Activities at Simula: FEniCS and the Center for Biomedical Computing

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CAM Seminar Chalmers, September 26 2007

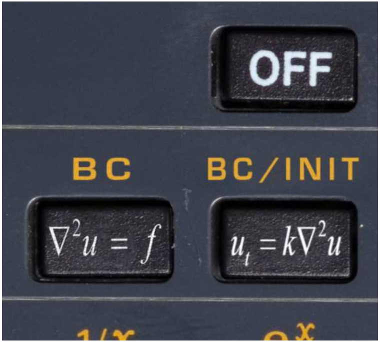
Outline

- FEniCS
  - Introduction
  - Examples
  - Design and implementation
- Simula Research Laboratory
  - About Simula
  - Center for Biomedical Computing
  - Simula School of Research & Innovation
- Recruitment

Solving differential equations

- Build a calculator
- One button for each equation?

- Too many equations
- Too many buttons

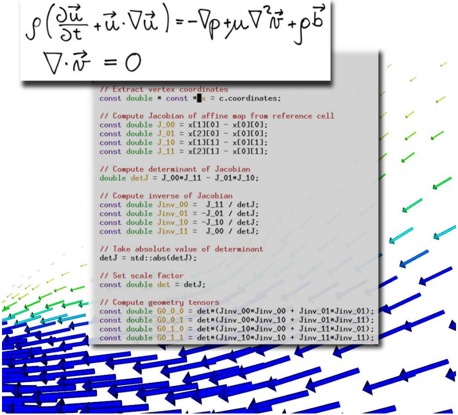


Automate the solution of differential equations

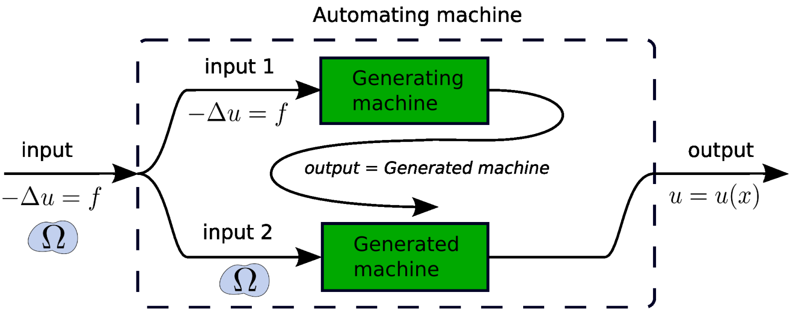
- Input: Differential equation
- Output: Solution

- Generate computer code
- Compute solution

- Build a calculator for each equation
- Automate the generation of calculators



Automate the solution of differential equations

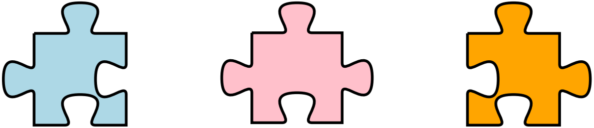


Generality *and* efficiency

- Any equation
- Any (finite element) method
- Maximum efficiency

Possible to combine generality with efficiency by generating code

Generality Efficiency



Compiler

Generality

- Any (multilinear) form
- Any element:

P_k	Arbitrary degree Lagrange elements
DG_k	Arbitrary degree discontinuous elements
BDM_k	Arbitrary degree Brezzi–Douglas–Marini
RT_k	Arbitrary degree Raviart–Thomas
CR_1	Crouzeix–Raviart
$\ldots$	(more in preparation)

- 2D (triangles) and 3D (tetrahedra)

Efficiency

- CPU time for computing the “element stiffness matrix”
- Straight-line C++ code generated by the FEniCS Form Compiler (FFC)
- Speedup vs a standard quadrature-based C++ code with loops over quadrature points

Form	$q = 1$	$q = 2$	$q = 3$	$q = 4$	$q = 5$	$q = 6$	$q = 7$	$q = 8$
Mass 2D	12	31	50	78	108	147	183	232
Mass 3D	21	81	189	355	616	881	1442	1475
Poisson 2D	8	29	56	86	129	144	189	236
Poisson 3D	9	56	143	259	427	341	285	356
Navier–Stokes 2D	32	33	53	37	—	—	—	—
Navier–Stokes 3D	77	100	61	42	—	—	—	—
Elasticity 2D	10	43	67	97	—	—	—	—
Elasticity 3D	14	87	103	134	—	—	—	—

The FEniCS project

- Initiated in 2003
- Collaborators (in order of appearance):
  - (Chalmers University of Technology)
  - University of Chicago
  - Argonne National Laboratory
  - (Toyota Technological Institute)
  - Delft University of Technology
  - Royal Institute of Technology (KTH)
  - Simula Research Laboratory
  - Texas Tech
  - University of Cambridge
- Automation of Computational Mathematical Modeling (ACMM)
- www.fenics.org

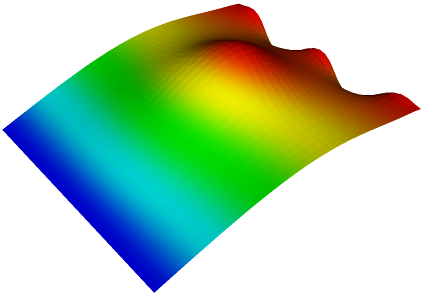
Poisson's equation

Differential equation

Differential equation:

$$-\Delta u = f$$

- Heat transfer
- Electrostatics
- Magnetostatics
- Fluid flow
- etc.



Poisson's equation

Variational formulation

Find $u \in V$ such that

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

where

$$a(v, u) = \int_\Omega \nabla v \cdot \nabla u \, \mathrm{d}x$$

$$L(v) = \int_\Omega v f \, \mathrm{d}x$$

Poisson’s equation

Implementation

```
element = FiniteElement("Lagrange", "triangle", 1)

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

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

Linear elasticity

Differential equation

Differential equation:

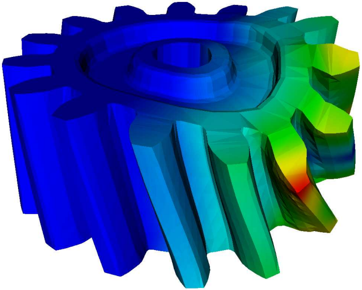
$$-\nabla \cdot \sigma(u) = f$$

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

Variational formulation

Find $u \in V$ such that

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

where

$$a(v,u) = \int_\Omega \nabla v : \sigma(u) \, \mathrm{d}x$$
$$L(v) = \int_\Omega v \cdot f \, \mathrm{d}x$$

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) + transp(grad(v)))

def sigma(v):
    return 2*mu*epsilon(v) + lmbda*mult(trace(epsilon(v)),I)

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

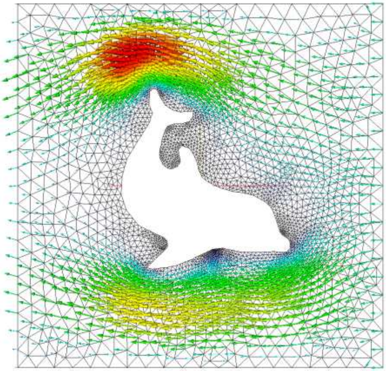
The Stokes equations

Differential equation

Differential equation:

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

- Fluid velocity $u = u(x)$
- Pressure $p = p(x)$



The Stokes equations

Variational formulation

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

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

where

$$a((v,q),(u,p)) = \int_\Omega \nabla v \cdot \nabla u - \nabla \cdot v\, p + q \nabla \cdot u \, \mathrm{d}x$$

$$L((v,q)) = \int_\Omega v \cdot f \, \mathrm{d}x$$

The Stokes equations

Implementation

```
P2 = VectorElement("Lagrange", "triangle", 2)
P1 = FiniteElement("Lagrange", "triangle", 1)
TH = P2 + P1

(v, q) = TestFunctions(TH)
(u, p) = TrialFunctions(TH)

f = Function(P2)

a = (dot(grad(v), grad(u)) - div(v)*p + q*div(u))*dx
L = dot(v, f)*dx
```

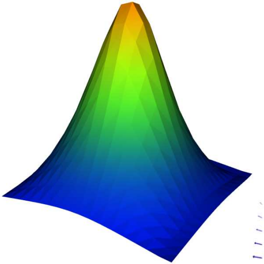
Mixed Poisson with $H(\mathrm{div})$ elements

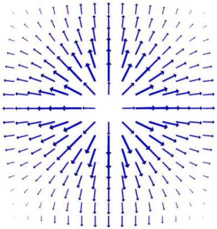
Differential equation

Differential equation:

$$\sigma + \nabla u = 0$$
$$\nabla \cdot \sigma = f$$

- $u \in L_2$
- $\sigma \in H(\mathrm{div})$





Mixed Poisson with $H(\mathrm{div})$ elements

Variational formulation

Find $(\sigma, u) \in V$ such that

$$a((\tau, w), (\sigma, u)) = L((\tau, w)) \quad \forall (\tau, w) \in \hat{V}$$

where

$$\begin{aligned} a((\tau, w), (\sigma, u)) &= \int_\Omega \tau \cdot \sigma - \nabla \cdot \tau \, u + w \nabla \cdot \sigma \, \mathrm{d}x \\ L((\tau, w)) &= \int_\Omega w f \, \mathrm{d}x \end{aligned}$$

Mixed Poisson with $H(\mathrm{div})$ elements

Implementation

```
BDM1 = FiniteElement("Brezzi-Douglas-Marini","triangle",1)
DG0 = FiniteElement("Discontinuous Lagrange","triangle",0)

element = BDM1 + DG0

(tau, w) = TestFunctions(element)
(sigma, u) = TrialFunctions(element)

f = Function(DG0)

a = (dot(tau, sigma) - div(tau)*u + w*div(sigma))*dx
L = w*f*dx
```

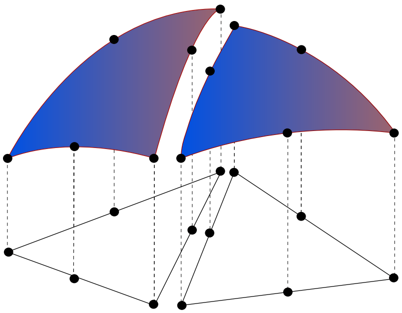
Poisson's equation with DG elements

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

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

where

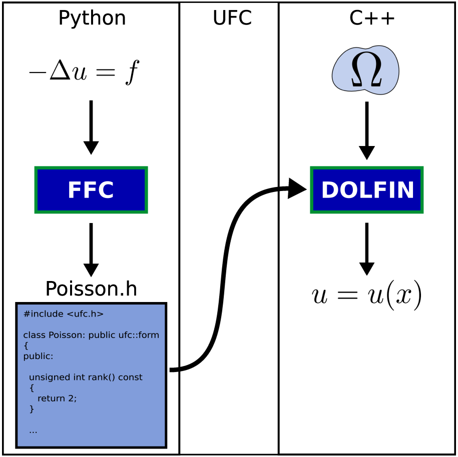
$$\begin{aligned}
a(v,u) = &\int_\Omega \nabla v \cdot \nabla u \,\mathrm{d}x \\
&+ \sum_S \int_S -\langle \nabla v \rangle \cdot [\![u]\!]_n - [\![v]\!]_n \cdot \langle \nabla u \rangle + (\alpha/h) [\![v]\!]_n \cdot [\![u]\!]_n \,\mathrm{d}S \\
&+ \int_{\partial\Omega} -\nabla v \cdot [\![u]\!]_n -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

Poisson's equation with DG elements

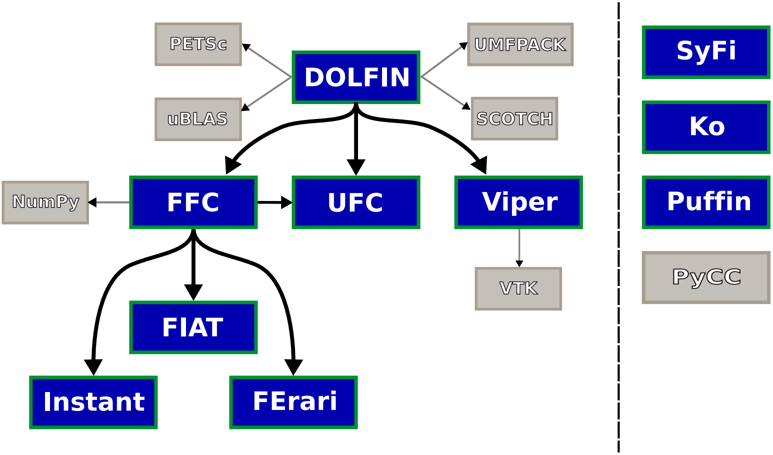
Implementation

```
DG1 = FiniteElement("Discontinuous Lagrange", "triangle", 1)

v = TestFunction(DG1)
u = TrialFunction(DG1)

f = Function(DG1)
g = Function(DG1)
n = FacetNormal("triangle")
h = MeshSize("triangle")

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

Code generation system



Software map



Recent updates

- UFC, a framework for finite element assembly
- DG, BDM and RT elements
- A new improved mesh library, adaptive refinement
- Mesh and graph partitioning
- Improved linear algebra supporting PETSc and uBLAS
- Optimized code generation (FErari)
- Improved ODE solvers
- Python bindings
- Bugzilla database, pkg-config, improved manual, compiler support, demos, file formats, built-in plotting, . . .

Future plans (highlights)

- Full support for parallel computing
- UFL/UFC
- Automation of error control
  - Automatic generation of dual problems
  - Automatic generation of a posteriori error estimates
- Improved geometry support (MeshBuilder)
- Debian/Ubuntu packages
- Finite element exterior calculus

$\longrightarrow$ `www.fenics.org` $\longleftarrow$

About Simula

- Established in 2001
- Located at Fornebu in Oslo
- Owners:
  - Norwegian government (80%)
  - SINTEF + Norwegian Computing Center (20%)
- Financing:
  - Base funding from Norwegian government
  - External funding

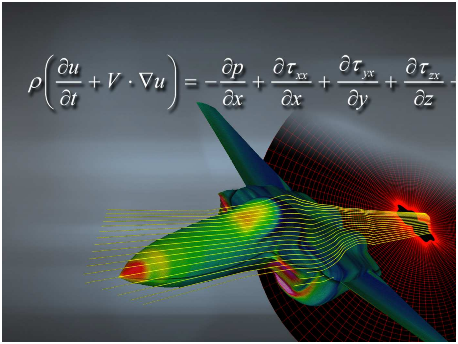
Organization

- Research divisions
  - Networks and distributed systems
  - Scientific computing (CBC)
  - Software engineering
- Simula School of Research & Innovation
- Simula Innovation AS

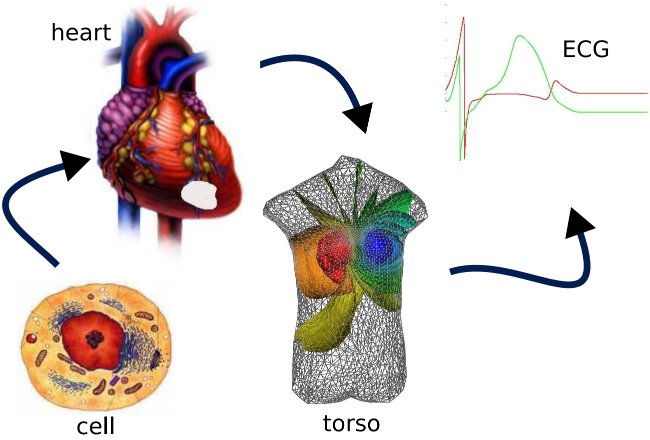


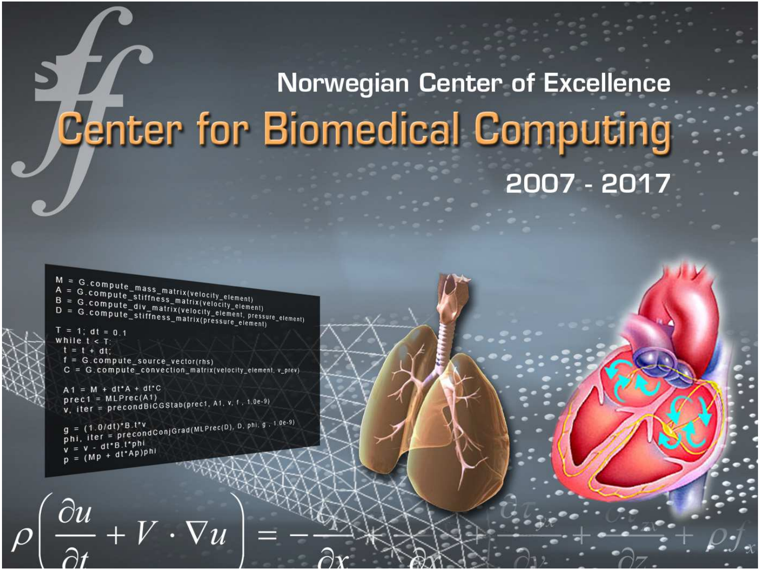
Principles

- Directed basic research (grundforskning)
- Large and focused projects
- The “full day researcher”



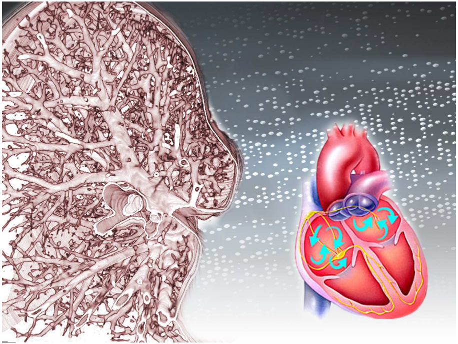
Computing the electrical activity of the heart




Norwegian Center of Excellence
Center for Biomedical Computing
2007 - 2017
M = G.compute_mass_matrix(velocity_element)
A = G.compute_stiffness_matrix(velocity_element)
B = G.compute_div_matrix(velocity_element, pressure_element)
D = G.compute_stiffness_matrix(pressure_element)
T = 1; dt = 0.1
while t < T:
t = t + dt;
f = G.compute_source_vector(rhs)
C = G.compute_convection_matrix(velocity_element, v_prev)
A1 = M + dt*A + dt*C
prec1 = MLPrec(A1)
v, iter = precondBiCGStab(prec1, A1, v, f, 1.0e-9)
g = (1.0/dt)*B.t*v
phi, iter = precondConjGrad(MLPrec(D), D, phi, g, 1.0e-9)
v = v - dt*B.t*phi
p = (Mp + dt*Ap)phi
$\rho\left(\frac{\partial u}{\partial t} + V \cdot \nabla u\right) = -$

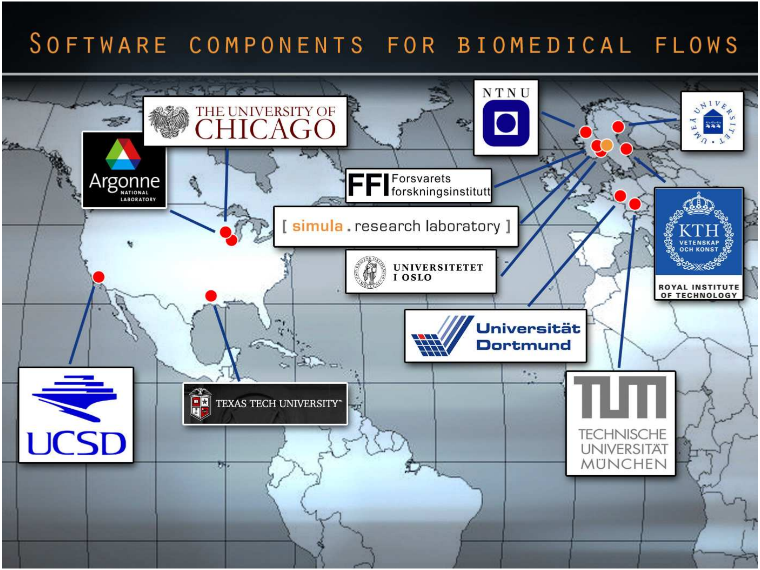
Center for Biomedical Computing (CBC)

- Center of Excellence: 2007-2017
- Funding: 10 MNOK / year
- Director: Hans Petter Langtangen
- Based at Simula with international partners



Organization

- Computational middleware
  - Problem solving environment for PDEs
  - General, simple, efficient
  - FEniCS
- Robust flow solvers
  - Adaptivity and error control
  - Fluid–structure interaction
  - Efficient algebraic solvers
  - Validation by experiments
- Biomedical flow applications
  - Drug inhalation
  - Aneurysms of the Circle of Willis
  - Multiscale 1D–3D flows
  - Flow around heart valves
  - Flow, deformation and electrophysiology of the heart
  - ...


SOFTWARE COMPONENTS FOR BIOMEDICAL FLOWS
THE UNIVERSITY OF CHICAGO
Argonne NATIONAL LABORATORY
NTNU
UMEÅ UNIVERSITET
FFI Forsvarets forskningsinstitutt
[simula . research laboratory]
UNIVERSITETET I OSLO
KTH VETENSKAP OCH KONST
ROYAL INSTITUTE OF TECHNOLOGY
Universität Dortmund
UCSD
TEXAS TECH UNIVERSITY
TUM TECHNISCHE UNIVERSITÄT MÜNCHEN

Simula School of Research & Innovation

- Opened in 2006
- Degrees awarded by the University of Oslo (Department of Informatics)

Postdoc	3 years	
PhD student	3 years	(3 months abroad)
Research trainee	1 year	(6 months practice)

- Close collaboration with Simula Innovation
- Main supervisor at Simula, external advisors

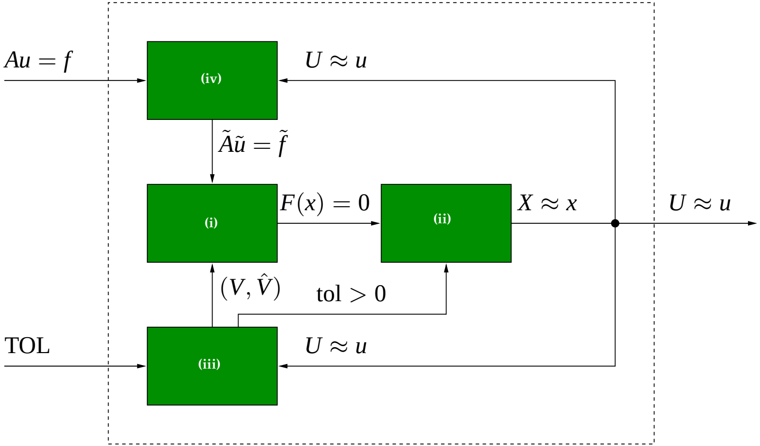
We are hiring!

- PhD students and postdocs
- Center for Biomedical Computing 2007–2017
  - 10 MNOK / year
- Outstanding Young Investigator award (Logg) 2008–2012
  - 2.5 MNOK / year
  - 3 PhD students, 2 postdocs

- Competitive salary and benefits
- For details, contact `logg@simula.no`

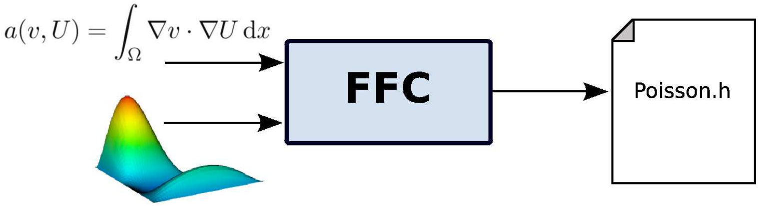
Additional slides

Automation of CMM



A common framework: UFL/UFC

- UFL - Unified Form Language
- UFC - Unified Form-assembly Code
- Unify, standardize, extend
- Working prototypes: FFC (Logg), SyFi (Mardal)



Compiling Poisson's equation: non-optimized, 16 ops

```
void eval(real block[], const AffineMap& map) const
{
  [...]

  block[0] = 0.5*G0_0_0 + 0.5*G0_0_1 +
             0.5*G0_1_0 + 0.5*G0_1_1;
  block[1] = -0.5*G0_0_0 - 0.5*G0_1_0;
  block[2] = -0.5*G0_0_1 - 0.5*G0_1_1;
  block[3] = -0.5*G0_0_0 - 0.5*G0_0_1;
  block[4] = 0.5*G0_0_0;
  block[5] = 0.5*G0_0_1;
  block[6] = -0.5*G0_1_0 - 0.5*G0_1_1;
  block[7] = 0.5*G0_1_0;
  block[8] = 0.5*G0_1_1;
}
```

Compiling Poisson's equation: `ffc -O`, 11 ops

```
void eval(real block[], const AffineMap& map) const
{
  [...]

  block[1] = -0.5*G0_0_0 + -0.5*G0_1_0;
  block[0] = -block[1] + 0.5*G0_0_1 + 0.5*G0_1_1;
  block[7] = -block[1] + -0.5*G0_0_0;
  block[6] = -block[7] + -0.5*G0_1_1;
  block[8] = -block[6] + -0.5*G0_1_0;
  block[2] = -block[8] + -0.5*G0_0_1;
  block[5] = -block[2] + -0.5*G0_1_1;
  block[3] = -block[5] + -0.5*G0_0_0;
  block[4] = -block[1] + -0.5*G0_1_0;
}
```

Compiling Poisson's equation: `ffc -f blas`, 36 ops

```
void eval(real block[], const AffineMap& map) const
{
  [...]

  cblas_dgemv(CblasRowMajor, CblasNoTrans,
              blas.mi, blas.ni, 1.0,
              blas.Ai, blas.ni, blas.Gi,
              1, 0.0, block, 1);
}
```

Key Features

- Simple and intuitive object-oriented API, C++ or Python
- Automatic and efficient evaluation of variational forms
- Automatic and efficient assembly of linear systems
- General families of finite elements, including arbitrary order continuous and discontinuous Lagrange elements, BDM, RT
- Arbitrary mixed elements
- High-performance parallel linear algebra
- General meshes, adaptive mesh refinement
- mcG(q)/mdG(q) and cG(q)/dG(q) ODE solvers
- Support for a range of output formats for post-processing, including DOLFIN XML, ParaView/Mayavi/VTK, OpenDX, Octave, MATLAB, GiD
- Built-in plotting

Linear algebra

- Complete support for PETSc
  - High-performance parallel linear algebra
  - Krylov solvers, preconditioners
- Complete support for uBLAS
  - BLAS level 1, 2 and 3
  - Dense, packed and sparse matrices
  - C++ operator overloading and expression templates
  - Krylov solvers, preconditioners added by DOLFIN
- Uniform interface to both linear algebra backends
- LU factorization by UMFPACK for uBLAS matrix types
- Eigenvalue problems solved by SLEPc for PETSc matrix types
- Matrix-free solvers ("virtual matrices")