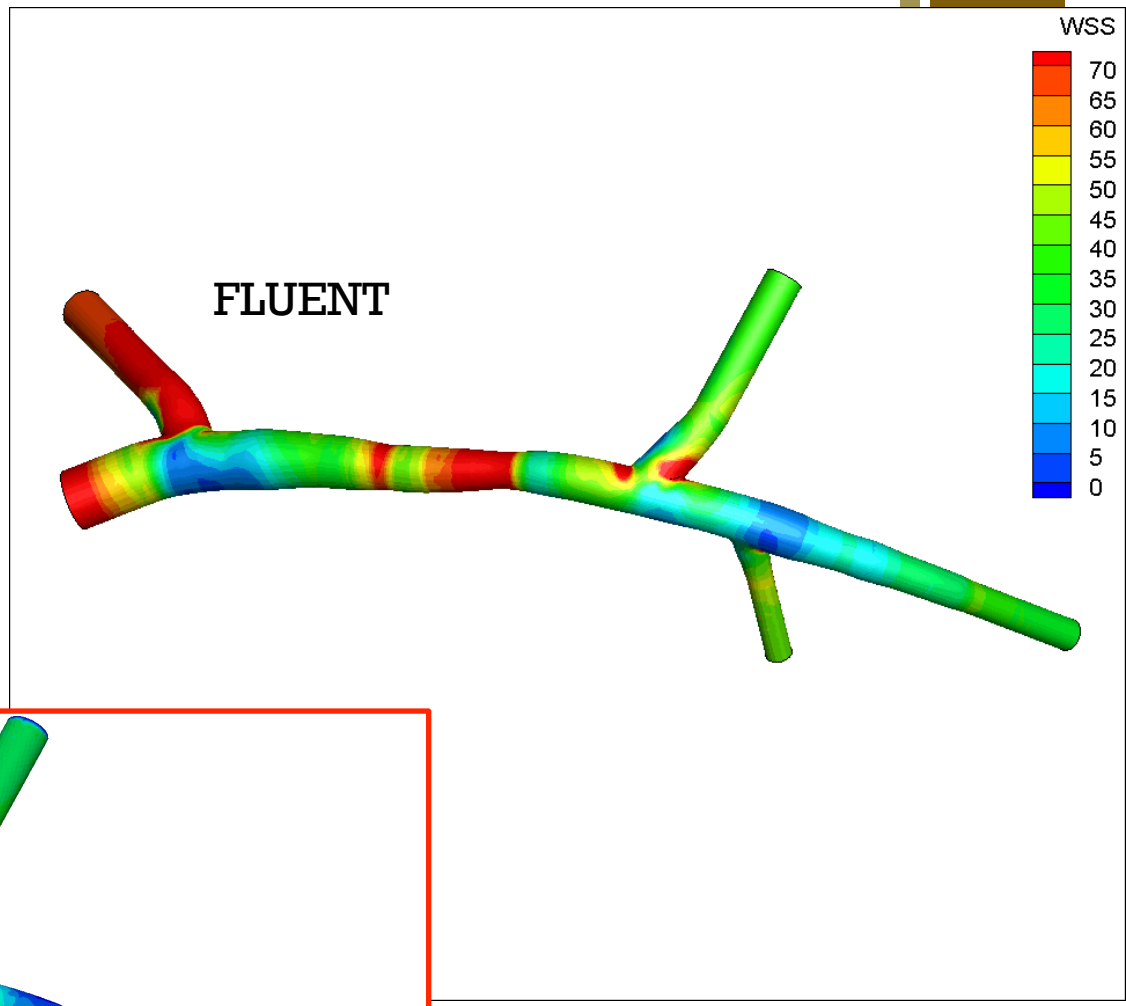
- a community of researchers
  - we make available (in principle) the tools we use to write papers

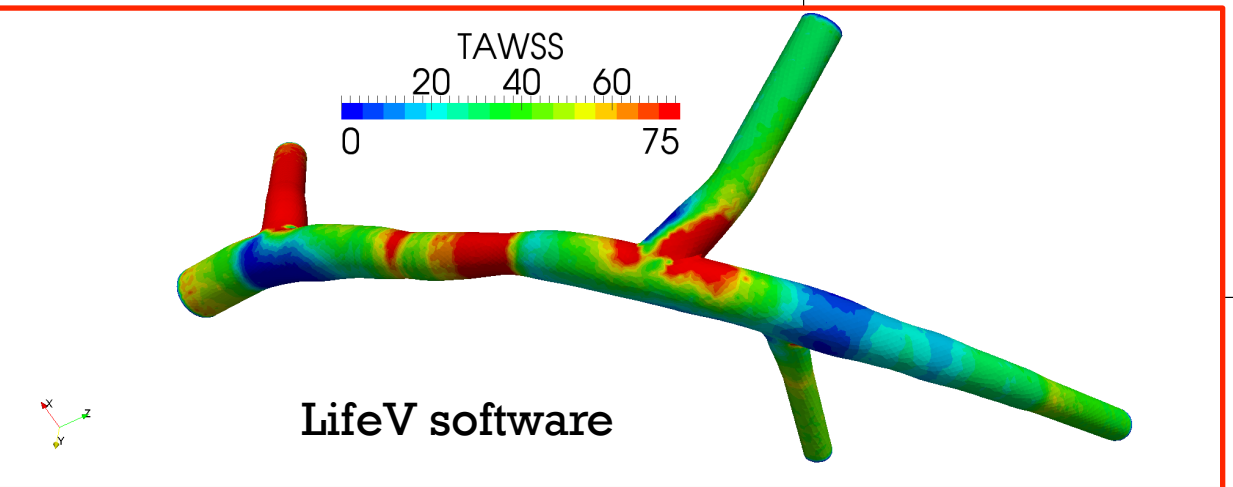
What LifeV is not (yet?)

- teaching / educational tool
  - Easily solve easy problems
- FEM for dummies
  - As we teach it, we code it
    - e.g. assembly routines, …
- seed for new collaborations
  - Enlarge the user base
- "software on demand"
  - Produce applications based on "LifeV as a library"
- collaborative development on a per-project basis
  - Shared code for shared papers
- …

Promoting LifeV (I)

- Be competitive
  - Verification, validation
- Be better
  - e.g. mass conservation (avg. mass balance 3e-7 g/s), not achieved to the same level of accuracy by the Fluent solver





Promoting LifeV (II)

- Be flexible

(tested machines, partial list)

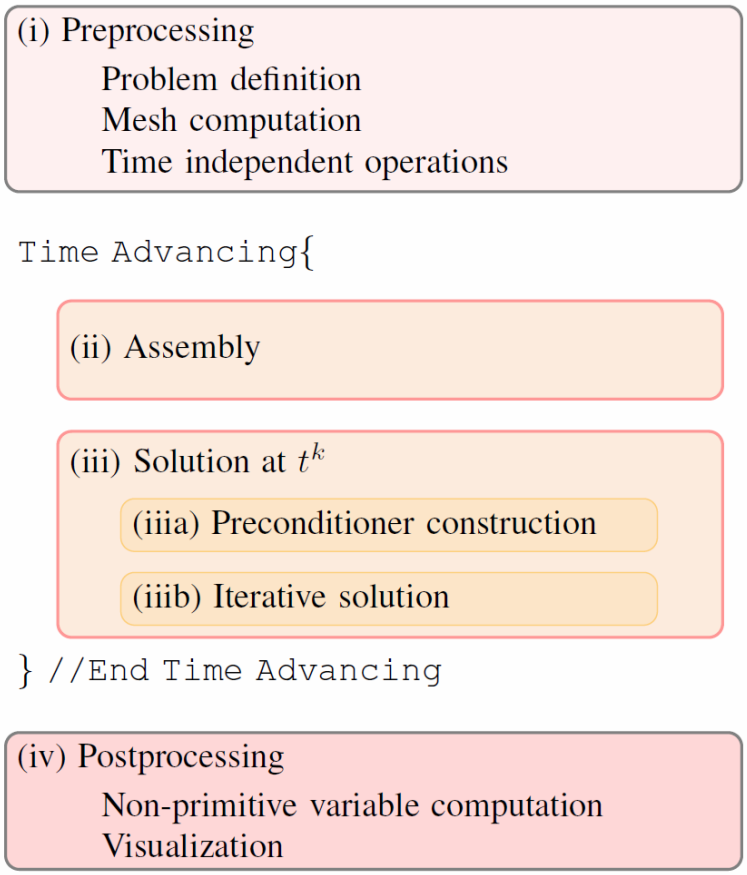
- puma: 32 (2xDualCore) nodes, 128 cores, 8GB RAM per node (theoretically 256GB tot)
- crunch: 8xQuadCore, 32 cores, 200GB RAM
- Emory's HPC facilities
  - Ellipse cluster: 256 nodes, 1024 cores
  - facilities at Emerson Center: heterogeneous cluster, up to 240 cores
- XSEDE HPC resources
  - Trestles @ San Diego Supercomputer Center: 324 compute nodes, 10368 cores
  - Lonestar4 @ Texas Advanced Computing Center: 1888 nodes, 22656 cores
  - Steele @ Purdue University: 902 nodes, 7216 cores
- Collaboration with Italian HPC center Cilea
  - HP cluster Lagrange: 208 nodes, 1664 cores
- Amazon EC2
- …

Promoting LifeV (III)

- A clear and easy design

The basic steps of the simulation:

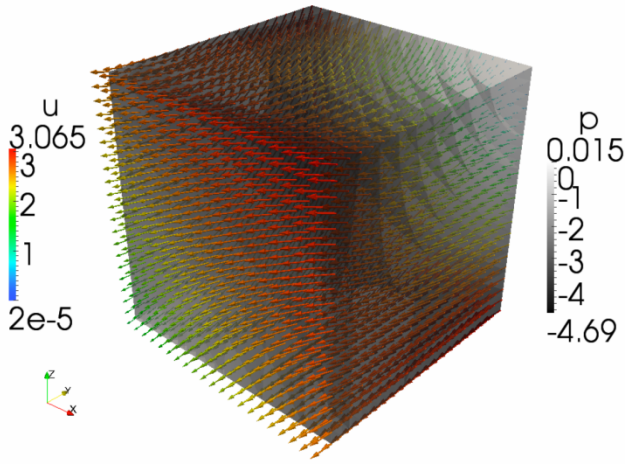
i. Mesh generation/reading
ii. Mesh → matrices & vectors
iii. Linear system solve
   a. Preconditioner update
   b. Solve
iv. Processing & exporting



LifeV Application

NavierStokesApplicat | data | NavierStokesApplicat | write_boundary_point | data | TimeA

```
1  #include "TestNavierStokes.hpp"
2  #include <boost/scoped_ptr.hpp>
3
4  using namespace LifeV;
5
6  // Do not edit
7  int main(int argc, char **argv)
8  {
9      using namespace LifeV;
10 #ifdef HAVE_MPI
11     MPI_Init(&argc, &argv);
12     std::cout<< "MPI Initialization\n";
13 #endif
14
15     boost::scoped_ptr<TestNavierStokes> testPtr( new TestNavierStokes( argc, argv ) );
16     testPtr->run();
17
18     int result( EXIT_FAILURE );
19     if( testPtr->checkErrors() )
20     {
21         result = EXIT_SUCCESS;
22     }
23     testPtr.reset();
24
25 #ifdef HAVE_MPI
26     MPI_Finalize();
27     std::cout<< "MPI Finalization \n";
28 #endif
29
30     return EXIT_SUCCESS;
31 }
```



(C. R. Ethier, D. Steinman, 1994)

LifeV Application

NavierStokesApplicat | data

```
45
46
47 void NavierStokesApplicatio
48 {
49     Debug() << "[NavierStok
50
51     readDataFile();
52
53     buildMesh();
54     buildFESpaces();
55     buildAssembler();
56     buildOperator();
57     this->buildExporter();
58
59     setupBDF();
60
61     this->initialize();
62
63     this->setBC();
64     this->timeLoop();
65 }
66
67
68 void NavierStokesApplicatio
69 {
70     Debug() << "[NavierStok
71
72     //=====================
73     //   Data File
74     //=====================
75     // boost::shared_ptr<Te
76     M_teuchosListPtr.reset(
77     Teuchos::updateParamete
78
```

```
48
49 class TestNavierStokes :
50 public NSApplication
51 {
52 public:
53
54     typedef LifeV::RossEthierSteinmanUnsteadyDec problem_type;
55
56
57     /** @name Constructors, destructor
58      */
59     //@{
60
61     TestNavierStokes( int argc, char** argv ) :
62         NSApplication( argc, argv ),
63         M_L2err_velocity(0.),
64         M_L2err_pressure(0.),
65         M_tolerance_velocity(0.),
66         M_tolerance_pressure(0.)
67     {}
68
69     virtual ~TestNavierStokes() {}
70     //@}
71
72     bool checkErrors();
73
74     virtual void initialize();
75     virtual void setBC();
76
77     virtual void postProcess( const Real& /*t*/ );
78
79 protected:
80     virtual void setProblemData();
81
82     void initializeErrorLog();
83     void printErrorLog();
84
85     LifeV::Real M_L2err_velocity, M_L2err_pressure;
86     LifeV::Real M_tolerance_velocity, M_tolerance_pressure;
87 };
88
```

Promoting LifeV (IV)

- Let the software circulate!
  - Lifev.org web portal
  - Personal/private pages
  - Public portals (github)

Example: lifev.org

Turek Cylinder Benchmark

cmcsforge.epfl.ch/lifev/dev/workgroups/ns/cylinder/?searchterm=turek

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  - Roadmap
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    - Core
    - Parallel
    - Serial
    - Mass Transport
    - Navier-Stokes
      - Meeting April 2006
      - NSPC and NSIP: preliminary analysis
      - Turek Cylinder Benchmark
      - NSPC and NSIP: preliminary analysis, continued
      - Turek Cylinder

Turek Cylinder Benchmark

Results of the Turek cylinder benchmark computations of LifeV Navier-Stokes solvers updated 17 November 2006 (old version here)

Testcase 3D-Z1 from Schaefer, Turek. See there for details about geometry etc.

The solution is steady, and it is found by running the time dependent solvers with 1st order BDF (=backward Euler) until t=10, about where a stationary state is reached. The timestep is chosen as equal to the largest mesh width, which is 12.5 times the smallest mesh width. With a maximal inflow velocity of 0.45, this would give a maximal CFL of 5.625. Note that the velocity is low where the mesh is fine (i. e. near the cylinder).

The drag and the lift have been evaluated by numerical integration of the stress on the cylinder. The pressure difference was calculated using a L^2 scalar product with two regularized delta functions located at the points of interest. The mass error is the integral over time of |inflow-outflow|. Implementation details can be found in life-playground/benchmark/cylinder/turek. I didn't want to put the finest mesh into cvs, you can find it here.

See the current results here, with the bounds indicated by Schaefer and Turek:

Solver	N_{dof}	h=Δt	drag	lift	Δp	mass error	cpu sec >per timestep<th>	Memory / MB
lower bound			6.05	0.0080	0.165			
upper bound			6.25	0.0100	0.175			
PC P1bubble-P1	36540	0.2	6.19	-0.0043	0.189	2.0e-6	42.9	46
	165236	0.1	6.10	-0.0094	0.172	2.3e-6	432.0	174

« January 2013 »

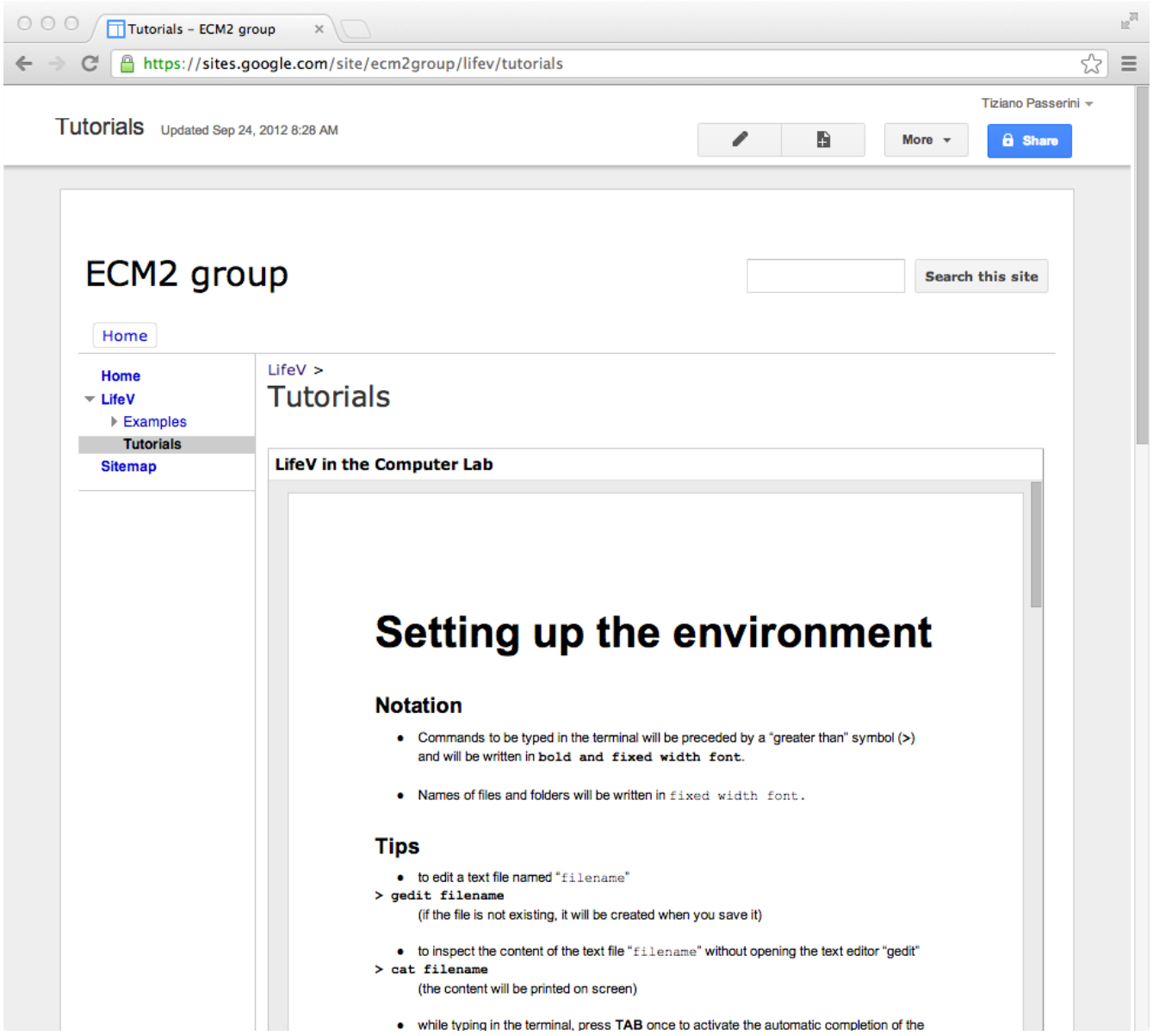
Mo	Tu	We	Th	Fr	Sa	Su
	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	31			

News

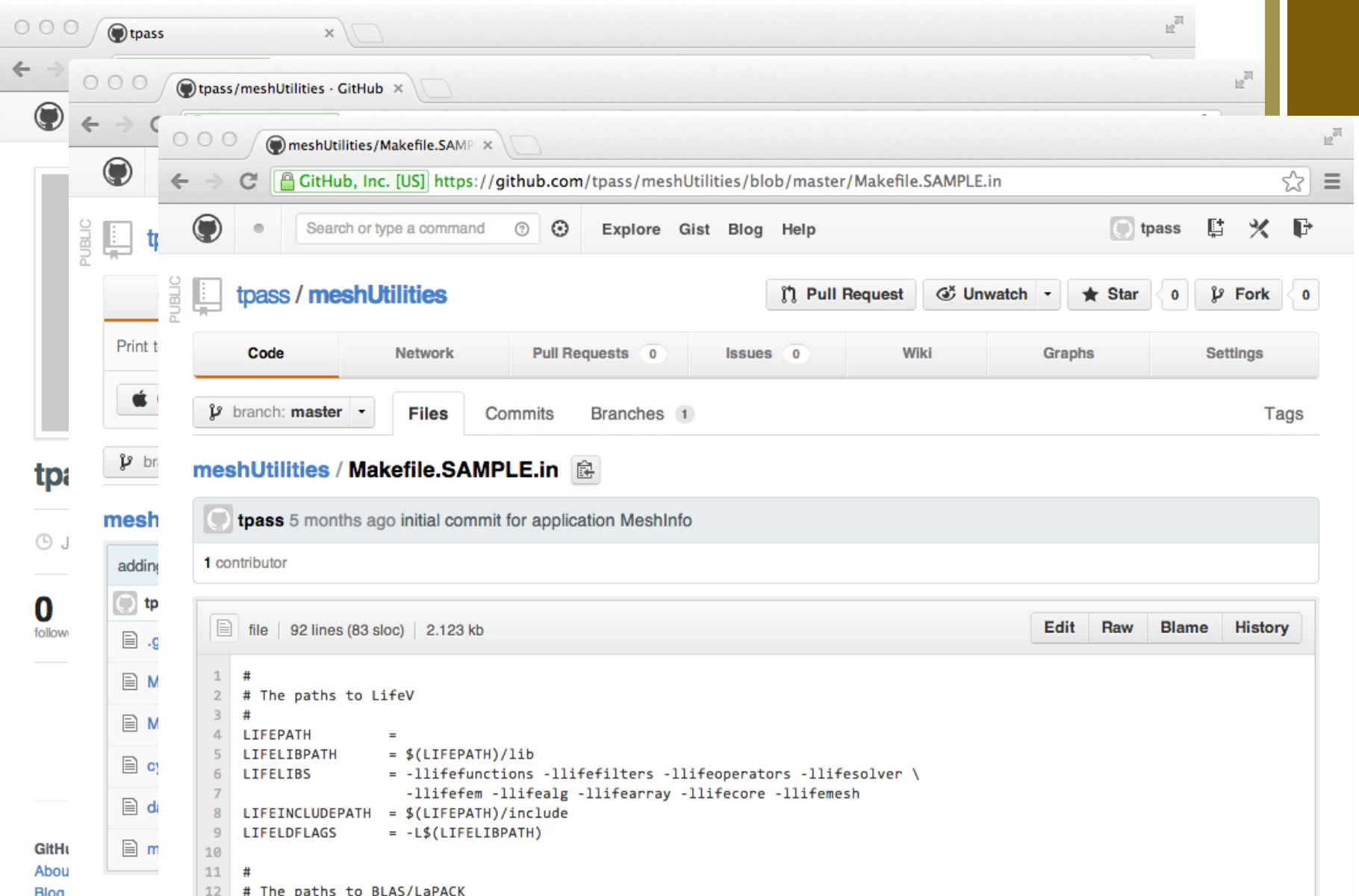
- Gallery updated Sep 16, 2010
- LifeV-Serial 1.0 released Apr 27, 2010
- LiveV workshop talks online Apr 22, 2010

More news...

Example: "private" web portals



Example: github



The ECM2 module

- A collection of code experiments
- A code forge (preliminary stage for the library)
- Playground / applications
- Content
  - A NS solver, various preconditioners (block operators)
  - A solver for linear elasticity (time advance)
  - A monolithic FSI solver (block operators)
  - Classes to simplify the implementation of "applications"
  - Classes/routines for manifold handling (boundary mesh extractor, assembler, FESpace,…)
  - Classes for BC / problem set up
  - …