Abstractions in FEM Software

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Outline

Motivation

- Success of the Finite Element Method(FEM) has led to a proliferation of FEM simulation software.
  - The FEniCS Project, Sundance, DEAL
  - Others: FreeFEM, FEMLab, ...
- No single package meets everyone's needs ... yet.
  - Sundance handles optimization well, but is limited in kinds of elements,
  - FEniCS gives a good smaller bundle that effeciently generates code,
  - DEAL handles a more elements and has a larger user community,
  - Both Sundance and FEniCS use easily readable code for user input.

Goals

- There seem to still be disjunctions between the math and the software.
  - Domains and meshes are not always identical.
  - Small variations of methods are hard or not possible.
  - ... other issues ....
- Some goals for this talk
  - Point out some rough spots in current software through my experiences.
  - Get feedback on validity and feasibility of ideas.
  - Challenge the next generation of FEM software to be more mathematically rigorous
    - Rigorous in code correctness.
    - Rigorous in correct mathematical abstractions from problems.

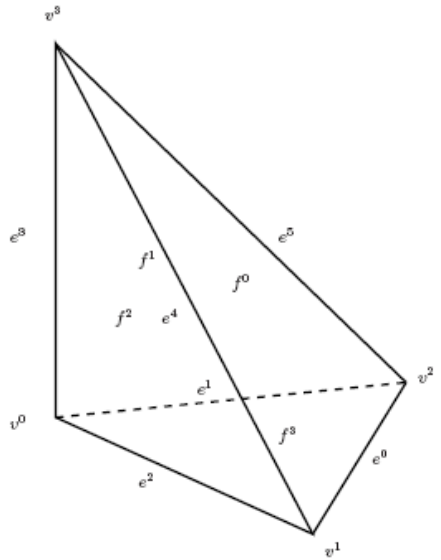
Analysis v. Simulation

Mathematically a finite element method is simply:

- A reference element, K
- A space of shape functions, $\mathcal{P}$
- A basis, $\mathcal{N}$

But it seems there is something missing:

- Links between elements,
- How the elements affect the solvers.



Alternate Methods

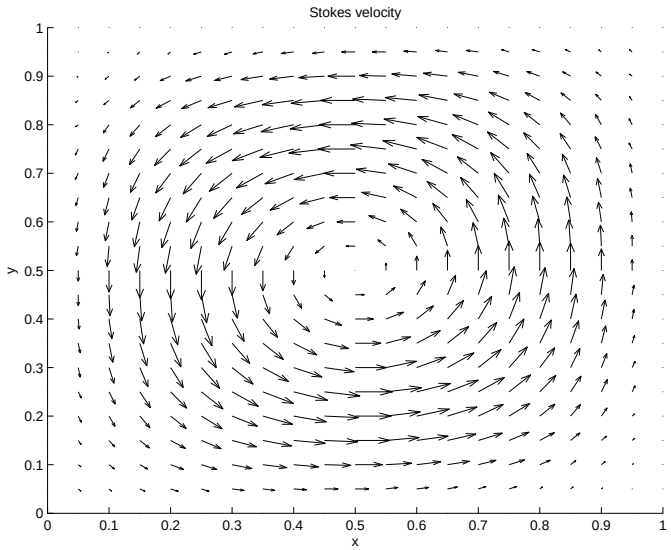
- It seems there is always someone who wants to do something different.
- How much control of you software to give the user, to play with new methods?
- Example: Mixed methods, do we just put the formulation in the software or give the user the matrices.

Example: Stokes Equations

$$\begin{aligned} -\Delta u + \nabla p &= f \\ \nabla \cdot u &= 0 \end{aligned}, \qquad u = \begin{bmatrix} \sin(\pi x)\cos(\pi y) \\ -\cos(\pi x)\sin(\pi y) \end{bmatrix}$$

Using Taylor-Hood elements with mixed formulation,

Number of Iterations		
mesh	P1/P2	P2/P3
4x4	14	22
8x8	24	54
16x16	83	283
32x32	328	1319

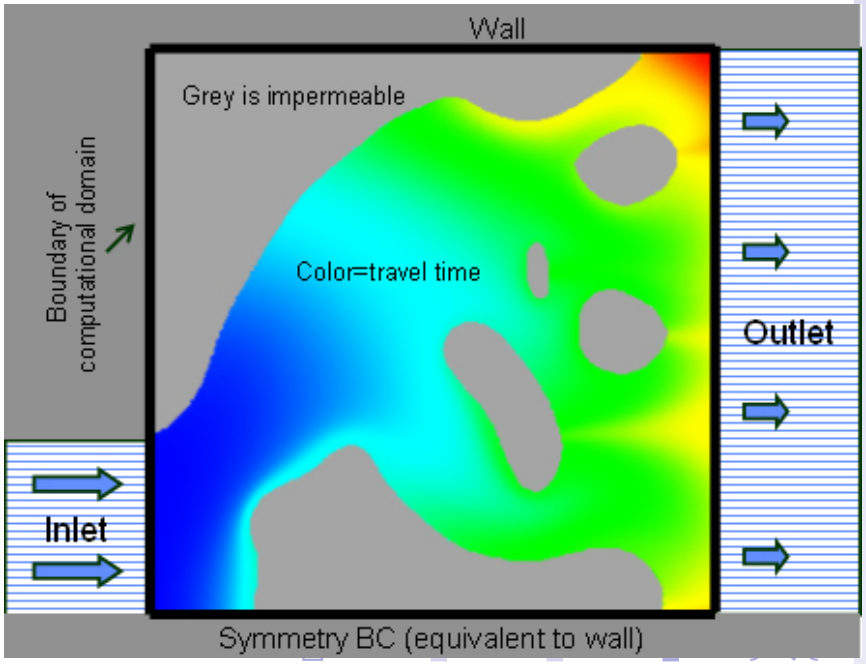


How about optimization problems?

- Use Automatic Differentiation tools on produced code - expensive on user side
- Create a symbolics engine that can give derivatives - expensive on developer side

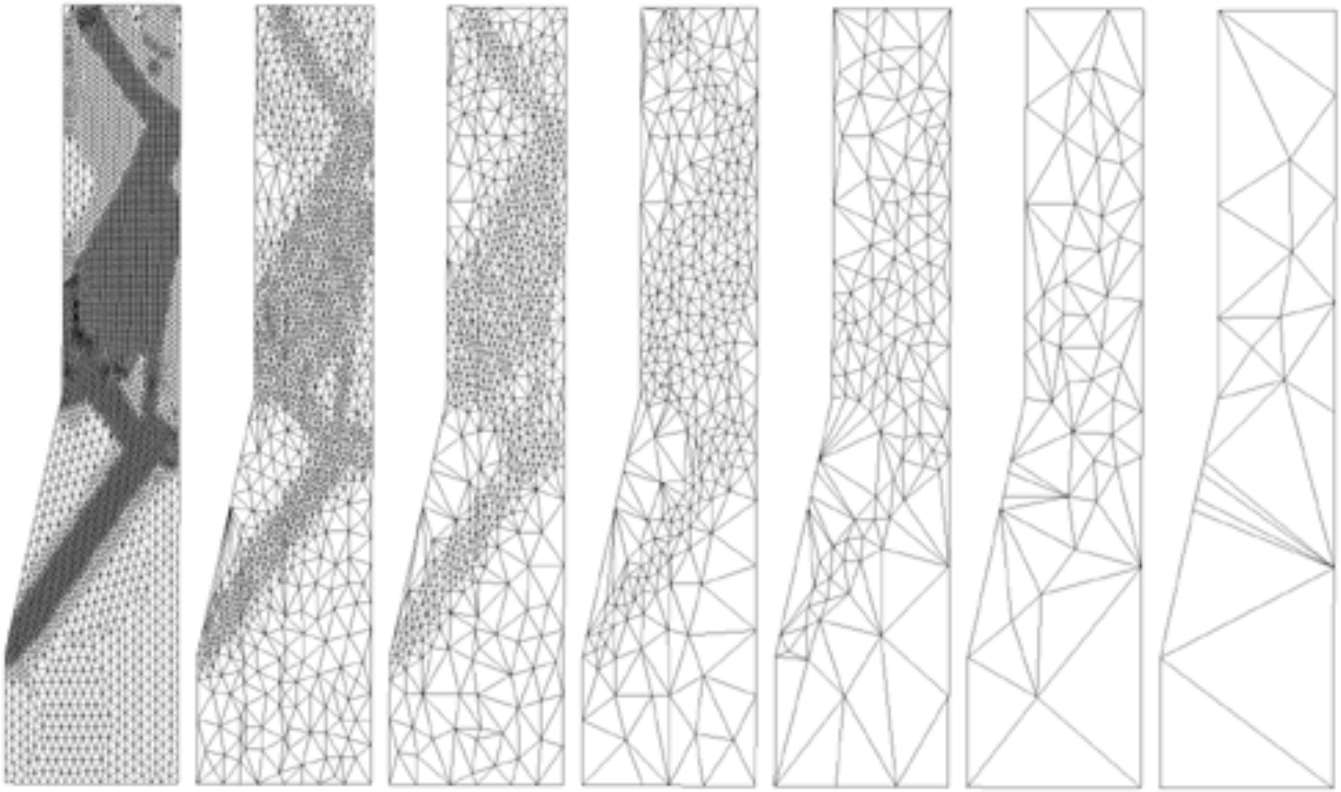
Example Problem in Microfluidic Devices

- To optimize flow, change channel geometry
- Most effective methods, use level set methods



What meshes can we handle?

None of these software packages are giving us great tools for multigrid adaptivity.



- courtesy Peter Brune.

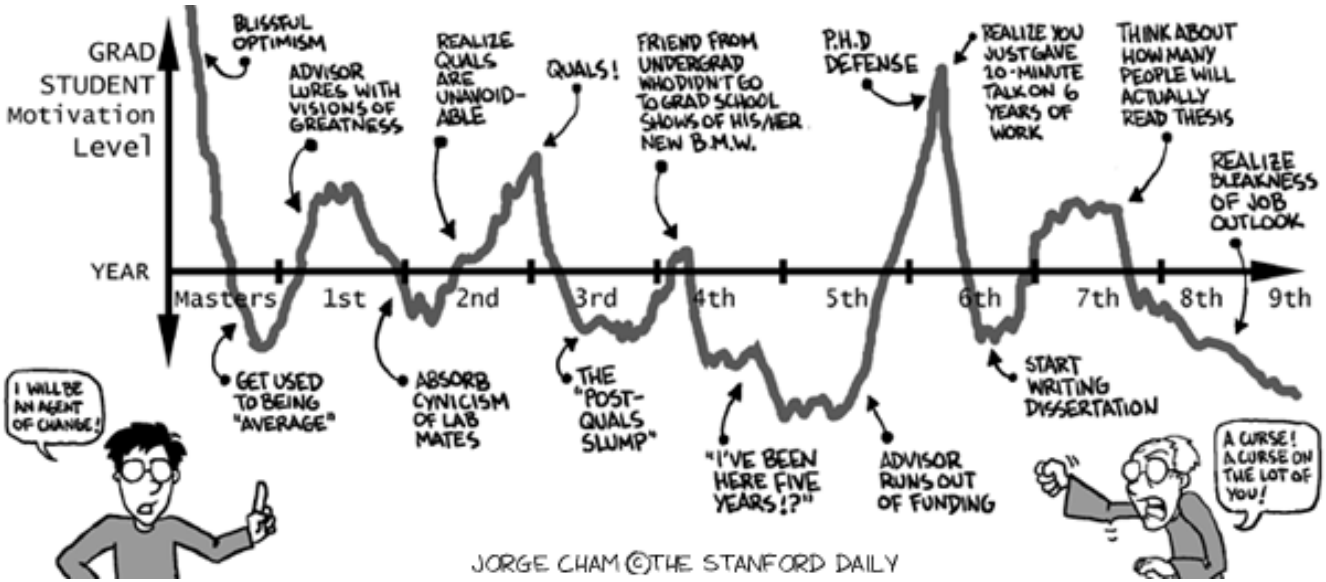
Why is Mathematical Software Hard?

The design space for mathematical software is multi-dimensional and not orthogonal.

- Mesh: uniform meshes, general geometry, adaptive meshes, unstructured meshes
- Function Space: linears, menu of options, arbitrary order, FIAT, exterior calculus
- Equation Description: menu, language, derived forms, error estimators
- Solver algorithms: menu, language
- Parallel Computing Support
- Boundary Conditions and embedded geometries.

Future

- Good mathematical abstractions have gotten us this far, where else can we go?
- How do these issues play well with software design principles?
- Is there a single solution to automated mathematical modelling?



Questions or Comments?
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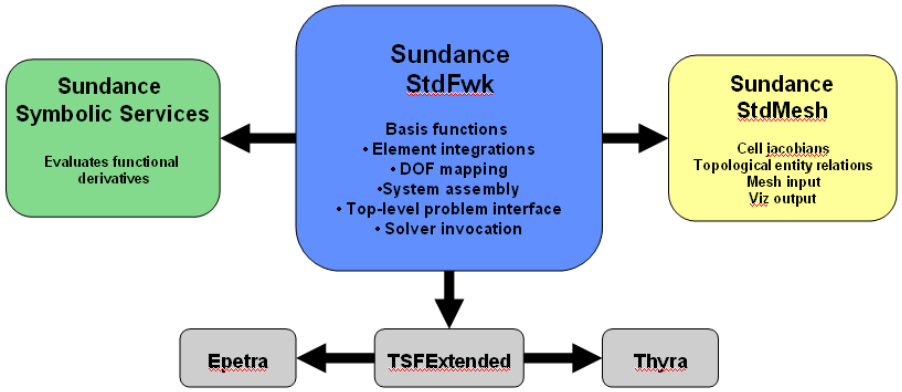
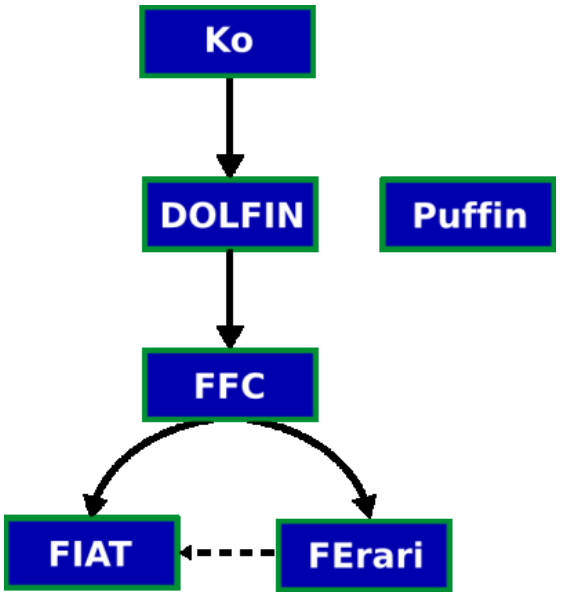
What about code complexity?

One bad estimate is lines of code:

- Dolfin + FFC $\sim$ 50K lines
- Sundance $\sim$ 100K lines
- DEAL $\sim$ 400K lines

Some Organization Charts





More Detailed Dependencies

An example of Dependencies for Sundance (not especially different from others)