

Automated Solution of Differential Equations

Anders Logg

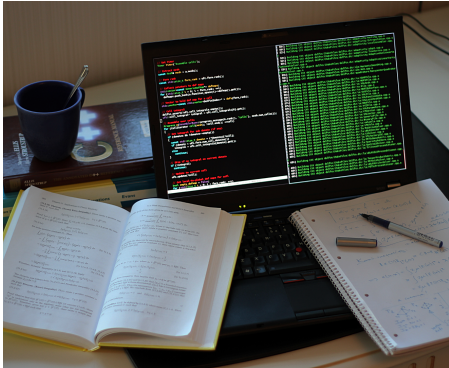
Mathematical Sciences
Chalmers University of Technology

Matematisk orientering TM1
8 december 2014

```
/// Constructor  
form() {}  
  
the global tensor  
virtual unsigned int rank() const = 0;  
  
/// Return the number of  
virtual unsigned int num_exterior_facet  
of exterior facet  
num_exterior_facet  
  
/// Create a new finite element  
virtual finite_element* create_finite_element(unsigned int n)  
  
/// Create a new dof map  
virtual dof_map* create_dof_map(unsigned int n)  
  
/// Create a new cell integral  
virtual cell_integral* create_cell_integral(unsigned int n)
```

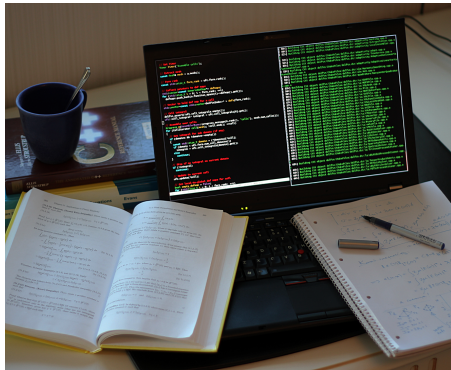
How to solve differential equations

(Using a numerical method)



How to solve differential equations

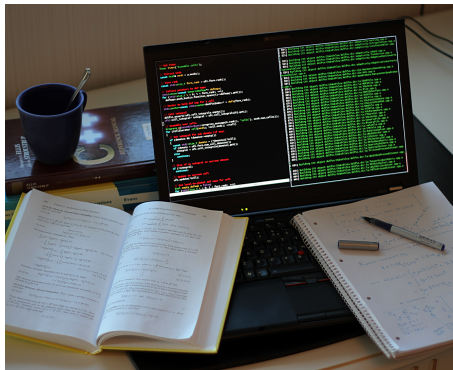
(Using a numerical method)



- ▶ Understand the model

How to solve differential equations

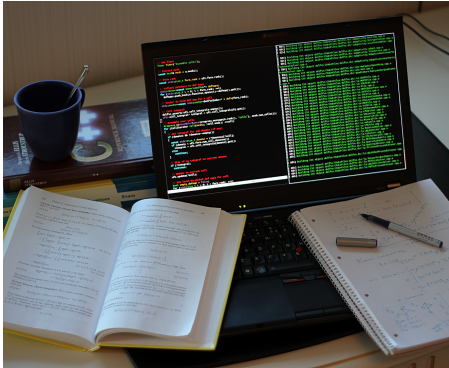
(Using a numerical method)



- ▶ Understand the model
- ▶ Develop the numerical method

How to solve differential equations

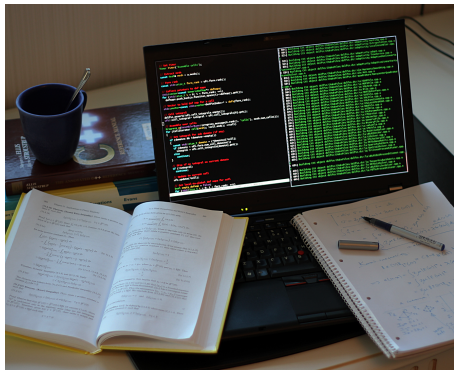
(Using a numerical method)



- ▶ Understand the model
- ▶ Develop the numerical method
- ▶ Write the code

How to solve differential equations

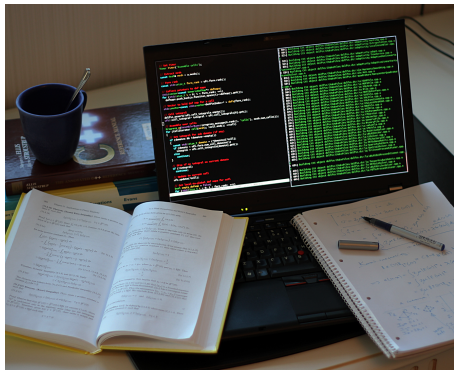
(Using a numerical method)



- ▶ Understand the model
- ▶ Develop the numerical method
- ▶ Write the code
- ▶ Compile the code

How to solve differential equations

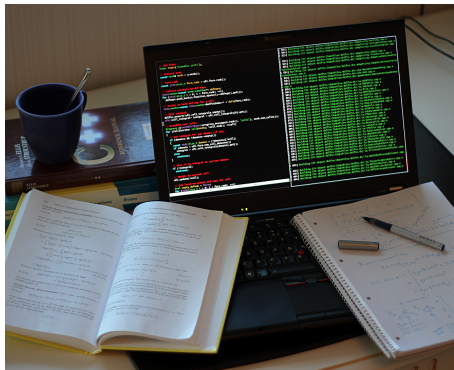
(Using a numerical method)



- ▶ Understand the model
- ▶ Develop the numerical method
- ▶ Write the code
- ▶ Compile the code
- ▶ Run the code

How to solve differential equations

(Using a numerical method)



- ▶ Understand the model
- ▶ Develop the numerical method
- ▶ Write the code
- ▶ Compile the code
- ▶ Run the code

- ▶ **Solving a single equation can take years!**

Let's look at an example (hyperelasticity)

$$F = I + \text{grad}(u)$$

$$C = F^T F$$

$$E = \frac{1}{2}(C - I)$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

$\begin{aligned} -\text{div } P &= B && \text{in } \Omega \\ u &= u_0 && \text{on } \partial\Omega \end{aligned}$

Let's look at an example (hyperelasticity)

$$F = I + \text{grad}(u)$$

$$C = F^T F$$

$$E = \frac{1}{2}(C - I)$$

● Strain measures



$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

$\begin{aligned} -\text{div } P &= B && \text{in } \Omega \\ u &= u_0 && \text{on } \partial\Omega \end{aligned}$

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● Strain measures



$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

● Strain energy



$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

$-\text{div } P = B \quad \text{in } \Omega$
$u = u_0 \quad \text{on } \partial\Omega$

Let's look at an example (hyperelasticity)

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$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

● Stress tensors

$-\text{div } P = B \quad \text{in } \Omega$
$u = u_0 \quad \text{on } \partial\Omega$

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● Strain energy

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● Stress tensors

$$P = FS$$

● Partial differential equation

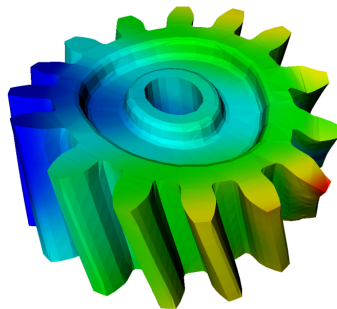
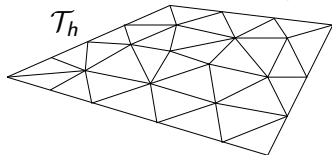
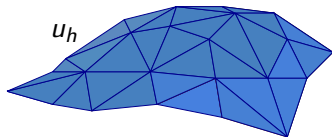
$-\text{div } P = B \quad \text{in } \Omega$
$u = u_0 \quad \text{on } \partial\Omega$

The mathematical model is reflected in the finite element discretization

Find $u \in V_h \subset V$ such that

$$\int_{\Omega} P : \text{grad } v \, dx = \int_{\Omega} B \cdot v \, dx$$

for all $v \in \hat{V}_h \subset \hat{V}$



But is obscured by the software implementation

```
1 subroutine quad(t,itype)
2 include 'commons'
3 integer t,itype,i,j,k,sub,qp
4 real x1,x2,x3,y1,y2,y3,
5 det,area,
6 dz1dx,dz2dx,dz3dx,
7 dz1dy,dz2dy,dz3dy,
8 qpx,qpy,
9 db1dx,db2dx,db1dy,db2dy
10 real bcrhs,cu
11 real qpf,qpp,qpq,qpr
12 logical bndsid(3)
13
14 x1=xvert(vertex(1,t))
15 x2=xvert(vertex(2,t))
16 x3=xvert(vertex(3,t))
17 y1=yvert(vertex(1,t))
18 y2=yvert(vertex(2,t))
19 y3=yvert(vertex(3,t))
20
21 det = x1*(y2-y3) +
22       x2*(y3-y1) + x3*(y1-y2)
23
24 area = abs(det/2.)
25
26 dz1dx = (y2-y3)/det
27 dz2dx = (y3-y1)/det
28 dz3dx = (y1-y2)/det
29 dz1dy = (x3-x2)/det
30 dz2dy = (x1-x3)/det
31 dz3dy = (x2-x1)/det
```

```
1 do 10 qp=1,nqpt
2   qpx = x1*quadpt(1,qp) +
3         x2*quadpt(2,qp) + x3*quadpt(3,qp)
4   qpy = y1*quadpt(1,qp) +
5         y2*quadpt(2,qp) + y3*quadpt(3,qp)
6   call pde(qpx,qpy,qpp,qpq,qpr,qpf)
7   do 20 i=1,nadd
8     db1dx = qpdbdz(1,row(i),qp)*dz1dx
9             + qpdbdz(2,row(i),qp)*dz2dx
10            + qpdbdz(3,row(i),qp)*dz3dx
11     db1dy = qpdbdz(1,row(i),qp)*dz1dy
12            + qpdbdz(2,row(i),qp)*dz2dy
13            + qpdbdz(3,row(i),qp)*dz3dy
14     db2dx = qpdbdz(1,col(i),qp)*dz1dx
15            + qpdbdz(2,col(i),qp)*dz2dx
16            + qpdbdz(3,col(i),qp)*dz3dx
17     db2dy = qpdbdz(1,col(i),qp)*dz1dy
18            + qpdbdz(2,col(i),qp)*dz2dy
19            + qpdbdz(3,col(i),qp)*dz3dy
20     add(i) = add(i) + quadw(qp)*
21             (qpp*db1dx*db2dx +
22              qpq*db1dy*db2dy +
23              qpr*qpbas(row(i),qp)*
24              qpbas(col(i),qp))
25   20 continue
26   do 30 i=1,naddrs
27     addrs(i) = addrs(i) + quadw(qp) *
28             qp * qpbas(rowrs(i),qp)
29   30 continue
30 10 continue
```

A new idea

R. C. Kirby, M. G. Knepley, A. Logg, L. R. Scott

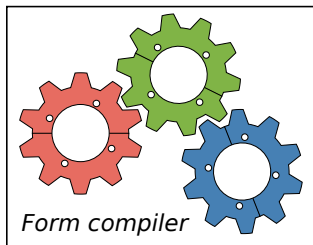
Optimizing the evaluation of finite element matrices
SIAM Journal on Scientific Computing 27 (2005)

R. C. Kirby and A. Logg

A compiler for variational forms
ACM Transactions on Mathematical Software 32 (2006)

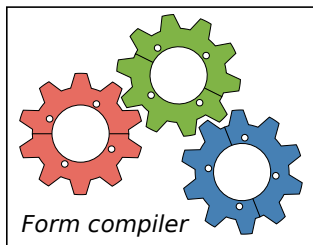
The code can be generated

$$\int_{\Omega} P : \text{grad } v \, dx = \int_{\Omega} B \cdot v \, dx$$



The code can be generated

$$\int_{\Omega} P : \text{grad } v \, dx = \int_{\Omega} B \cdot v \, dx$$



```
1 // Extract vertex coordinates
2 const double * const * x = c.coordinates;
3
4 // Compute Jacobian of affine map from
5 // reference cell
6 const double J_00 = x[1][0] - x[0][0];
7 const double J_01 = x[2][0] - x[0][0];
8 const double J_02 = x[3][0] - x[0][0];
9 const double J_10 = x[1][1] - x[0][1];
10 const double J_11 = x[2][1] - x[0][1];
11 const double J_12 = x[3][1] - x[0][1];
12 const double J_20 = x[1][2] - x[0][2];
13 const double J_21 = x[2][2] - x[0][2];
14 const double J_22 = x[3][2] - x[0][2];
15
16 // Compute sub determinants
17 const double d_00 = J_11*J_22 - J_12*J_21;
18 const double d_01 = J_12*J_20 - J_10*J_22;
19 const double d_02 = J_10*J_21 - J_11*J_20;
20 const double d_10 = J_02*J_21 - J_01*J_22;
21 const double d_11 = J_00*J_22 - J_02*J_20;
22 const double d_12 = J_01*J_20 - J_00*J_21;
23 const double d_20 = J_01*J_12 - J_02*J_11;
24 const double d_21 = J_02*J_10 - J_00*J_12;
25 const double d_22 = J_00*J_11 - J_01*J_10;
26
27 // Compute determinant of Jacobian
28 double detJ = J_00*d_00 + J_10*d_10 +
29 // Compute inverse of Jacobian
30 const double K_00 = d_00 / detJ;
31 ... [7328 lines of code]
```

**This is 7328 lines of code
that no one had to write**

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

$$C = F^{\top} F$$

$$E = \frac{1}{2}(C - I)$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

And we recover the mathematical notation

$$F = I + \text{grad}(u) \qquad \mathbf{F} = \mathbf{I} + \text{grad}(u)$$

$$C = F^\top F$$

$$E = \frac{1}{2}(C - I)$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

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$$P = FS$$

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

$$F = I + \text{grad}(u)$$

$$C = F^T F$$

$$C = F \cdot T * F$$

$$E = \frac{1}{2}(C - I)$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$S = \frac{\partial W}{\partial E}$$

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And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

$$F = I + \text{grad}(u)$$

$$C = F^T F$$

$$C = F.T*F$$

$$E = \frac{1}{2}(C - I)$$

$$E = \text{variable}(0.5*(C - I))$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

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$$C = F^T F$$

$$C = F.T*F$$

$$E = \frac{1}{2}(C - I)$$

$$E = \text{variable}(0.5*(C - I))$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2) \quad W = \text{lmda}/2*(\text{tr}(E)**2) + \text{mu}*tr(E*E)$$

$$S = \frac{\partial W}{\partial E}$$

$$P = FS$$

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

$$F = I + \text{grad}(u)$$

$$C = F^T F$$

$$C = F.T * F$$

$$E = \frac{1}{2}(C - I)$$

$$E = \text{variable}(0.5 * (C - I))$$

$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

$$W = \text{lmda}/2 * (\text{tr}(E)**2) + \text{mu} * \text{tr}(E * E)$$

$$S = \frac{\partial W}{\partial E}$$

$$S = \text{diff}(W, E)$$

$$P = FS$$

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

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$$S = \frac{\partial W}{\partial E}$$

$$S = \text{diff}(W, E)$$

$$P = FS$$

$$P = F * S$$

$$\int_{\Omega} P : \text{grad } v \, dx - \int_{\Omega} B \cdot v \, dx = 0$$

And we recover the mathematical notation

$$F = I + \text{grad}(u)$$

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$$E = \frac{1}{2}(C - I)$$

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$$W = \frac{\lambda}{2}(\text{tr}(E))^2 + \mu \text{tr}(E^2)$$

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$$S = \frac{\partial W}{\partial E}$$

$$S = \text{diff}(W, E)$$

$$P = FS$$

$$P = F * S$$

$$\int_{\Omega} P : \text{grad } v \, dx - \int_{\Omega} B \cdot v \, dx = 0$$

\Leftrightarrow

$$\text{inner}(P, \text{grad}(v)) * dx - \text{dot}(B, v) * dx == 0$$

**Can we completely automate the solution of
differential equations?**

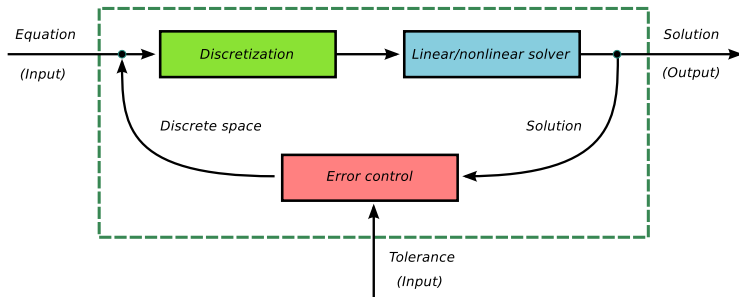
Automated solution of differential equations

Input

- ▶ $A(u) = f$
- ▶ $\epsilon > 0$

Output

- ▶ $u_h \approx u$
- ▶ $\|u - u_h\| \leq \epsilon$



Automated solution of differential equations

Key steps

- (i) Automated discretization ✓ (2006)
- (ii) Automated error control ✓ (2010)
- (iii) Automated generation of well-posed discretizations

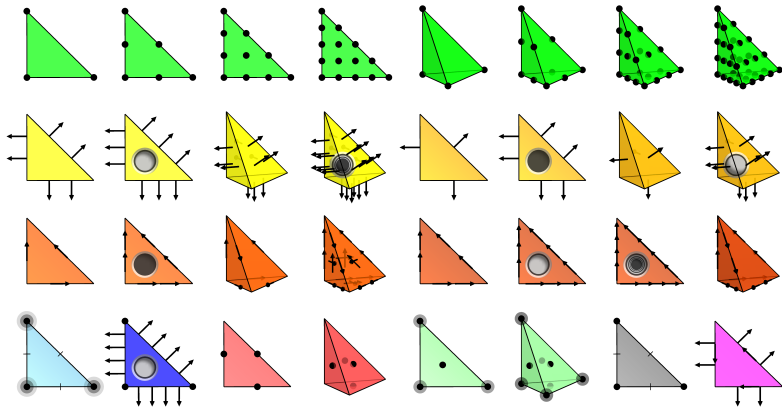
Key techniques

- ▶ Adaptive finite element methods
- ▶ Automatic code generation

(i) Automated discretization

Automated discretization by automated FEM

- ▶ Automated generation of basis functions
- ▶ Automated evaluation of variational forms
- ▶ Automated finite element assembly



The Finite Element Method (FEM)

Differential equation (strong form)

$$-\Delta u = f$$

Weak form

$$\text{Find } u \in V : \underbrace{\langle \text{grad } u, \text{grad } v \rangle}_{a(u,v)} = \underbrace{\langle f, v \rangle}_{L(v)} \quad \forall v \in V$$

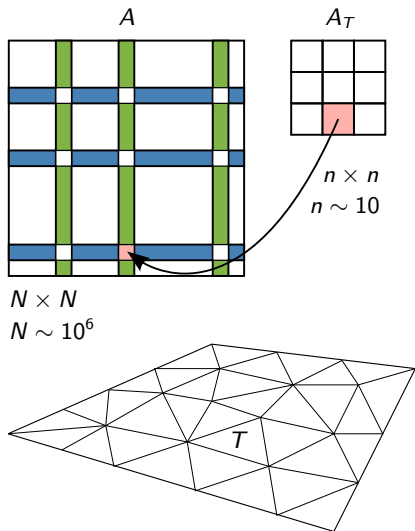
Finite element method

$$\text{Find } u_h \in V_h : \langle \text{grad } u_h, \text{grad } v \rangle = \langle f, v \rangle \quad \forall v \in V_h$$

Solution algorithm (for $u_h = \sum_{j=1}^N U_j \phi_j$)

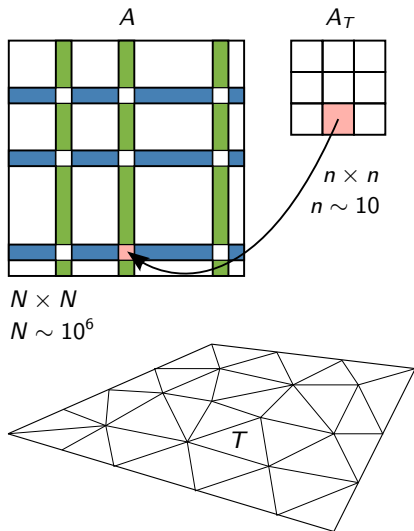
$$AU = b \quad A_{ij} = \langle \text{grad } \phi_j, \text{grad } \phi_i \rangle \quad b_i = \langle f, \phi_i \rangle$$

Finite element assembly



- Compute $A_{ij} = a(\phi_j, \phi_i)$

Finite element assembly

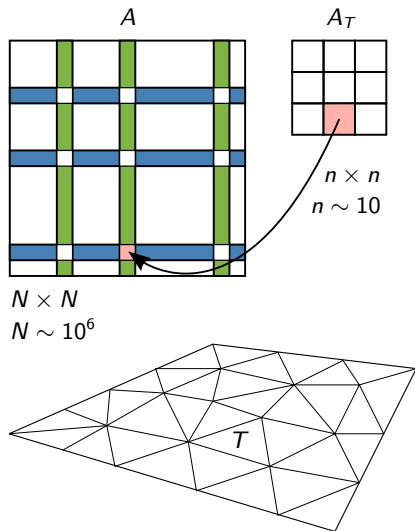


- ▶ Compute $A_{ij} = a(\phi_j, \phi_i)$
- ▶ Compute the element matrix

$$A_{T,ij} = a_T(\phi_j, \phi_i)$$

on each triangle T

Finite element assembly



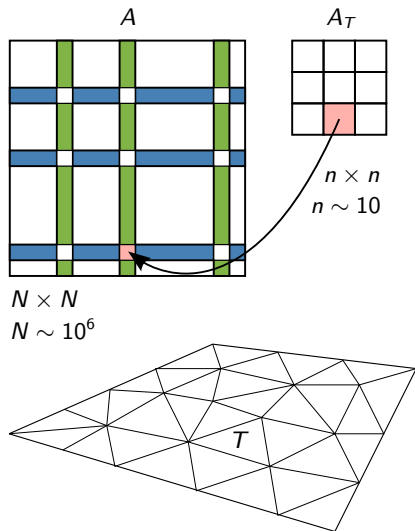
- ▶ Compute $A_{ij} = a(\phi_j, \phi_i)$
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$$A_{T,ij} = a_T(\phi_j, \phi_i)$$

on each triangle T

- ▶ Assemble $\{A_T\}_T$ into the global matrix A

Finite element assembly



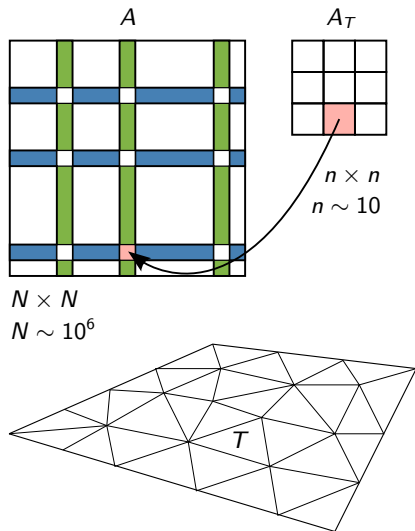
- ▶ Compute $A_{ij} = a(\phi_j, \phi_i)$
- ▶ Compute the element matrix

$$A_{T,ij} = a_T(\phi_j, \phi_i)$$

on each triangle T

- ▶ Assemble $\{A_T\}_T$ into the global matrix A
- ▶ Generate code for the evaluation of A_T

Finite element assembly



- ▶ Compute $A_{ij} = a(\phi_j, \phi_i)$
- ▶ Compute the element matrix

$$A_{T,ij} = a_T(\phi_j, \phi_i)$$

on each triangle T

- ▶ Assemble $\{A_T\}_T$ into the global matrix A
- ▶ Generate code for the evaluation of A_T
- ▶ Use the structure of A_T to generate *optimized* code

Automatic code generation

Input

Equation (variational problem)

Output

Efficient application-specific code

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{b}$$
$$\nabla \cdot \vec{u} = 0$$

```
// Extract affine coordinates
const double * const x = c.coordinates;

// Compute Jacobian of affine map from reference cell
const double J_00 = x[1]*01 - x[0]*01;
const double J_01 = x[2]*01 - x[0]*01;
const double J_10 = x[1]*11 - x[0]*11;
const double J_11 = x[2]*11 - x[0]*11;

// Compute determinant of Jacobian
double detJ = J_00*J_11 - J_01*J_10;

// Compute inverse of Jacobian
const double Jinv_00 = J_11 / detJ;
const double Jinv_01 = -J_01 / detJ;
const double Jinv_10 = -J_10 / detJ;
const double Jinv_11 = J_00 / detJ;

// Take absolute value of determinant
detJ = std::abs(detJ);

// Set scale factor
const double det = detJ;

// Compute geometry tensors
const double G0_0_0 = det*(Jinv_00*Jinv_00 + Jinv_01*Jinv_01);
const double G0_0_1 = det*(Jinv_00*Jinv_10 + Jinv_01*Jinv_11);
const double G0_1_0 = det*(Jinv_10*Jinv_00 + Jinv_11*Jinv_01);
const double G0_1_1 = det*(Jinv_10*Jinv_10 + Jinv_11*Jinv_11);
```

Equation (variational form)

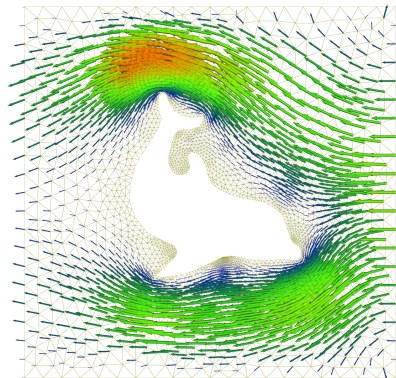
Form compiler

Application-specific code

Example: the Stokes equations

Differential equation

$$\begin{aligned} -\operatorname{div} \operatorname{grad} u + \operatorname{grad} p &= f \\ \operatorname{div} u &= 0 \end{aligned}$$



Example: the Stokes equations

Weak form

Find $(u, p) \in V \times Q$ such that

$$a((u, p), (v, q)) = L((v, q)) \quad \forall (v, q) \in \hat{V} \times \hat{Q}$$

where

$$a((u, p), (v, q)) = \int_{\Omega} \text{grad } u : \text{grad } v - p \text{ div } v + \text{div } u q \, dx$$
$$L((v, q)) = \int_{\Omega} f v \, dx$$

Example: the Stokes equations

Implementation

Python code

```
1 P2 = VectorElement("Lagrange", triangle, 2)
2 P1 = FiniteElement("Lagrange", triangle, 1)
3 TH = P2 * P1
4
5 (u, p) = TrialFunctions(TH)
6 (v, q) = TestFunctions(TH)
7
8 f = Coefficient(P2)
9
10 a = (inner(grad(u), grad(v)) - p*div(v) + div(u)*q)*dx
11 L = dot(f, v)*dx
```

Example: the Stokes equations

Implementation

Python code

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1 P2 = VectorElement("Lagrange", triangle, 2)
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3 TH = P2 * P1
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5 (u, p) = TrialFunctions(TH)
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8 f = Coefficient(P2)
9
10 a = (inner(grad(u), grad(v)) - p*div(v) + div(u)*q)*dx
11 L = dot(f, v)*dx
```

$$a = \int_{\Omega} \text{grad } u : \text{grad } v - p \text{div } v + \text{div } u q \, dx$$

(ii) Automated error control

Automated goal-oriented error control

Input

- ▶ Variational problem: Find $u \in V$: $a(u, v) = L(v) \quad \forall v \in V$
- ▶ Quantity of interest: $\mathcal{M} : V \rightarrow \mathbb{R}$
- ▶ Tolerance: $\epsilon > 0$

Objective

Find $V_h \subset V$ such that $|\mathcal{M}(u) - \mathcal{M}(u_h)| < \epsilon$ where

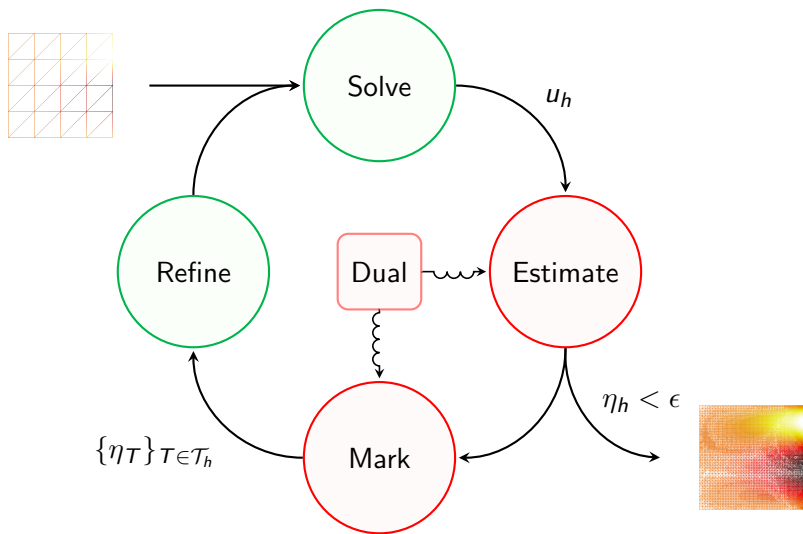
$$a(u_h, v) = L(v) \quad \forall v \in V_h$$

Automated in FEniCS (for linear and nonlinear PDE)

Python code

```
1 solve(a == L, u, M=M, tol=1e-3)
```

Adaptivity = solve – estimate – mark – refine



Error analysis

Define (weak) residual:

$$r(v) = L(v) - a(u_h, v)$$

Introduce dual problem:

$$\text{Find } z \in V: \quad a^*(z, v) = \mathcal{M}(v) \quad \forall v \in V$$

Error representation:

$$\begin{aligned} \mathcal{M}(u) - \mathcal{M}(u_h) &= \mathcal{M}(e) \\ &= a^*(z, e) \\ &= a(e, z) \\ &= a(u, z) - a(u_h, z) \\ &= L(z) - a(u_h, z) \\ &\equiv r(z) \end{aligned}$$

A posteriori error estimate for Poisson

$$a(u, v) = \int_{\Omega} \text{grad } u \cdot \text{grad } v \, dx \quad L(v) = \int_{\Omega} f v \, dx$$

Recall error representation:

$$\mathcal{M}(u) - \mathcal{M}(u_h) = r(z) = \int_{\Omega} f z - \text{grad } u_h \cdot \text{grad } z \, dx$$

Residual decomposition:

$$r(v) = \sum_{T \in \mathcal{T}_h} \int_T \underbrace{(f + \Delta u_h)}_{R_T} v \, dx - \int_{\partial T} \underbrace{\text{grad } u_h \cdot n}_{R_{\partial T}} v \, ds$$

Error indicators:

$$\eta_T = |\langle R_T, z - \pi_h z \rangle_T + \langle \llbracket R_{\partial T} \rrbracket, z - \pi_h z \rangle_{\partial T}|$$

Key steps to automated error control

- ▶ Automated linearization
- ▶ Automated generation of the dual problem
- ▶ Automated integration by parts:

$$r_T(v) = \int_T R_T \cdot v \, dx + \int_{\partial T} R_{\partial T} \cdot v \, ds$$

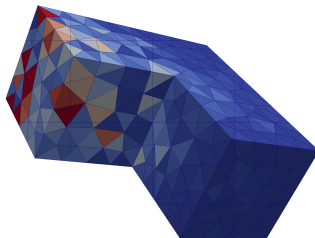
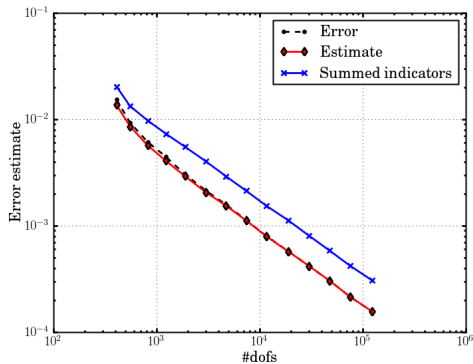
Test against bubble functions to solve for R_T and $R_{\partial T}$

- ▶ Automated computation of error indicators:

$$\eta_T = |\langle R_T, \tilde{z}_h - z_h \rangle_T + \langle \llbracket R_{\partial T} \rrbracket, \tilde{z}_h - z_h \rangle_{\partial T}|$$

- ▶ Automated mesh refinement
- ▶ Dual problem solved on same function space and extrapolated

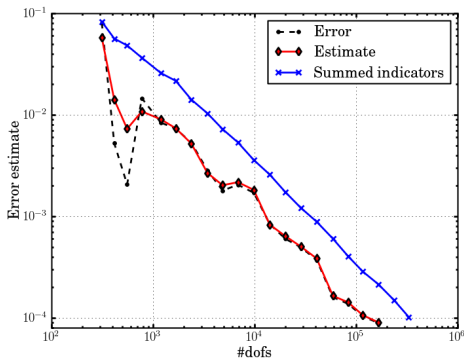
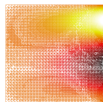
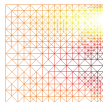
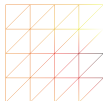
Poisson's equation



$$a(u, v) = \langle \text{grad } u, \text{grad } v \rangle$$

$$\mathcal{M}(u) = \int_{\Gamma} u \, ds, \quad \Gamma \subset \partial\Omega$$

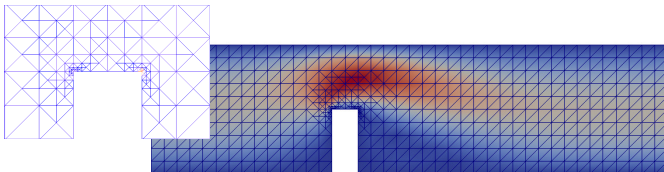
A three-field mixed elasticity formulation



$$a((\sigma, u, \gamma), (\tau, v, \eta)) = \langle A\sigma, \tau \rangle + \langle u, \operatorname{div} \tau \rangle + \langle \operatorname{div} \sigma, v \rangle + \langle \gamma, \tau \rangle + \langle \sigma, \eta \rangle$$

$$\mathcal{M}((\sigma, u, \eta)) = \int_{\Gamma} g \sigma \cdot n \cdot t \, ds$$

Incompressible Navier–Stokes



Outflux $\approx 0.4087 \pm 10^{-4}$

Uniform

1.000.000 dofs, N hours

Adaptive

5.200 dofs, 127 seconds

Python code

```
1 from dolfin import *
2
3 class Noslip(SubDomain): ...
4
5 mesh = Mesh("channel-with-flap.xml.gz")
6 V = VectorFunctionSpace(mesh, "CG", 2)
7 Q = FunctionSpace(mesh, "CG", 1)
8 W = V*Q
9
10 # Define test functions and unknown(s)
11 (v, q) = TestFunctions(W)
12 w = Function(W)
13 (u, p) = split(w)
14
15 # Define (non-linear) form
16 n = FacetNormal(mesh)
17 p0 = Expression("(4.0 - x[0])/4.0")
18 F = (0.02*inner(grad(u), grad(v)) + inner(grad(u)*u), v)*dx
19     - p*div(v) + div(u)*q + dot(v, n)*p0*ds
20
21 # Define goal functional
22 M = u[0]*ds(0)
23
24 # Compute solution
25 tol = 1e-4
26 solve(F == 0, w, bcs, M, tol)
```

The FEniCS Project

FEniCS is an automated programming environment for differential equations

- ▶ C++/Python FEM library
- ▶ Initiated 2003 in Chicago
- ▶ 1000–2000 monthly downloads
- ▶ Part of Debian and Ubuntu
- ▶ Licensed under the GNU LGPL

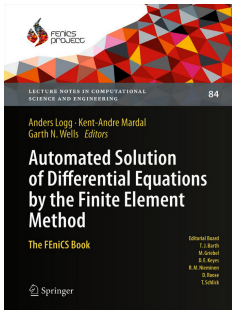


<http://fenicsproject.org/>

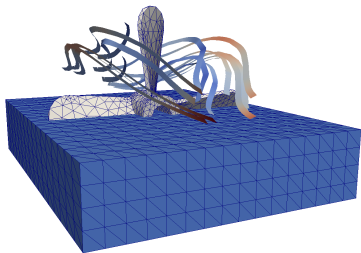
Collaborators (in order of appearance)

Chalmers University of Technology, University of Chicago, KTH Royal Institute of Technology, Simula Research Laboratory, University of Cambridge, Texas Tech University, University of Texas at Austin, Baylor University

Key features

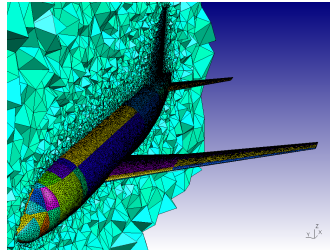
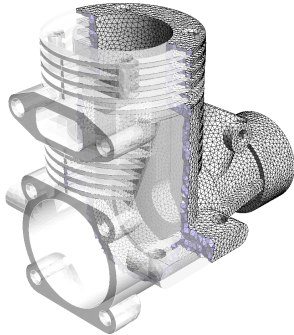
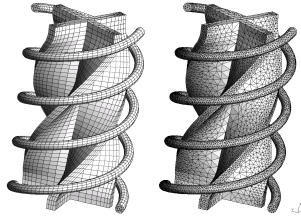
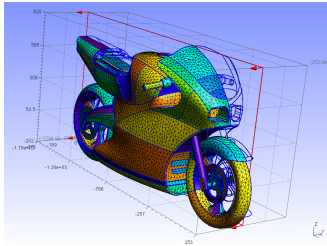


- ▶ Automated discretization
- ▶ Automated error control
- ▶ General families of finite elements, including arbitrary order continuous and discontinuous Lagrange elements, BDM, RT, Nédélec, . . .
- ▶ General mixed elements
- ▶ Distributed (clusters) and shared memory (multicore) parallelism
- ▶ High performance linear algebra (PETSc, Trilinos)
- ▶ Mesh generation, adaptive mesh refinement
- ▶ Extensive documentation

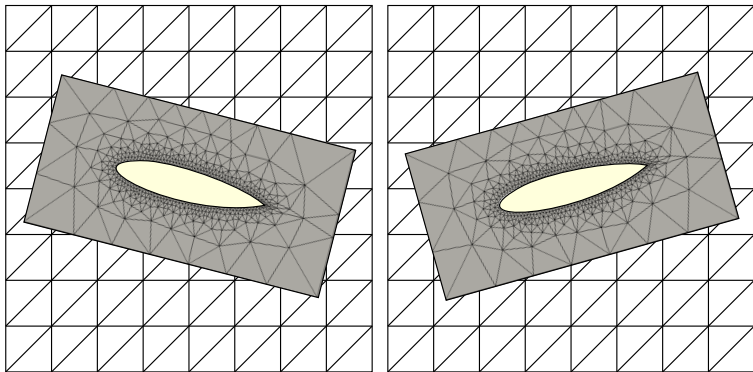


Multimesh FEM for multiphysics

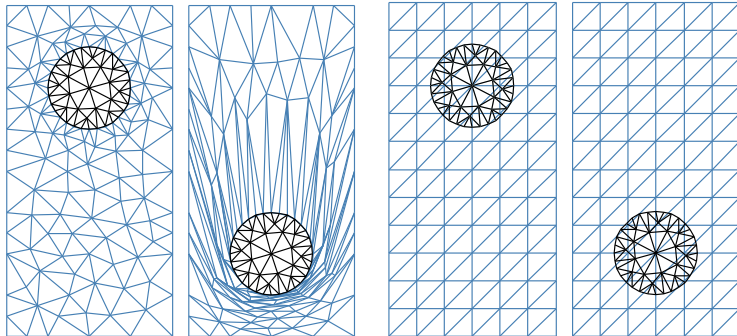
Challenge 1: Mesh generation



Challenge 2: Geometry-dependent parameter studies



Challenge 3: Evolving geometries



Multimesh finite element methods

- ▶ Galerkin framework based on Nitsche's method
- ▶ Arbitrary combination of overlapping and intersecting meshes
- ▶ Proper method design leads to a theoretical basis including
 - ▶ Inf-sup stability
 - ▶ Optimal a priori error estimates
 - ▶ Optimal algebraic condition number estimates

Theoretical program by Burman, Hansbo, Hansbo, Larson

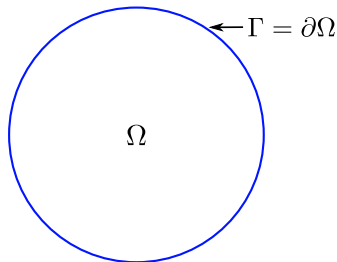
- ▶ Efficient and robust implementation in 3D
- ▶ Application to fluid flow and FSI
- ▶ Distributed as free/open-source software as part of FEniCS

Collaborators: Larson, Massing, Rognes, Johansson, Lundholm

Nitsche's method for Dirichlet boundary conditions

Differential equation

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega \\ u &= g & \text{on } \Gamma \end{aligned}$$



Weak form

Find $u \in V_h$ s.t.

$$a(u, v) = L(v) \quad \forall v \in V_h$$

$$\begin{aligned} a(u, v) &= \int_{\Omega} \nabla u \cdot \nabla v \, dx - \underbrace{\int_{\Gamma} \nabla u \cdot \mathbf{n} v \, dS}_{\text{Consistency}} - \underbrace{\int_{\Gamma} \nabla v \cdot \mathbf{n} u \, dS}_{\text{Symmetrization}} + \underbrace{\gamma \int_{\Gamma} h^{-1} uv \, dS}_{\text{Penalization}} \\ L(v) &= \int_{\Omega} f v \, dx - \underbrace{\int_{\Gamma} \nabla v \cdot \mathbf{n} g \, dS}_{\text{Symmetrization}} + \underbrace{\gamma \int_{\Gamma} h^{-1} g v \, dS}_{\text{Penalization}} \end{aligned}$$

Nitsche's method for interface conditions

Domain decomposition

Find (u_1, u_2) such that

$$-\Delta u_i = f_i \quad \text{in } \Omega_i, \quad i = 1, 2$$

$$[\nabla u \cdot \mathbf{n}] = 0 \quad \text{on } \Gamma$$

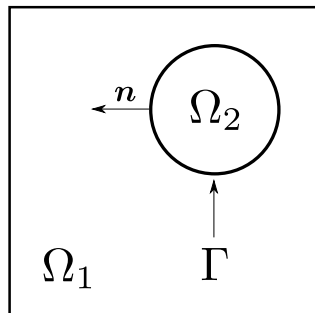
$$[u] = 0 \quad \text{on } \Gamma$$

Variational formulation

$$a(u, v) = \sum_{i=1,2} \int_{\Omega_i} \nabla u \cdot \nabla v \, dx$$

$$- \underbrace{\int_{\Gamma} \langle \nabla u \cdot \mathbf{n} \rangle [v] \, dS}_{\text{Consistency}} - \underbrace{\int_{\Gamma} \langle \nabla v \cdot \mathbf{n} \rangle [u] \, dS}_{\text{Symmetrization}} + \underbrace{\gamma \int_{\Gamma} h^{-1} [u][v] \, dS}_{\text{Penalty/Stabilization}}$$

$$L(v) = \int_{\Omega} f v \, dx$$



Multimesh FEM for Stokes

Interface formulation

$$\begin{aligned} -\Delta \mathbf{u}_i + \nabla p_i &= \mathbf{f}_i & \text{in } \Omega_i, & \quad i = 1, 2 \\ \mathbf{n} \cdot \mathbf{u}_i &= 0 & \text{in } \Omega_i, & \quad i = 1, 2 \\ [\mathbf{u}] &= 0 & \text{on } \Gamma \\ [\partial_{\mathbf{n}} \mathbf{u} - p \mathbf{n}] &= 0 & \text{on } \Gamma \\ \mathbf{u} &= 0 & \text{on } \partial \Omega \end{aligned}$$

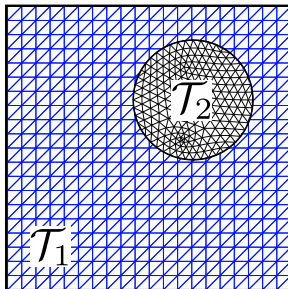
Finite element method

$$a_h(\mathbf{u}_h, \mathbf{v}_h) = (\nabla \mathbf{u}_h, \nabla \mathbf{v}_h)_{\Omega_1 \cup \Omega_2} - (\langle \partial_{\mathbf{n}} \mathbf{u}_h \rangle, [\mathbf{v}_h])_{\Gamma}$$

$$- (\langle \partial_{\mathbf{n}} \mathbf{v}_h \rangle, [\mathbf{u}_h])_{\Gamma} + \gamma (h^{-1} [\mathbf{u}_h], [\mathbf{v}_h])_{\Gamma}$$

$$b_h(\mathbf{v}_h, q_h) = -(\nabla \cdot \mathbf{v}_h, q_h)_{\Omega_1 \cup \Omega_2} + (\mathbf{n} \cdot [\mathbf{v}_h], \langle q_h \rangle)_{\Gamma}$$

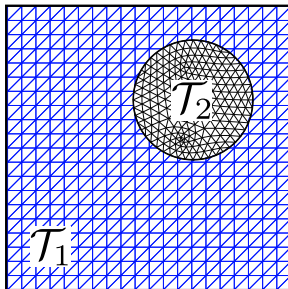
$$S_h(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) = \delta \underbrace{\sum_{i=1,2} \sum_{T \in \mathcal{T}_i \cap \Omega_i} h_T^2 (-\Delta \mathbf{u}_h + \nabla p_h, -\alpha \Delta \mathbf{v}_h + \beta \nabla q_h)_T}_{\text{Stabilization}}$$



Multimesh FEM for Stokes

Interface formulation

$$\begin{aligned} -\Delta \mathbf{u}_i + \nabla p_i &= \mathbf{f}_i & \text{in } \Omega_i, \quad i = 1, 2 \\ \mathbf{n} \cdot \mathbf{u}_i &= 0 & \text{in } \Omega_i, \quad i = 1, 2 \\ [\mathbf{u}] &= 0 & \text{on } \Gamma \\ [\partial_{\mathbf{n}} \mathbf{u} - p \mathbf{n}] &= 0 & \text{on } \Gamma \\ \mathbf{u} &= 0 & \text{on } \partial \Omega \end{aligned}$$



Finite element method

$$a_h(\mathbf{u}_h, \mathbf{v}_h) = (\nabla \mathbf{u}_h, \nabla \mathbf{v}_h)_{\Omega_1 \cup \Omega_2} - (\langle \partial_{\mathbf{n}} \mathbf{u}_h \rangle, [\mathbf{v}_h])_{\Gamma}$$

$$- (\langle \partial_{\mathbf{n}} \mathbf{v}_h \rangle, [\mathbf{u}_h])_{\Gamma} + \gamma (h^{-1} [\mathbf{u}_h], [\mathbf{v}_h])_{\Gamma}$$

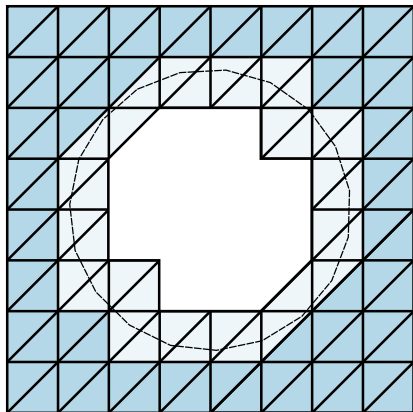
$$b_h(\mathbf{v}_h, q_h) = -(\nabla \cdot \mathbf{v}_h, q_h)_{\Omega_1 \cup \Omega_2} + (\mathbf{n} \cdot [\mathbf{v}_h], \langle q_h \rangle)_{\Gamma}$$

$$S_h(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) = \delta \underbrace{\sum_{T \in \mathcal{T}_1^* \cup \mathcal{T}_2} h_T^2 (-\Delta \mathbf{u}_h + \nabla p_h, -\alpha \Delta \mathbf{v}_h + \beta \nabla q_h)_T}_{\text{Stabilization and ghost penalty } p}$$

$$s_h(\mathbf{u}_h, \mathbf{v}_h) = \underbrace{(\nabla(\mathbf{u}_{h,1} - \mathbf{u}_{h,2}), \nabla(\mathbf{v}_{h,1} - \mathbf{v}_{h,1}))_{\Omega_O}}_{\text{Ghost penalty for } u}$$

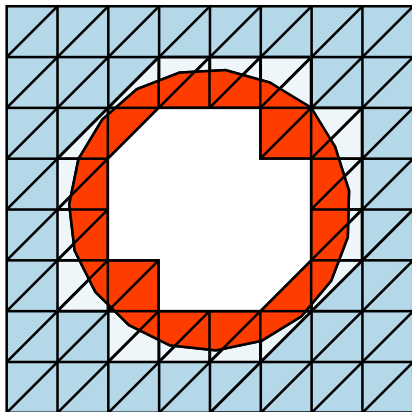
Ghost penalty for u

Ghost penalties are added in the interface zone



$$\delta \sum_{T \in \mathcal{T}_1^* \cup \mathcal{T}_2} h_T^2 (-\Delta \mathbf{u}_h + \nabla p_h, -\alpha \Delta \mathbf{v}_h + \beta \nabla q_h)_T$$

Ghost penalty for p



$$(\nabla(\mathbf{u}_{h,1} - \mathbf{u}_{h,2}), \nabla(\mathbf{v}_{h,1} - \mathbf{v}_{h,1}))_{\Omega_O}$$

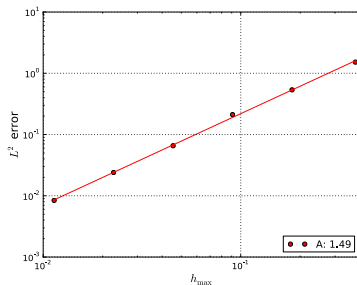
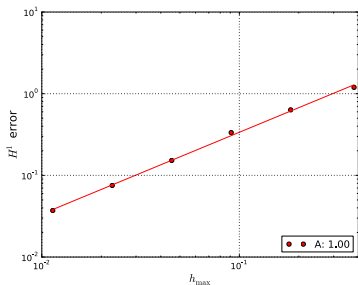
Ghost penalty for u

Optimal a priori error estimate

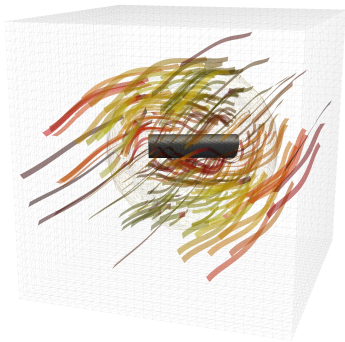
Theorem

Let $k, l \geq 1$ and assume that $(\mathbf{u}, p) \in [H^{k+1}(\Omega)]^d \times H^{l+1}(\Omega)$ is a (weak) solution of the Stokes problem. Then the finite element solution $(\mathbf{u}_h, p_h) \in V_h^k \times Q_h^l$ satisfies the following error estimate:

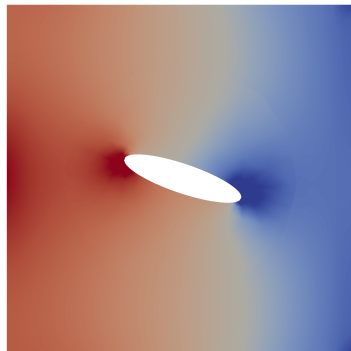
$$\|(\mathbf{u} - \mathbf{u}_h, p - p_h)\| \lesssim h^k |\mathbf{u}|_{k+1, \Omega} + h^{l+1} |p|_{l+1, \Omega}.$$



Application: Stokes flow around an airfoil

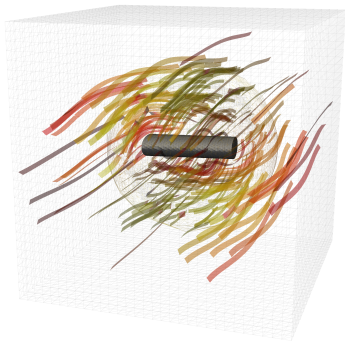


Velocity streamlines

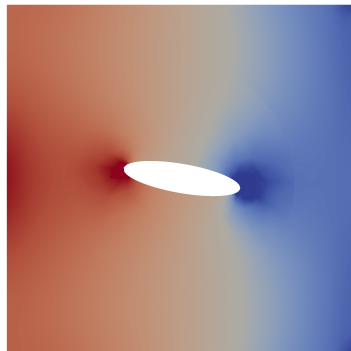


Pressure

Application: Stokes flow around an airfoil

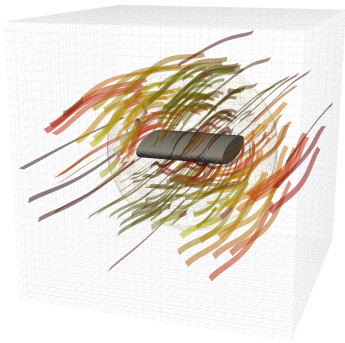


Velocity streamlines

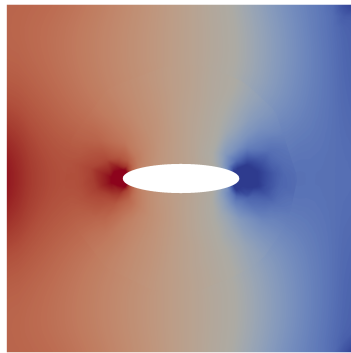


Pressure

Application: Stokes flow around an airfoil

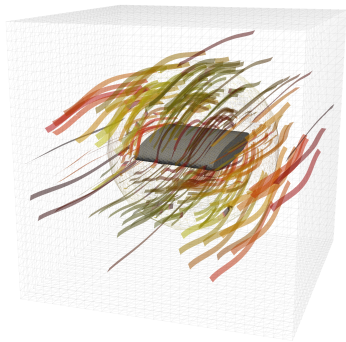


Velocity streamlines

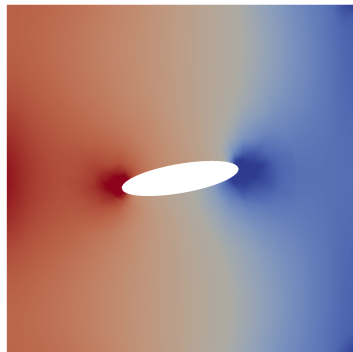


Pressure

Application: Stokes flow around an airfoil

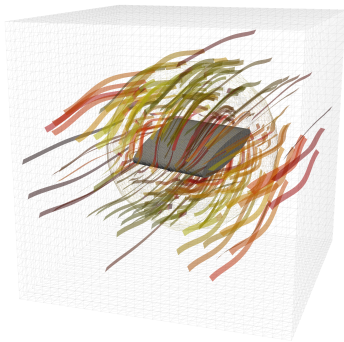


Velocity streamlines

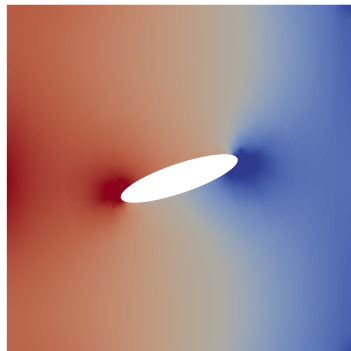


Pressure

Application: Stokes flow around an airfoil



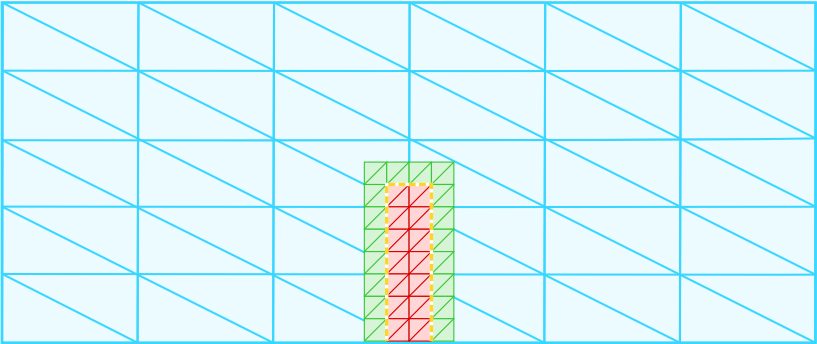
Velocity streamlines



Pressure


Fluid–structure interaction on cut meshes

Multimesh FEM for FSI



 *Fluid*

 *Mesh + Fluid*

 *Structure*

 *Interface*

A stationary FSI problem: state equations

$$\begin{array}{l} \text{Fluid} \\ (F) \end{array} \quad \begin{array}{l} \nabla \cdot \sigma_F(u_F, p_F) = 0 \\ \nabla \cdot u_F = 0 \end{array}$$

$$\nabla \cdot \tilde{\sigma}_M(\tilde{u}_M) = 0$$

Mesh
(M)

$$\nabla \cdot \hat{\Pi}(\hat{u}_S) = 0$$

Structure
(S)

A stationary FSI problem: state equations

Fluid
(F)

$$\begin{aligned} \nabla \cdot \sigma_F(u_F, p_F) &= 0 \\ \nabla \cdot u_F &= 0 \end{aligned}$$

Interface
(I)

$$\begin{aligned} \tilde{u}_M &= \hat{u}_S \\ u_F &= 0 \\ \hat{\Pi}(\hat{u}_S) \cdot \hat{n}_S &= \tilde{J}_M \tilde{\sigma}(\tilde{u}_F, \tilde{p}_F) \tilde{F}_M^{-T} \hat{n}_S \end{aligned}$$

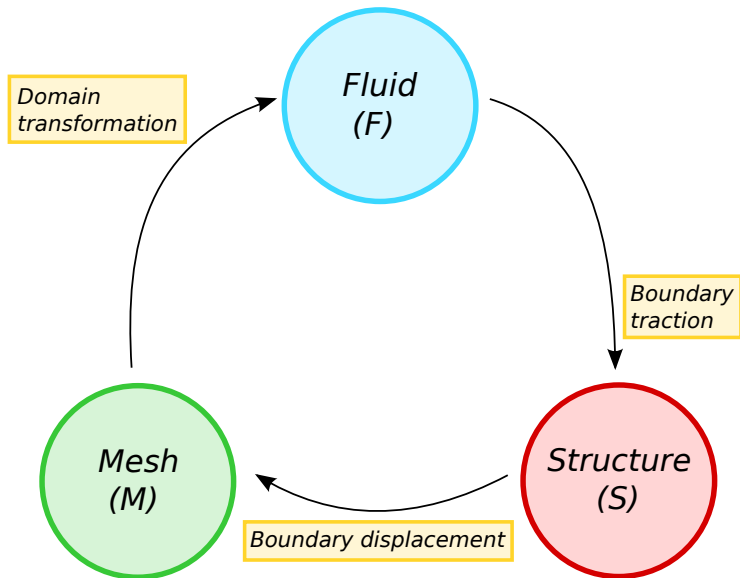
$$\nabla \cdot \tilde{\sigma}_M(\tilde{u}_M) = 0$$

Mesh
(M)

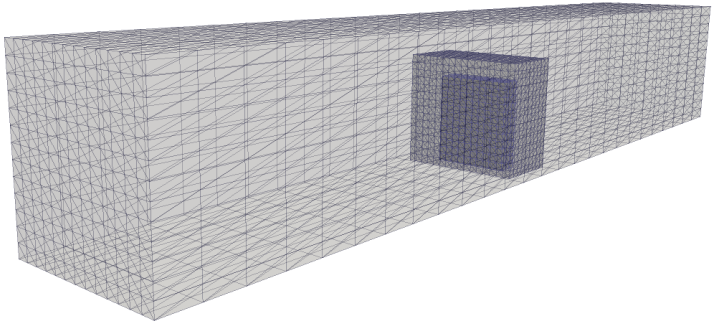
$$\nabla \cdot \hat{\Pi}(\hat{u}_S) = 0$$

Structure
(S)

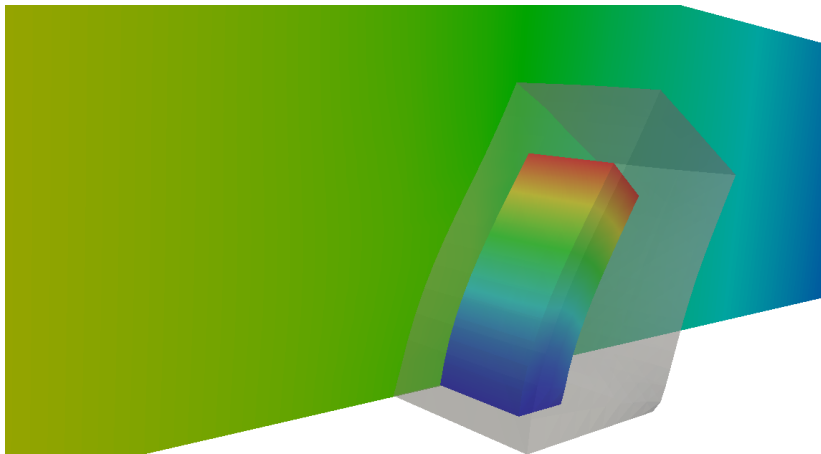
The stationary FSI problem can be solved by a classical fixed-point method



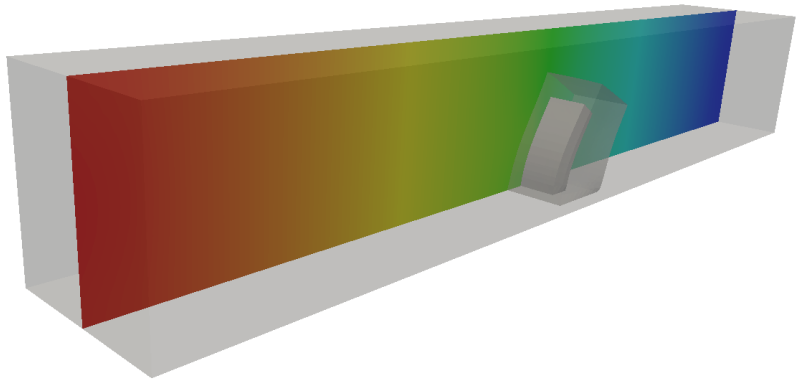
Application: elastic flap in channel



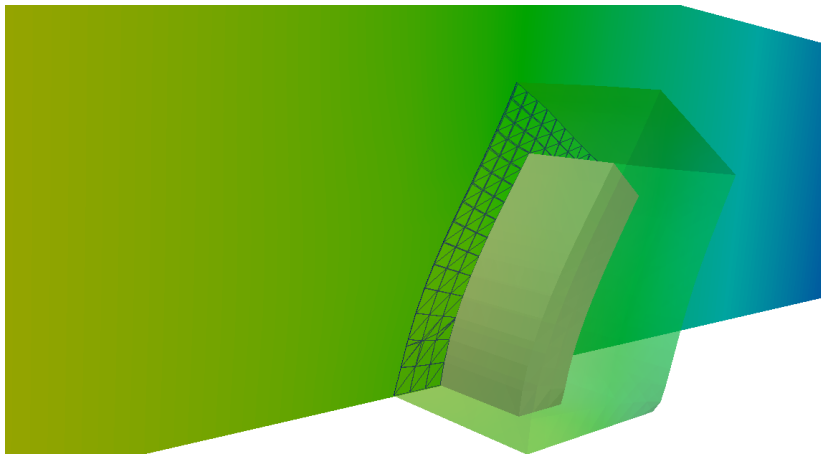
Flap in channel: Displacement



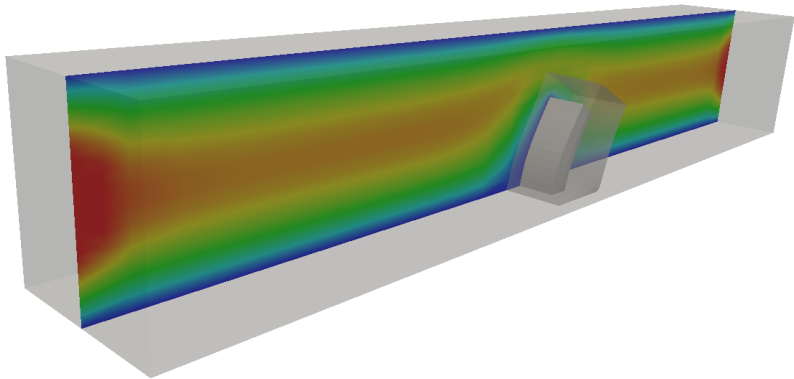
Flap in channel: Pressure



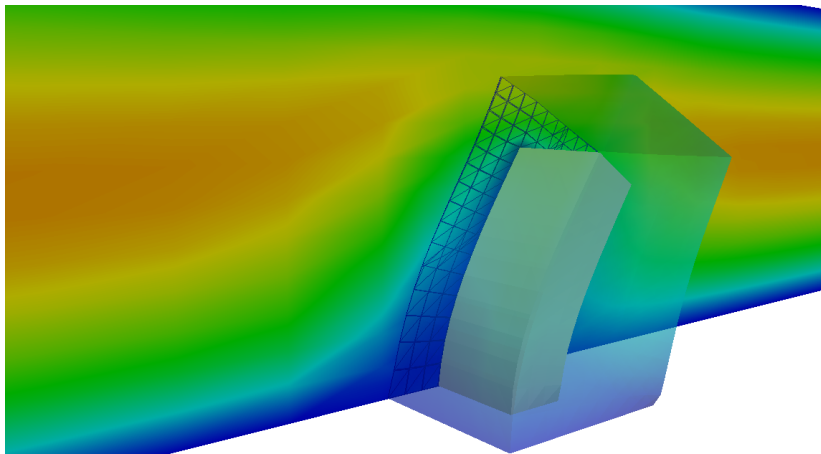
Flap in channel: Pressure



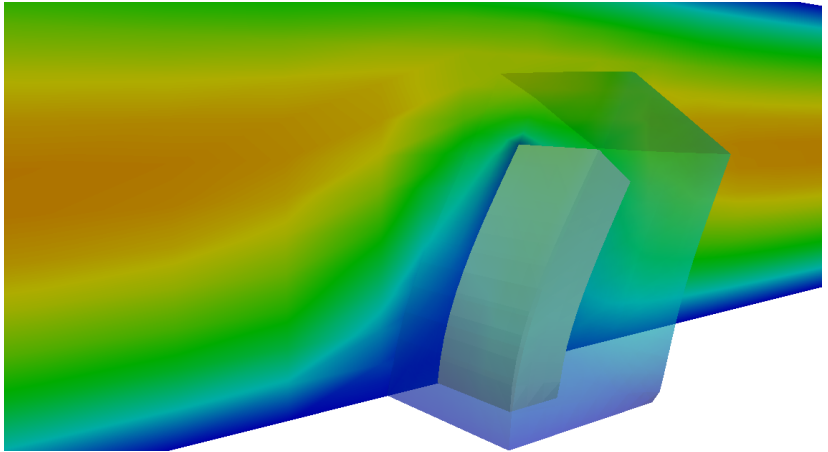
Flap in channel: Velocity



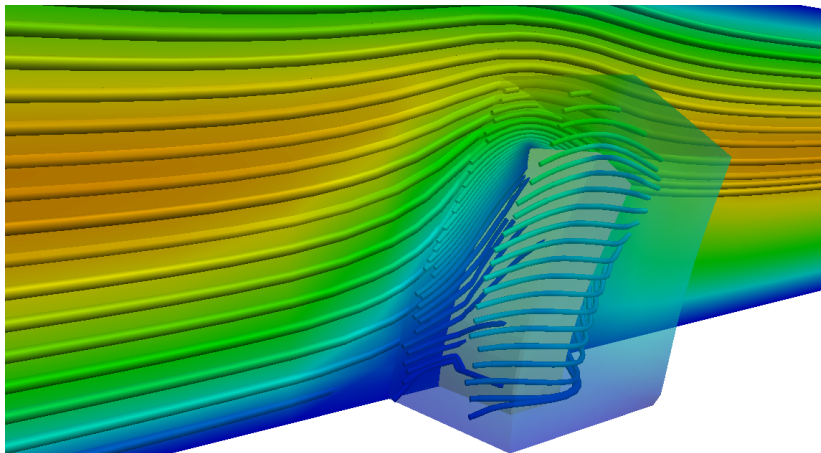
Flap in channel: Velocity



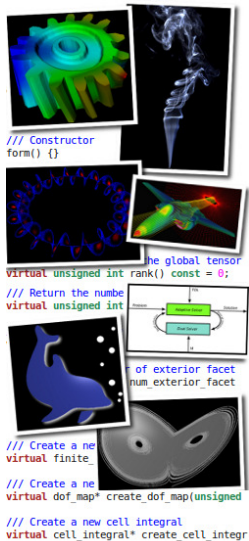
Flap in channel: Velocity



Flap in channel: Velocity



Summary



- ▶ The solution of PDEs can be **automated**
- ▶ Based on **automatic code generation**
- ▶ New tools for:
 - ▶ Application scientists and engineers
 - ▶ Numerical analysts
- ▶ New possibilities for:
 - ▶ Mathematical modeling
 - ▶ Teaching of PDE and FEM

<http://fenicsproject.org/>