# Mathematical Interfaces of Automated Scientific Computing

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# Acknowledgments


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- Anders Logg (Simula Research Lab)

# Outline

1. Science and Computing
   - Big Science
   - Little Science
2. The Automation of Scientific Computing
   - Algebraic Solvers
   - Functional Spaces
   - Equation Descriptions
   - Domain Representations
3. The Future of Scientific Computing

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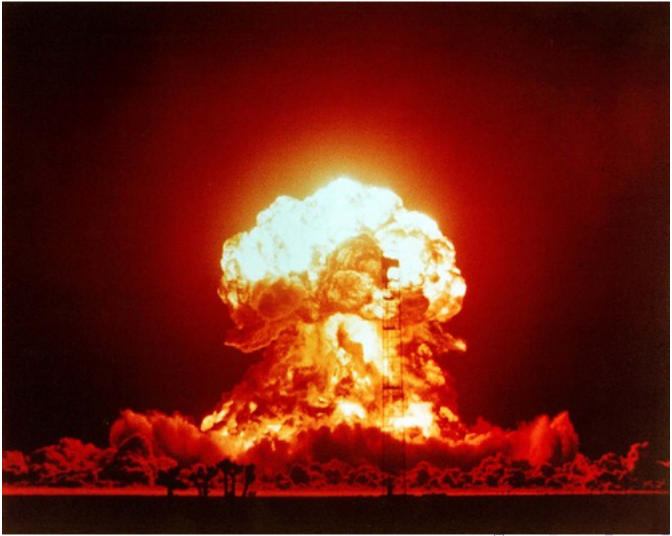
# Why do simulations?

# Why do simulations?

Because experiments are expensive

# Why do simulations?

Because experiments are dangerous



# Why do simulations?

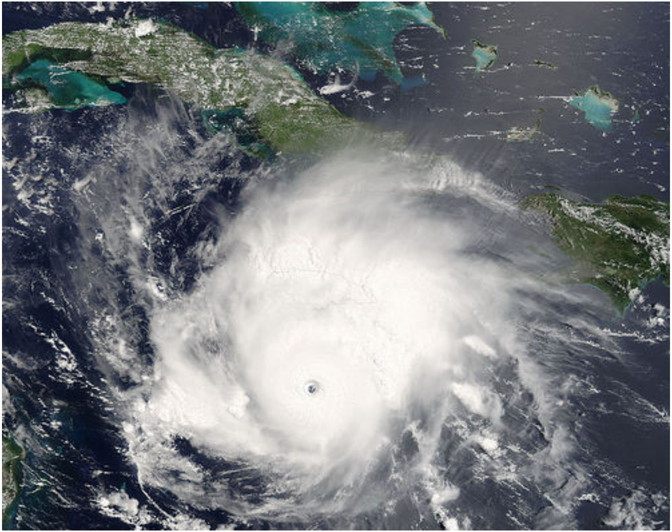
Because experiments are not possible

# Why do simulations?

Because simulations are faster

# Why do simulations?

Because we need the data ASAP



# Simulation: Third Tier of Science

- D'Alembert's Paradox
- Mass of Neutrino
- Rayleigh-Taylor Constant

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# Big vs Little Science

*The goal of this session is explore whether, when and why universities should do big or little science. Panelists may discuss why big science wastes money, exploits graduate students and makes research too short range. They may argue that little science produces results that are too deep and narrow, oblivious to global systems issues, not properly validated, and too out of touch with reality to ever be practical. Panelists may also find some advantages to both kinds of science.*

ACM SIGARCH Computer Architecture News
Volume 18, Issue 3a, June 1990

# Big Science and Big Computers

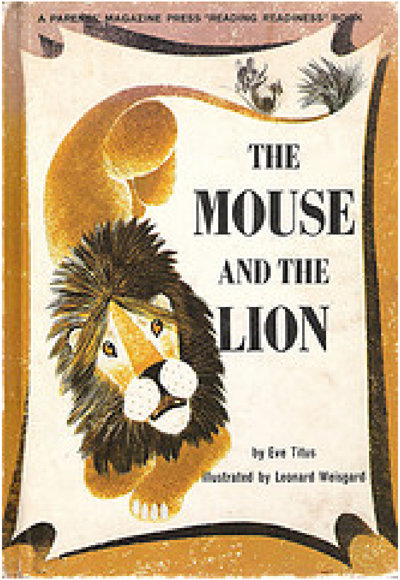
- Requires large coding projects that are highly specialized
- Incredibly hard to design for maintainability, feature addition, and new hardware paradigms
- Expensive
- Resolves large open phenomena (or asks for more money)

# Little Science and Rapid Development

- Able to use inefficient methods
- Usually only test on small or simple problems
- Can use (somewhat) exhaustive search of different possible methods.
- High Productivity Environment

# Automation becomes the Thorn

- Pervasive abstractions
- Write general code, Generate specific code
- Fails due to bad interfaces



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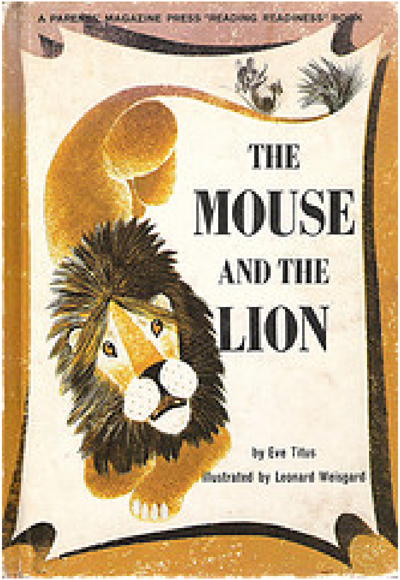

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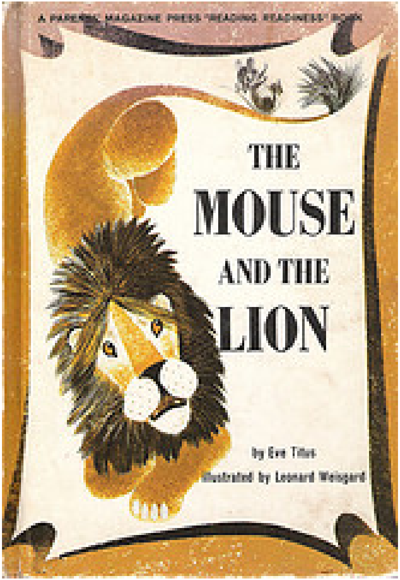

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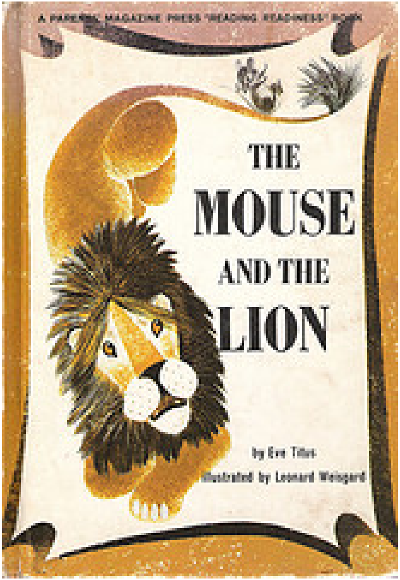


# Outline

# The Productivity Factors



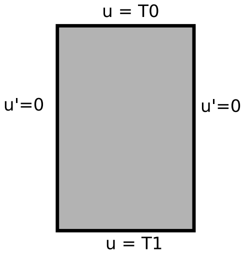
How much code do I have to write:

| **Written Code** | **Generated Code** |
|---|---|
| ANSI C: 50 lines | Assembler: 200 lines |
| FFC: 10 lines | C++: 20K lines |
| Quantum Chemistry: 6 symbols | FORTRAN: 1M lines |

# The FEM-PDE model

Find u on domain Ω, given f and BC

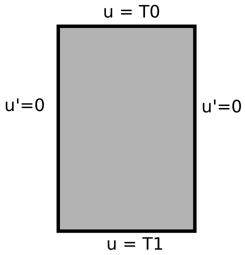
$$-\Delta u = f$$



# The FEM-PDE model

Find u on domain Ω, given f and BC, such that for all v in the function space S

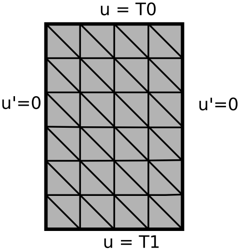
$$a(u,v) = (f,v)$$



# The FEM-PDE model

Find u_h on a triangulization of domain Ω, given f and BC,
such that for all v in the function space S

a(u_h,v) = (f,v)



# The FEM-PDE model

Find u_h on a triangulization of domain Ω,
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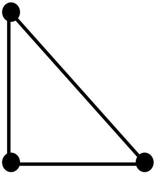
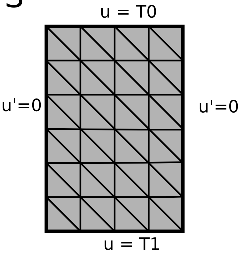
in the function space V ⊂ S

a(u_h,v_h) = (f,v_h)

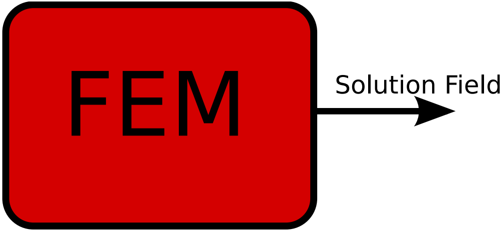




# The FEM-PDE model

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \begin{bmatrix} x \end{bmatrix} = \begin{bmatrix} b \end{bmatrix}$$

# The FEM-PDE model



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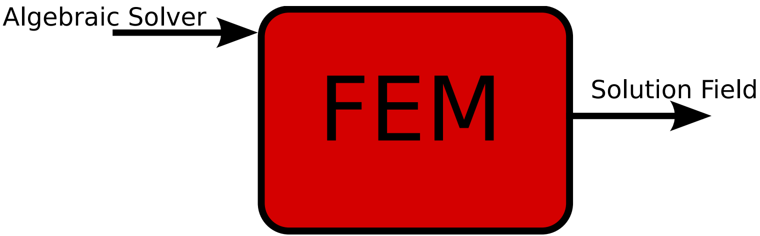

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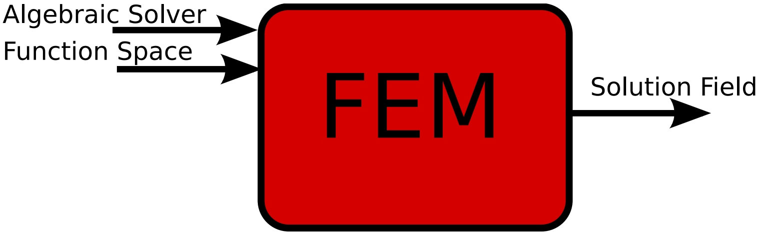

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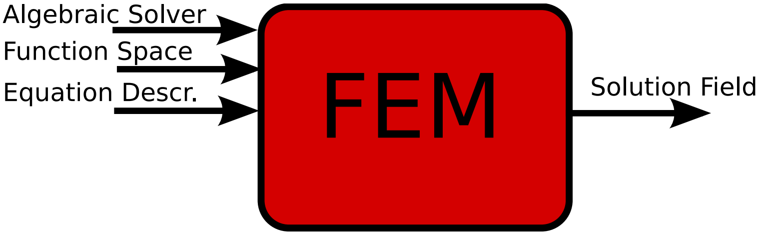

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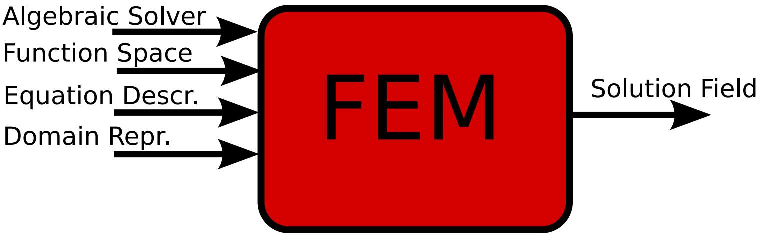

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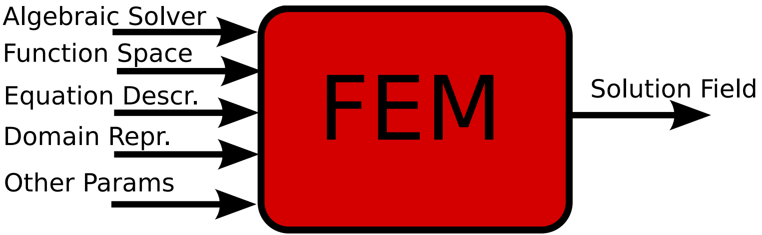
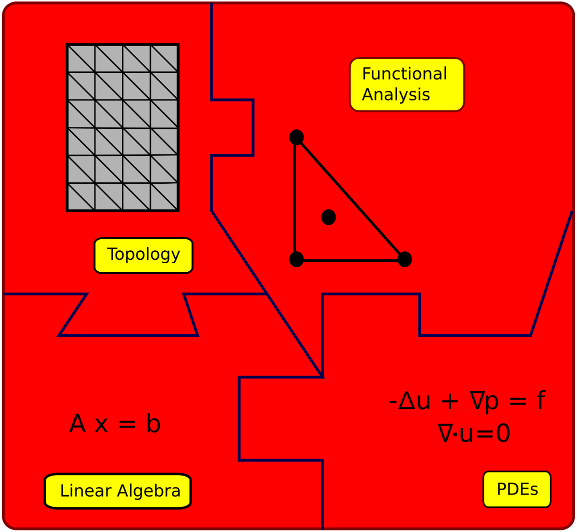


# Mathematics Necessary



# Algebraic Solvers

# Why use Ax=b?

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}\begin{bmatrix} \\ x \\ \\ \end{bmatrix} = \begin{bmatrix} \\ b \\ \\ \end{bmatrix}$$

- Model is able to capture lots of computations
- Reisz Representation Theorem

# The Large Scale Success Story

- BLAS
- LAPACK
- Scalapack
- Atlas
- Flame
- Trilinos
- PETSc
- Hypre
- ... More to come (Salsa)

# Functional Spaces

# Function Space Matters

Stokes Equation

- Taylor-Hood
- Crouzeix-Raviart
- Iterated Penalty

$$\begin{aligned} -\Delta \mathbf{u} + \nabla \mathbf{p} &= f \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

# Function Space Matters

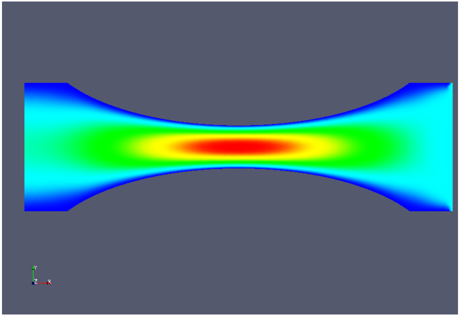
$$\frac{du}{dt} + u \cdot \nabla u = -\frac{\nabla \mathbf{p}}{\rho} + \nu \Delta \mathbf{u}$$

Navier-Stokes

- Stokes Solver
- Nonlinear Solver
- Time Stepping

**Stokes Equation**
Taylor-Hood
Crouzeix-Raviart
Iterated Penalty

# Function Space Matters



**Navier-Stokes**
Stokes Solver
Nonlinear Solver
Time Stepping

**Stokes Equation**
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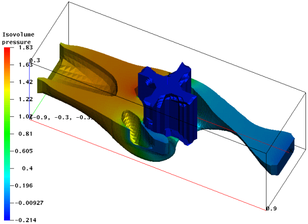
Non-Newtonian Flow

- Oldroyd-B
- Grade 2

# Function Space Matters




**Stokes Equation**
Taylor-Hood
Crouzeix-Raviart
Iterated Penalty

**Navier-Stokes**
Stokes Solver
Nonlinear Solver
Time Stepping

**Non-Newtonian**
Odroyd-B
Grade 2
...

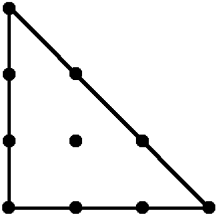
Fluid Solid Interfaces

- Free Boundary Problems
- Couple to legacy Codes

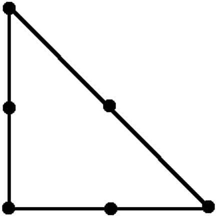
# Success Story

- FIAT Algorithm [Kirby 2005]
- Syfi [Mardel et al 2007]

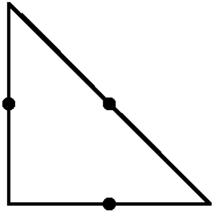
# Stokes Function Spaces



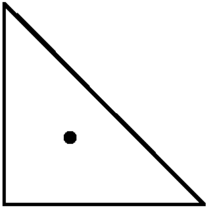
(a) $P_3$ for $V$



(b) $P_2$ for $\Pi$



(c) Crouzeix-Raviart for $V$

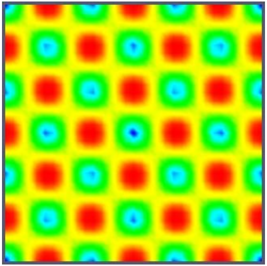


(d) $P_0$ for $\Pi$

# Problem statement

$$\mathbf{u} = \left[ \begin{array}{c} \sin(3\pi x)\cos(3\pi y) \\ -\cos(3\pi x)\sin(3\pi y) \end{array} \right]$$

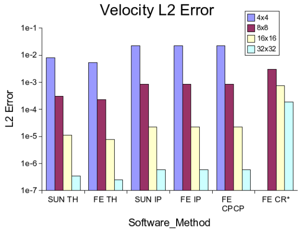
$$p = \sin(3\pi x)\sin(3\pi y)$$

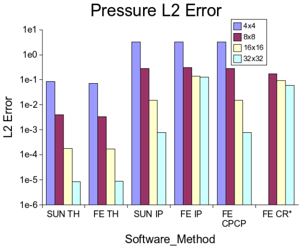


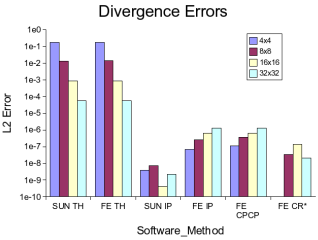
# Important Numbers.

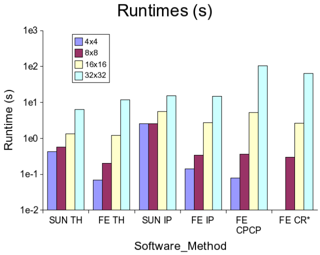


## Comparison of Fourth Order



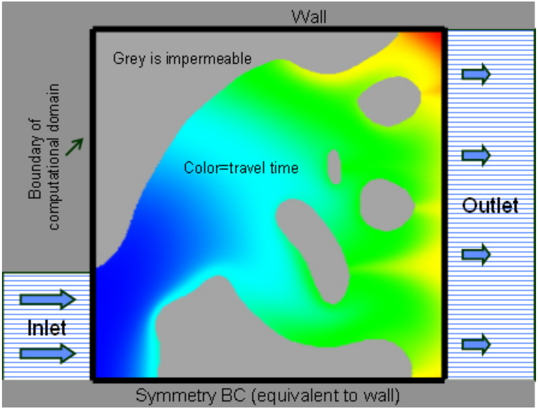



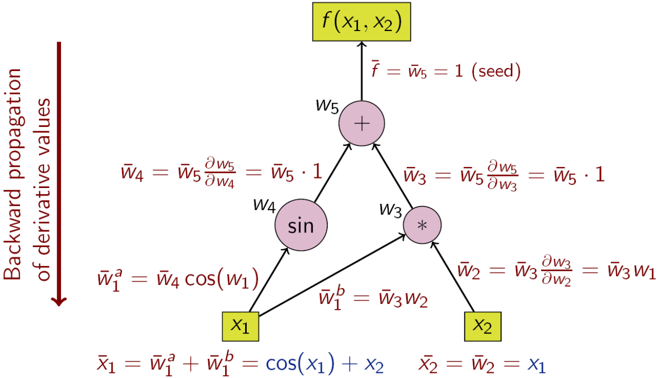



# Equation Description

# Optimization



# Automatic Differentiation



# Domain Representation

# Two Applications

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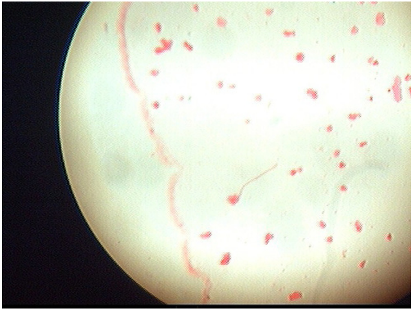
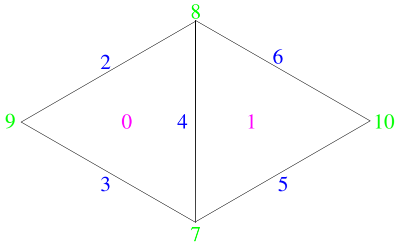
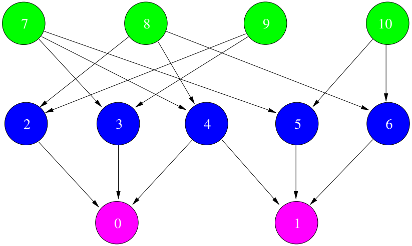
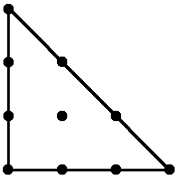


# Sieve



# Easy General Mesh



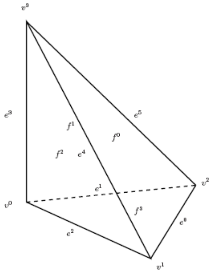
**Simple Mesh**

Points: 1,2,3
Edges: (1,2),(1,3),(2,3)
Face: (1,2,3)

**Sieve Mesh**

Points: 1,2,3
Edges: support(Points)
Face: support(Edges)

# Easy General Mesh



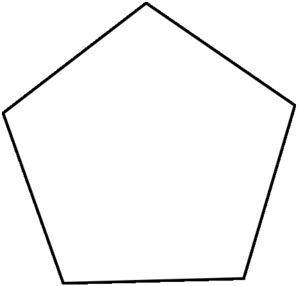
**Simple Mesh**

Points: 1,2,3,4
Edges: (1,2),(1,3),
(1,4),(2,3),(2,4),(3,4)
Face: (1,2,3),(1,2,4),
(1,3,4),(2,3,4)

**Sieve Mesh**

Points: 1,2,3,4
Edges: support(Points)
Faces: support(Edges)

# Easy General Mesh



**Sieve Mesh**

Points: 1,2,3,4,5
Edges: support(Points)
Faces: support(Edges)

**Simple Mesh**

Unsupported.

# Outline

# Automation Standard

Already Matlab is standard. Why?

# Automation Standard

Already Matlab is standard. Why?

Because with '\', the user does not have to chose between the following algorithms:

- Cholesky factorization
- QR factorization
- LU factorization
- Gaussian elimination with partial pivoting
- Least Squares fitting

# Computing = Big Computing

We should not settle for less

# Questions

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