Automated Solution of Differential Equations with Application to Fluid–Structure Interaction on Cut Meshes

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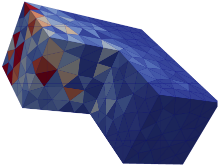
* Credits: `http://fenicsproject.org/about/team.html`

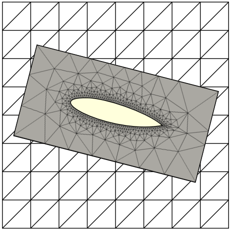
Topics

The FEniCS Project

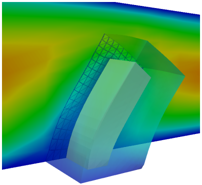
Adaptivity



Cut FEM



FSI



What is FEniCS?

FEniCS is an automated programming environment for differential equations

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

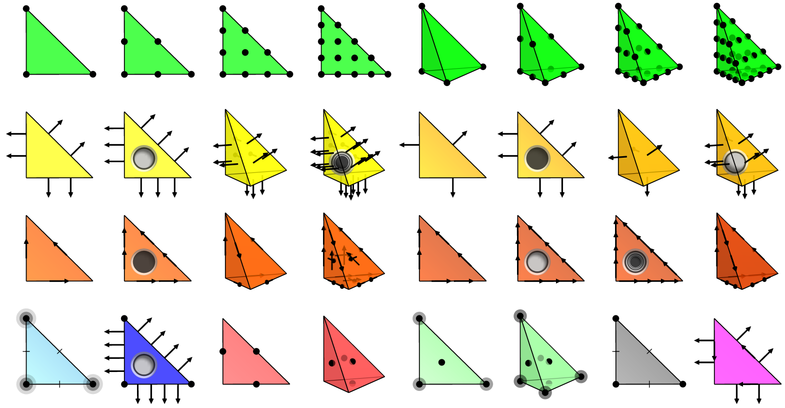
`http://fenicsproject.org/`

Collaborators

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

FEniCS is automated FEM

- Automated generation of basis functions
- Automated evaluation of variational forms
- Automated finite element assembly
- Automated adaptive error control



FEniCS is automated scientific computing

Input

- $A(u) = f$
- $\epsilon > 0$

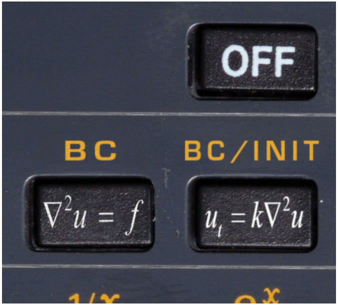
Output

- Approximate solution:

$$u_h \approx u$$

- Guaranteed accuracy:

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



How to use FEniCS?

Installation

- Official packages for Debian and Ubuntu
- Drag and drop installation on Mac OS X
- Binary installer for Windows
- Automated installation from source

Hello World in FEniCS: problem formulation

Poisson's equation

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Finite element formulation

Find $u \in V$ such that

$$\underbrace{\int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x}_{a(u,v)} = \underbrace{\int_\Omega f \, v \, \mathrm{d}x}_{L(v)} \quad \forall \, v \in V$$

Hello World in FEniCS: implementation

```
from dolfin import *

mesh = UnitSquare(32, 32)

V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

a = dot(grad(u), grad(v))*dx
L = f*v*dx

bc = DirichletBC(V, 0.0, DomainBoundary())

u = Function(V)
solve(a == L, u, bc)
plot(u)
```

Linear elasticity

Differential equation

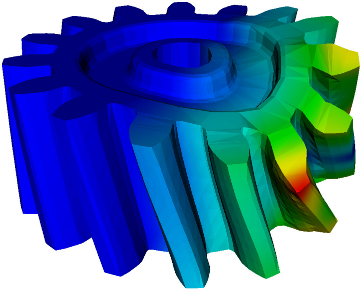
Differential equation:

$$-\nabla \cdot \sigma(u) = f$$

where

$$\sigma(v) = 2\mu\epsilon(v) + \lambda \mathrm{tr}\,\epsilon(v)\,I$$
$$\epsilon(v) = \frac{1}{2}(\nabla v + (\nabla v)^\top)$$

- Displacement $u = u(x)$
- Stress $\sigma = \sigma(x)$



Linear elasticity
Implementation

```
element = VectorElement("Lagrange", "tetrahedron", 1)

v = TestFunction(element)
u = TrialFunction(element)
f = Function(element)

def epsilon(v):
    return 0.5*(grad(v) + grad(v).T)

def sigma(v):
    return 2.0*mu*epsilon(v) + lmbda*tr(epsilon(v))*I

a = inner(sigma(u), epsilon(v))*dx
L = dot(f, v)*dx
```

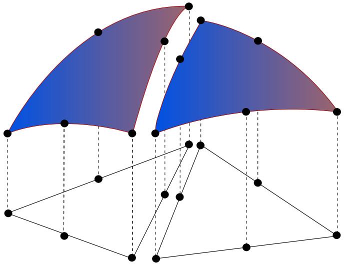
Poisson's equation with DG elements

Differential equation

Differential equation:

$$-\Delta u = f$$

- $u \in L^2$
- u discontinuous across element boundaries



Poisson's equation with DG elements

Variational formulation (interior penalty method)

Find $u \in V$ such that

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

where

$$\begin{aligned} a(u, v) &= \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x \\ &\quad + \sum_S \int_S -\langle \nabla u \rangle \cdot [\![v]\!]_n - [\![u]\!]_n \cdot \langle \nabla v \rangle + (\alpha/h) [\![u]\!]_n \cdot [\![v]\!]_n \, \mathrm{d}S \\ &\quad + \int_{\partial\Omega} -\nabla u \cdot [\![v]\!]_n - [\![u]\!]_n \cdot \nabla v + (\gamma/h) u v \, \mathrm{d}s \\ L(v) &= \int_\Omega f v \, \mathrm{d}x + \int_{\partial\Omega} g v \, \mathrm{d}s \end{aligned}$$

Poisson's equation with DG elements

Implementation

```
V = FunctionSpace(mesh, "DG", 1)

u = TrialFunction(V)
v = TestFunction(V)

f = Expression(...)
g = Expression(...)
n = FacetNormal(mesh)
h = CellSize(mesh)

a = dot(grad(u), grad(v))*dx
  - dot(avg(grad(u)), jump(v, n))*dS
  - dot(jump(u, n), avg(grad(v)))*dS
  + alpha/avg(h)*dot(jump(u, n), jump(v, n))*dS
  - dot(grad(u), jump(v, n))*ds
  - dot(jump(u, n), grad(v))*ds
  + gamma/h*u*v*ds
```

Oelgaard, Logg, Wells, *Automated Code Generation for Discontinuous Galerkin Methods* (2008)

Simple prototyping and development in Python

```
# Tentative velocity step (sigma formulation)
U = 0.5*(u0 + u)
F1 = rho*(1/k)*inner(v, u - u0)*dx +
rho*inner(v, grad(u0)*(u0 - w))*dx \
   + inner(epsilon(v), sigma(U, p0))*dx \
   + inner(v, p0*n)*ds - mu*inner(grad(U).T*n, v)*ds \
   - inner(v, f)*dx
a1 = lhs(F1)
L1 = rhs(F1)
```

```
class StVenantKirchhoff(MaterialModel):

    def model_info(self):
        self.num_parameters = 2
        self.kinematic_measure = \
          "GreenLagrangeStrain"

    def strain_energy(self, parameters):
        E = self.E
        [mu, lmbda] = parameters
        return lmbda/2*(tr(E)**2) + mu*tr(E*E)
```

```
class GentThomas(MaterialModel):

    def model_info(self):
        self.num_parameters = 2
        self.kinematic_measure = \
          "CauchyGreenInvariants"

    def strain_energy(self, parameters):
        I1 = self.I1
        I2 = self.I2

        [C1, C2] = parameters
        return C1*(I1 - 3) + C2*ln(I2/3)
```

```
# Time-stepping loop
while True:

    # Fixed point iteration on FSI problem
    for iter in range(maxiter):

        # Solve fluid subproblem
        F.step(dt)

        # Transfer fluid stresses to structure
        Sigma_F = F.compute_fluid_stress(u_F0, u_F1,
                                         p_F0, p_F1,
                                         U_M0, U_M1)
        S.update_fluid_stress(Sigma_F)

        # Solve structure subproblem
        U_S1, P_S1 = S.step(dt)

        # Transfer structure displacement to fluidmesh
        M.update_structure_displacement(U_S1)

        # Solve mesh equation
        M.step(dt)

        # Transfer mesh displacement to fluid
        F.update_mesh_displacement(U_M1, dt)
```

```
# Fluid residual contributions
R_F0 = w*inner(EZ_F - Z_F, Dt_U_F - div(Sigma_F))*dx_F
R_F1 = avg(w)*inner(EZ_F('+') - Z_F('+'),
                    jump(Sigma_F, N_F))*dS_F
R_F2 = w*inner(EZ_F - Z_F, dot(Sigma_F, N_F))*ds
R_F3 = w*inner(EY_F - Y_F,
               div(J(U_M)*dot(inv(F(U_M)), U_F)))*dx_F
```

Simple development of specialized applications

```python
# Define Cauchy stress tensor
def sigma(v,w):
    return 2.0*mu*0.5*(grad(v) + grad(v).T)  -
w*Identity(v.cell().d)

# Define symmetric gradient
def epsilon(v):
    return  0.5*(grad(v) + grad(v).T)

# Tentative velocity step (sigma formulation)
U = 0.5*(u0 + u)
F1 = rho*(1/k)*inner(v, u - u0)*dx +
rho*inner(v, grad(u0)*(u0 - w))*dx \
   + inner(epsilon(v), sigma(U, p0))*dx \
   + inner(v, p0*n)*ds - mu*inner(grad(U).T*n, v)*ds \
   - inner(v, f)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# Pressure correction
a2 = inner(grad(q), k*grad(p))*dx
L2 = inner(grad(q), k*grad(p0))*dx - q*div(u1)*dx

# Velocity correction
a3 = inner(v, u)*dx
L3 = inner(v, u1)*dx + inner(v, k*grad(p0 - p1))*dx
```

- The Navier–Stokes solver is implemented in Python/FEniCS
- FEniCS allows solvers to be implemented in a minimal amount of code
- Simple integration with application specific code and data management

Valen-Sendstad, Mardal, Logg, *Computational hemodynamics* (2011)

FEniCS under the hood

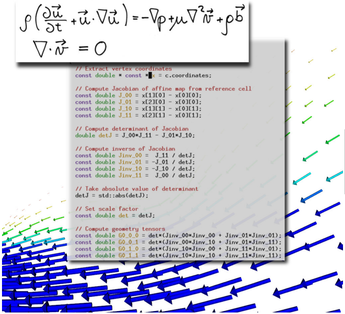
Automatic code generation

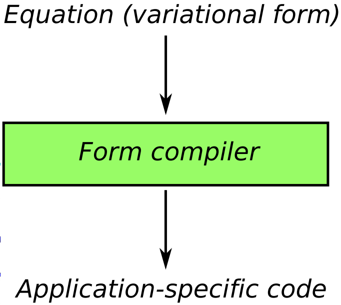
Input

Equation (variational problem)

Output

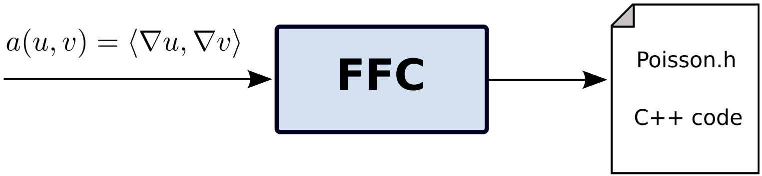
Efficient application-specific code





Code generation framework

- UFL - Unified Form Language
- UFC - Unified Form-assembly Code
- Form compilers: FFC, SyFi



Form compiler interfaces

Command-line

```
>> ffc poisson.ufl
```

Just-in-time

```
V = FunctionSpace(mesh, "CG", 3)
u = TrialFunction(V)
v = TestFunction(V)
A = assemble(dot(grad(u), grad(v))*dx)
```

Code generation system

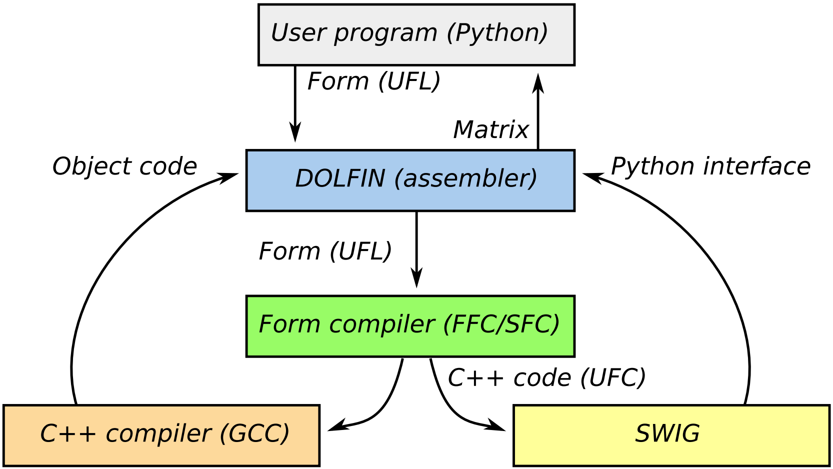
```
mesh = UnitSquare(32, 32)

V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

a = dot(grad(u), grad(v))*dx
L = f*v*dx

bc = DirichletBC(V, 0.0, DomainBoundary())

A = assemble(a)
b = assemble(L)
bc.apply(A, b)

u = Function(V)
solve(A, u.vector(), b)
```

Code generation system

```
mesh = UnitSquare(32, 32)

V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

a = dot(grad(u), grad(v))*dx
L = f*v*dx

bc = DirichletBC(V, 0.0, DomainBoundary())

A = assemble(a)
b = assemble(L)
bc.apply(A, b)

u = Function(V)
solve(A, u.vector(), b)
```

(Python, C++–SWIG–Python, Python–JIT–C++–GCC–SWIG–Python)

Just-In-Time (JIT) compilation



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: $\mathcal{M} : V \to \mathbb{R}$
- 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)

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

Key steps to automated error control

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

$$r_T(v) = \int_T R_T \cdot v \, \mathrm{d}x + \int_{\partial T} R_{\partial T} \cdot v \, \mathrm{d}s$$

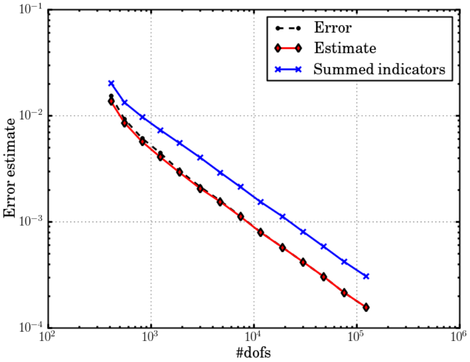
  Test against bubble functions to solve for R_T and $R_{\partial T}$
- Automated computation of error indicators:

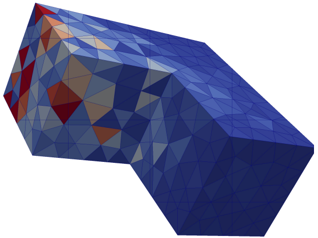
$$\eta_T = |\langle R_T, \tilde{z}_h - z_h \rangle_T + \langle [\![R_{\partial T}]\!], \tilde{z}_h - z_h \rangle_{\partial T}|$$

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

Rognes, Logg, *Automated Goal-Oriented Error Control I: Stationary Variational Problems* (2010)

Poisson's equation

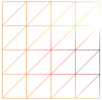


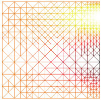


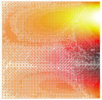
$$a(u,v) = \langle \nabla u, \nabla v \rangle$$

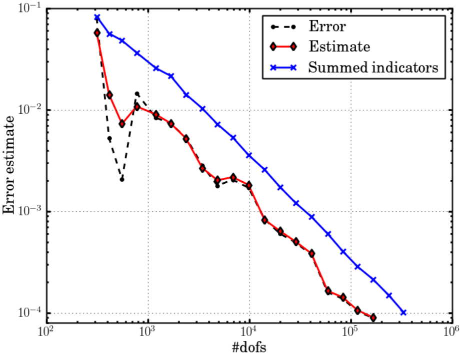
$$\mathcal{M}(u) = \int_\Gamma u \, \mathrm{d}s, \quad \Gamma \subset \partial\Omega$$

A three-field mixed elasticity formulation





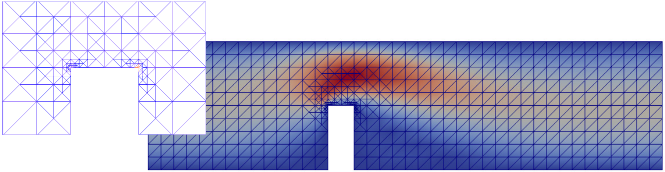




$$a((\sigma, u, \gamma), (\tau, v, \eta)) = \langle A\sigma, \tau \rangle + \langle u, \operatorname{div} \tau \rangle + \langle \operatorname{div} \sigma, v \rangle + \langle \gamma, \tau \rangle + \langle \sigma, \eta \rangle$$

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

Incompressible Navier–Stokes



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

Uniform

1.000.000 dofs, N hours

Adaptive

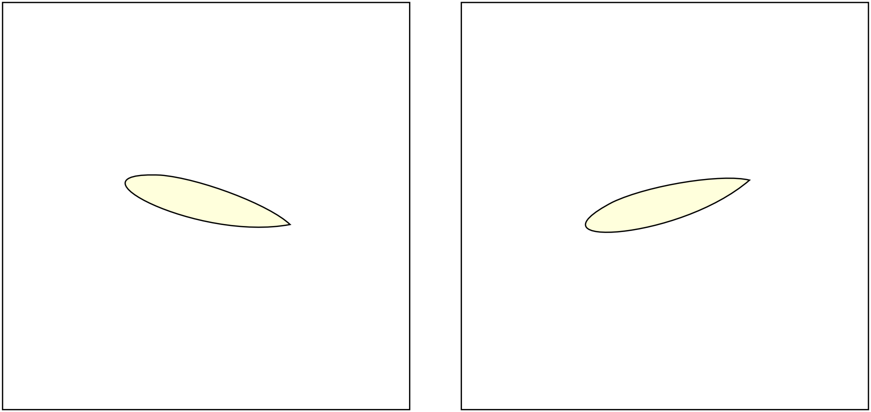
5.200 dofs, 127 seconds

```
from dolfin import *

class Noslip(SubDomain): ...

mesh = Mesh("channel-with-flap.xml.gz")
V = VectorFunctionSpace(mesh, "CG", 2)
Q = FunctionSpace(mesh, "CG", 1)
W = V*Q

# Define test functions and unknown(s)
(v, q) = TestFunctions(W)
w = Function(W)
(u, p) = split(w)

# Define (non-linear) form
n = FacetNormal(mesh)
p0 = Expression("(4.0 - x[0])/4.0")
F = (0.02*inner(grad(u), grad(v)) + inner(grad(u)*u), v)*dx
    - p*div(v) + div(u)*q + dot(v, n)*p0*ds

# Define goal functional
M = u[0]*ds(0)

# Compute solution
tol = 1e-4
solve(F == 0, w, bcs, M, tol)
```

Rognes, Logg, *Automated Goal-Oriented Error Control I* (2010)

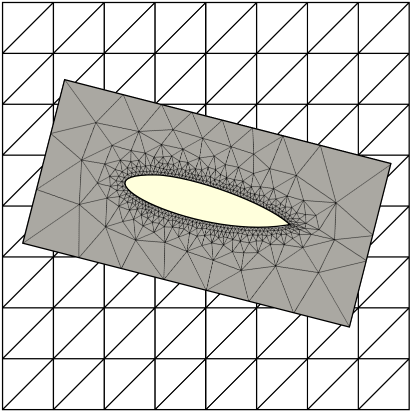
Cut finite elements

Multiple geometries – multiple meshes



Massing, Larson, Logg, Rognes, *A Nitsche overlapping mesh method for the Stokes problem* (2012)

Multiple geometries – multiple meshes



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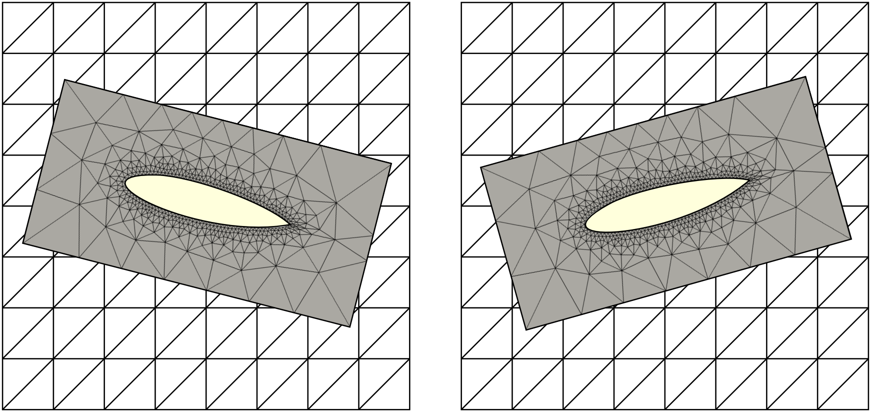
Multiple geometries – multiple meshes



Massing, Larson, Logg, Rognes, *A Nitsche overlapping mesh method for the Stokes problem* (2012)

A Nitsche formulation for the Stokes problem

Variational formulation

Find $(\boldsymbol{u}_h, p_h) \in V_h^k \times Q_h^l$ such that $\forall\, (\boldsymbol{v}_h, q_h) \in V_h^k \times Q_h^l$:

$$a_h(\boldsymbol{u}_h, \boldsymbol{v}_h) + b_h(\boldsymbol{v}_h, p_h) + b_h(\boldsymbol{u}_h, q_h) + s_h(\boldsymbol{u}_h, \boldsymbol{v}_h) - S_h(\boldsymbol{u}_h, p_h; \boldsymbol{v}_h, q_h) = L_h(\boldsymbol{v}_h, q_h)$$

where

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

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

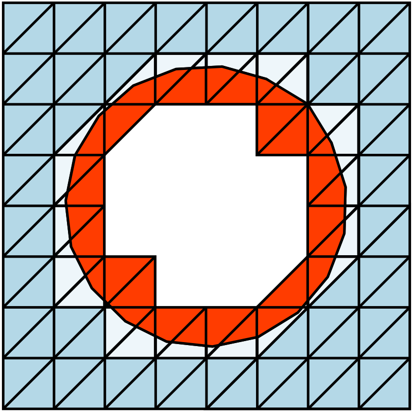
$$b_h(\boldsymbol{v}_h, q_h) = -(\nabla \cdot \boldsymbol{v}_h, q_h)_{\Omega_1 \cup \Omega_2} + \underbrace{(\boldsymbol{n} \cdot [\boldsymbol{v}_h], \langle q_h \rangle)_\Gamma}_{\text{Nitsche terms}},$$

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

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

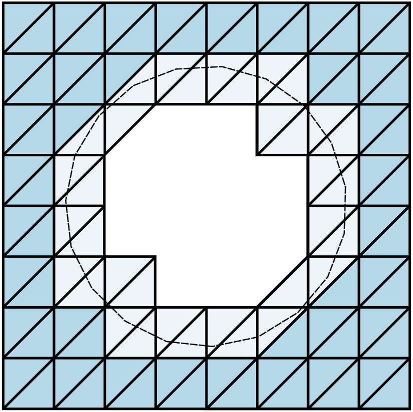
$$L_h(\boldsymbol{v}, q) = (\boldsymbol{f}, \boldsymbol{v}) - \delta \sum_{T \in \mathcal{T}_1^* \cup \mathcal{T}_2} h_T^2 (\boldsymbol{f}, -\alpha \Delta \boldsymbol{v}_h + \beta \nabla q_h)_T.$$

Ghost-penalties added in the interface zone



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

Ghost penalty for u



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

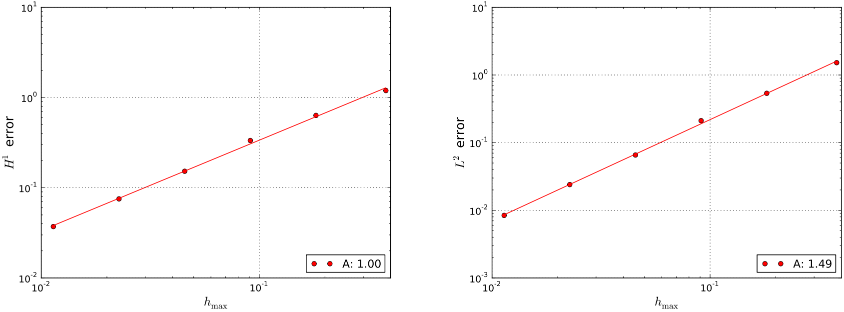
Ghost penalty for p

Optimal *a priori* estimates

Theorem

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

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

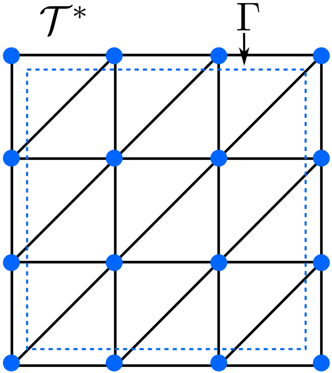


Bounded condition numbers

Theorem

There is a constant $C > 0$ independent of the position of Γ, s.t. the condition number of the stiffness matrix $\mathcal{A}$ associated with the Nitsche fictitious domain method satisfies

$$\kappa(\mathcal{A}) \leqslant Ch^{-2},$$



Bounded condition numbers

Theorem

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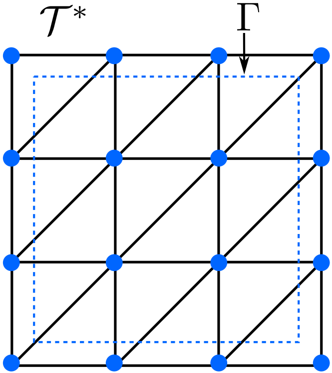
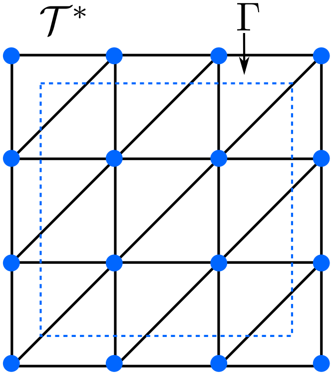


Bounded condition numbers

Theorem

There is a constant $C > 0$ independent of the position of Γ, s.t. the condition number of the stiffness matrix $\mathcal{A}$ associated with the Nitsche fictitious domain method satisfies

$$\kappa(\mathcal{A}) \leqslant Ch^{-2},$$



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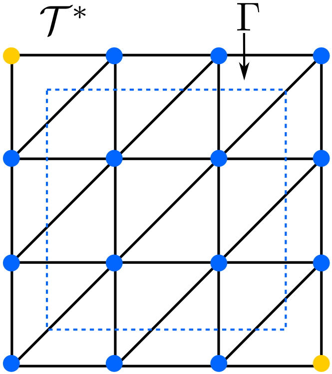
$$\kappa(\mathcal{A}) \leqslant C h^{-2},$$



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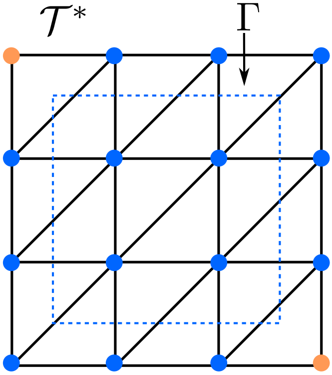

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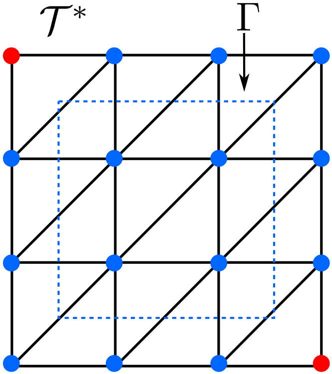

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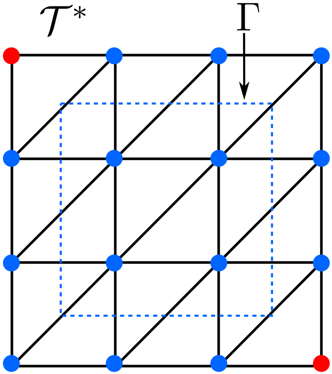

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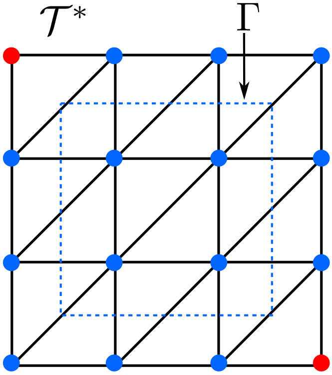
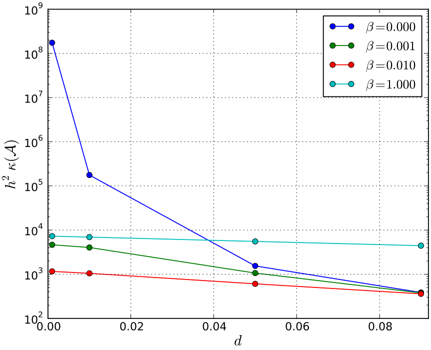
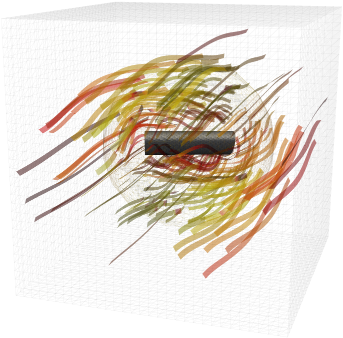
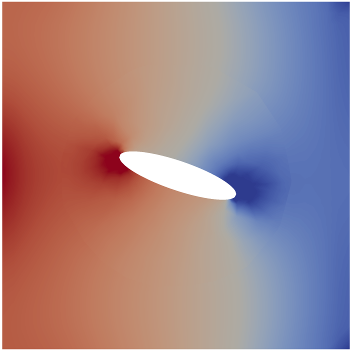




Stokes flow for different angles of attack

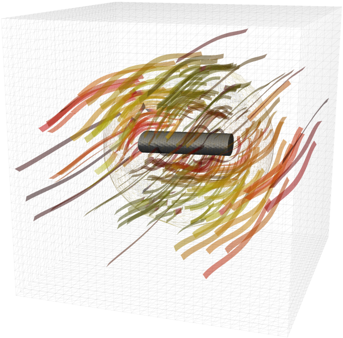




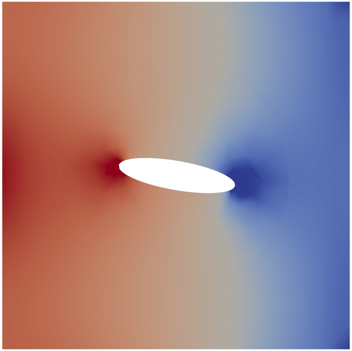
Velocity streamlines

Pressure

Stokes flow for different angles of attack



Velocity streamlines



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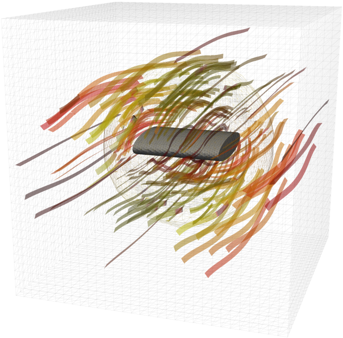
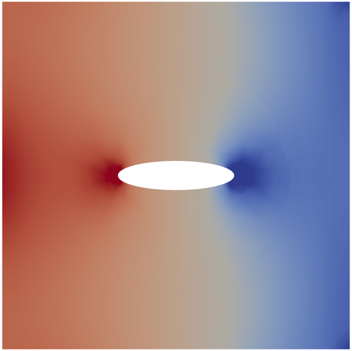


Velocity streamlines



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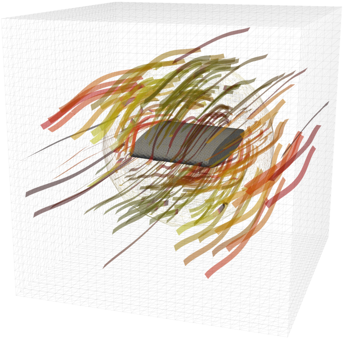

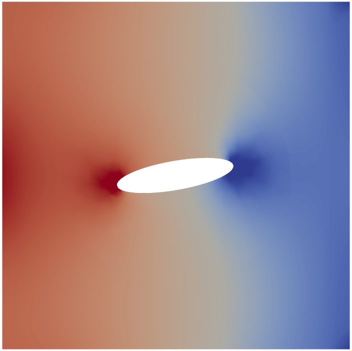

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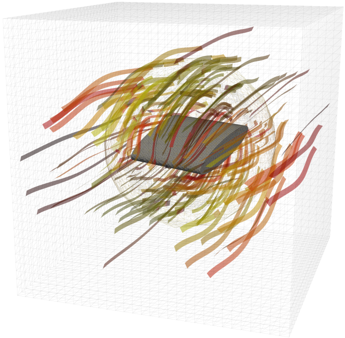

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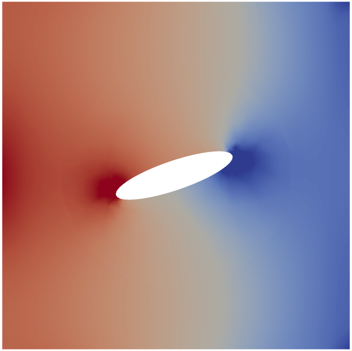
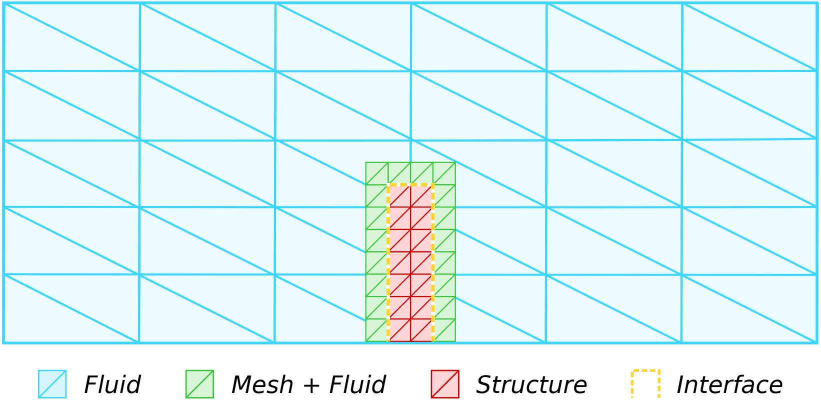


Pressure

Fluid–structure interaction on cut meshes



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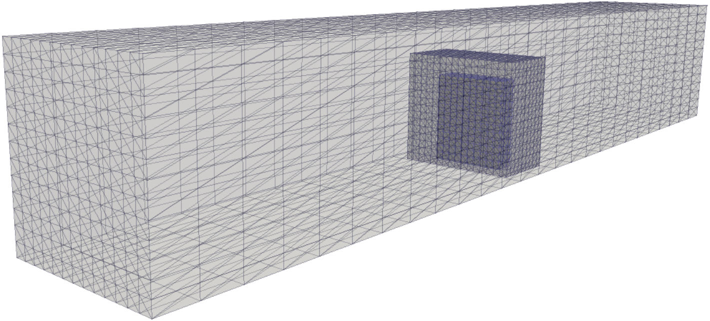
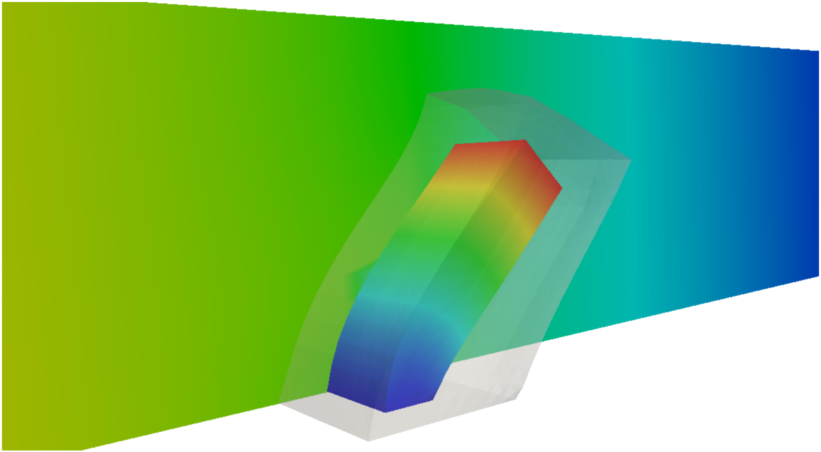


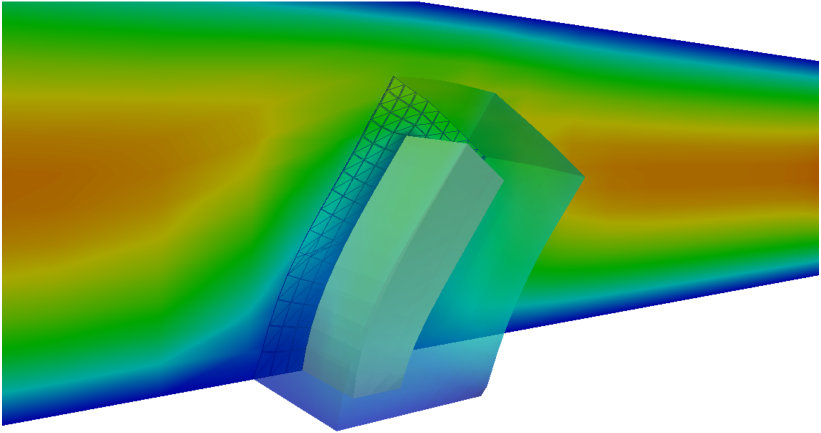
Larson, Logg, Massing, Rognes, *Fluid–structure interaction on cut meshes* (in preparation)

Fluid–structure interaction: displacement



Larson, Logg, Massing, Rognes, *Fluid–structure interaction on cut meshes* (in preparation)

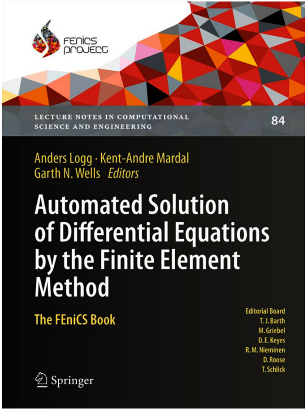
Fluid–structure interaction: velocity magnitude



Larson, Logg, Massing, Rognes, *Fluid–structure interaction on cut meshes* (in preparation)

Closing remarks

Ongoing activities



- Parallelization (2009)
- Automated error control (2010)
- Debian/Ubuntu (2010)
- Documentation (2011)
- FEniCS 1.0 (2011)
- The FEniCS Book (2012)

- **FEniCS'13**
  Cambridge March 2013
- Visualization, mesh generation
- Parallel AMR
- Hybrid MPI/OpenMP
- Overlapping/intersecting meshes

Summary

- Automated solution of PDE
- Easy install
- Easy scripting in Python
- Efficiency by automated code generation
- Free/open-source (LGPL)

`http://fenicsproject.org/`