Automatic Code Generation and the FEniCS Project

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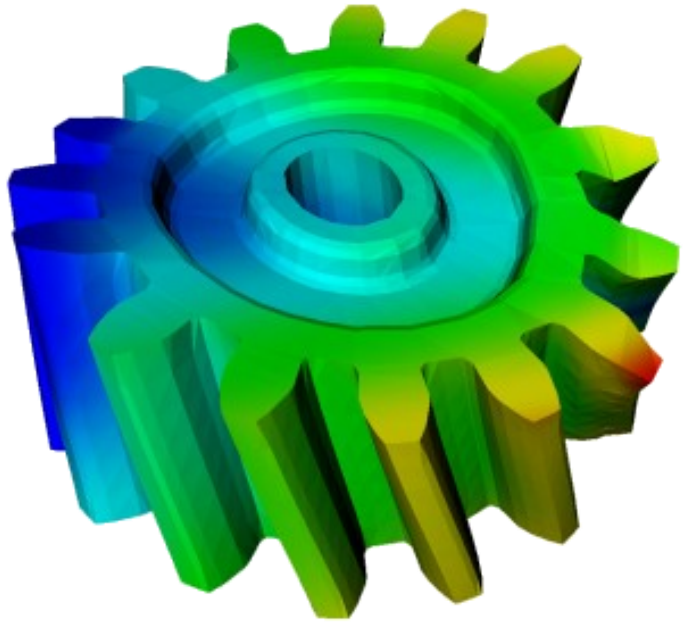

Anders Logg

Center for Biomedical Computing
Simula Research Laboratory

Department of Informatics
University of Oslo

Opportunities and Challenges in Computational Geodynamics
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The FEniCS Project

Free software for the Automation of CMM

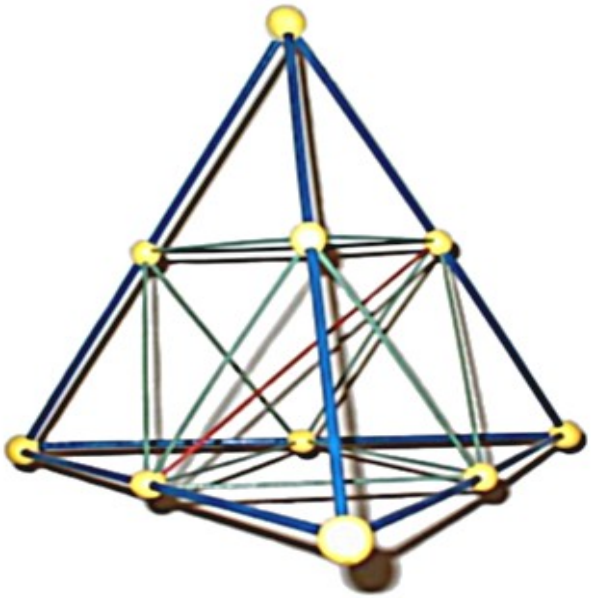
- Started 2003
- 12+ projects/components
- 15-20 active developers
- 1000+ monthly downloads
- 500+ monthly posts to mailing lists
- 10,000+ unique visitors each month
- 3500 changesets in 2008 (10 / day)

Project Team

- Chalmers University of Technology
- University of Chicago
- Argonne National Laboratory (ANL)
- Toyota Technological Institute at Chicago (TTI)
- Delft University of Technology
- Royal Institute of Technology (KTH)
- Simula Research Laboratory
- Texas Tech
- University of Cambridge
- Others

Main Features

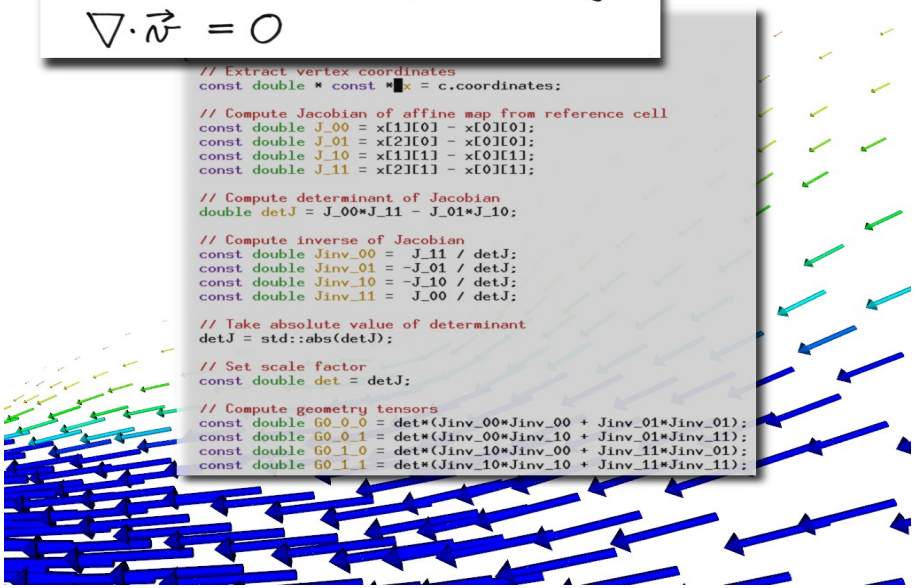
- **Generality**
  - **“Any” equation (expressive form language)**
  - **“Any” finite element method (CG, DG, BDM, Nedelec, ...)**
  - **“Any” mesh (simplex meshes in 1D, 2D, 3D)**
  - **“Any” linear algebra backend (PETSc, Epetra, uBLAS, MTL4)**
- **Efficiency**
  - **High performance assembly**
  - **High performance linear algebra**
  - **Automated domain-specific optimization**



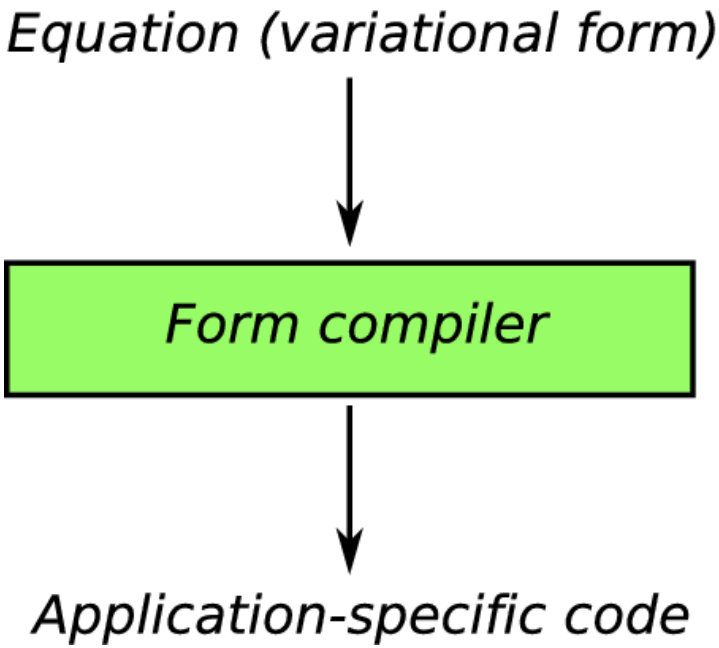
Automatic Code Generation

- Combining generality and efficiency
- Input: equation
- Output: efficient application-specific code

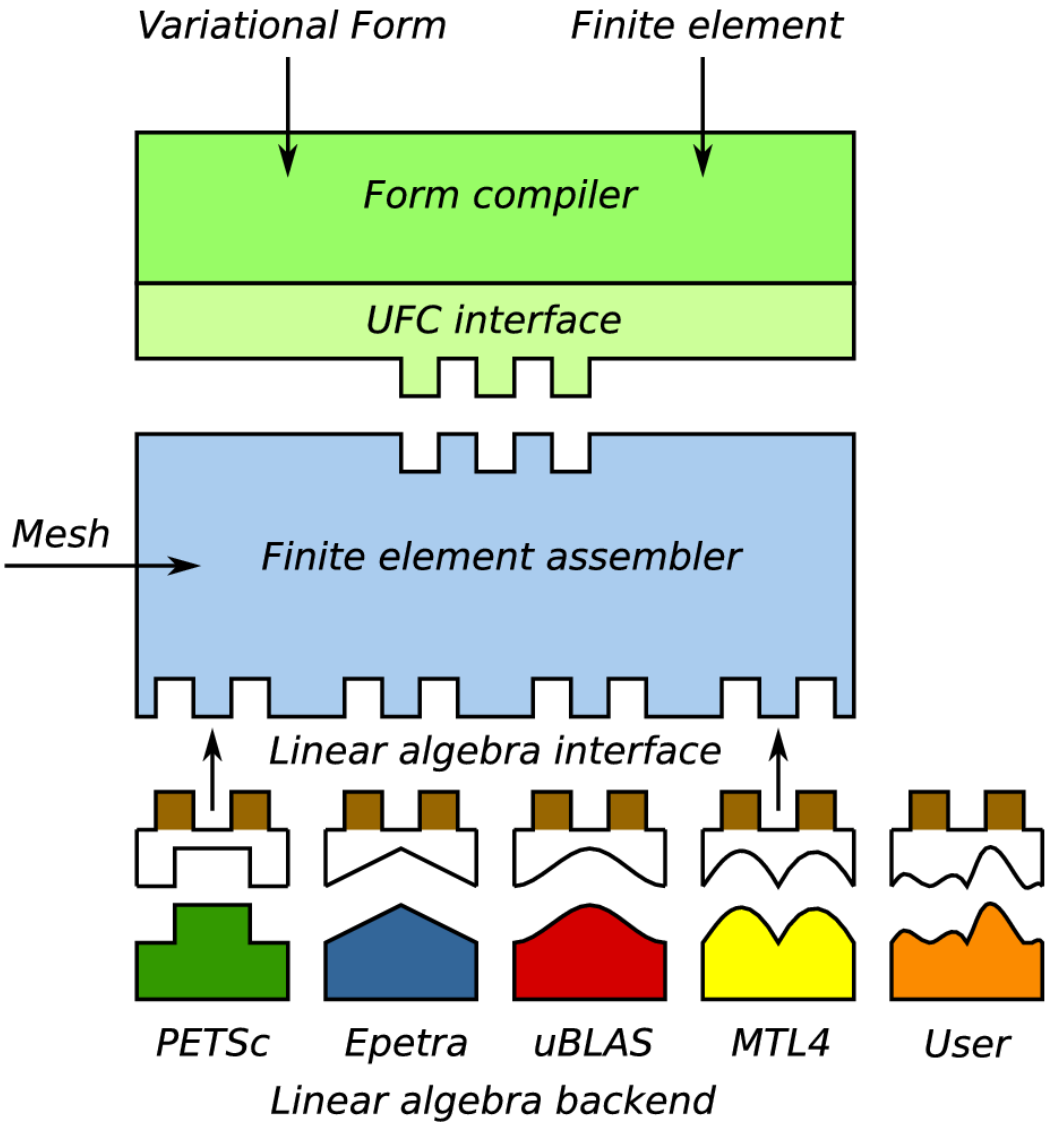
$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) = -\nabla p + \mu\nabla^2\vec{v} + \rho\vec{b}$$
$$\nabla\cdot\vec{v} = 0$$



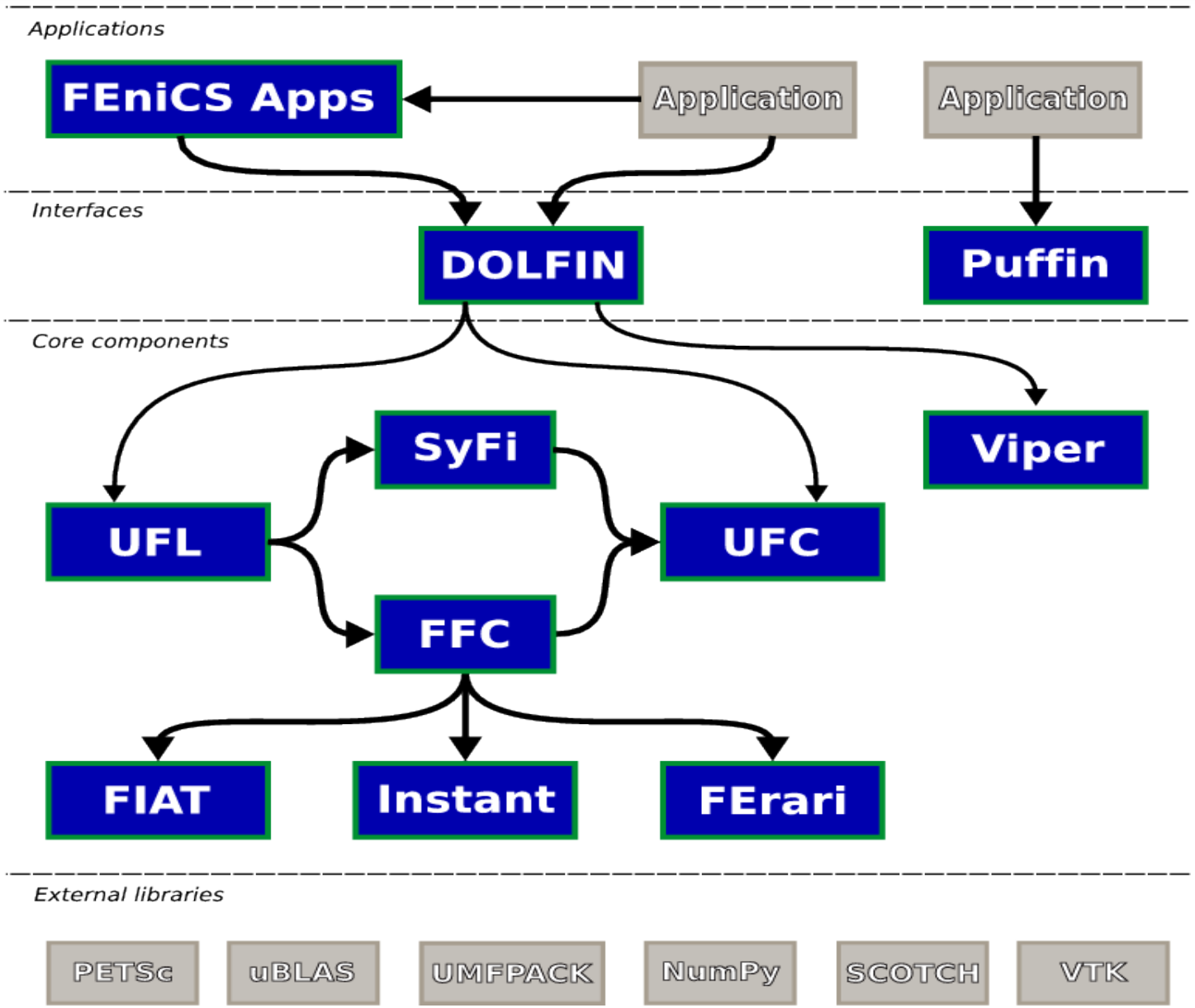
```
// Extract vertex coordinates
const double * const *x = c.coordinates;

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

// 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);
```



System Design



Software Components



Expressive Form Language

Mixed finite element methods for linear elasticity with weakly imposed symmetry, Arnold, Falk, Winther (2007)

```
S = VectorElement('BDM', triangle, k)
V = VectorElement('Discontinuous Lagrange', triangle, k - 1)
Q = TensorElement('Discontinuous Lagrange', triangle, k - 1)

element = MixedElement(S, V, Q)

(tau, v, eta) = TestFunctions(element)
(sigma, u, gamma) = TrialFunctions(element)

a = (sigma, tau) + (-tr(sigma), tr(tau)) \
  + (div(tau), u) + (-div(sigma), v) \
  + (tau, gamma) + (eta, sigma)
```

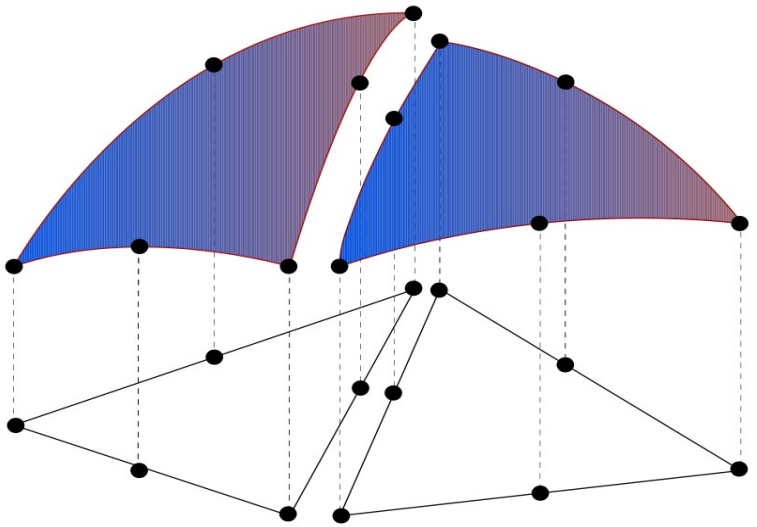
$$a((\tau, v, \eta), (\sigma, u, \gamma)) = (\sigma, \tau) - (\operatorname{tr}\sigma, \operatorname{tr}\tau)$$

$$+(\operatorname{div}\tau, u) - (\operatorname{div}\sigma, v) + (\tau, \gamma) + (\eta, \sigma)$$

Expressive Form Language

Discontinuous Galerkin formulation for Poisson (interior penalty method)

```
element = FiniteElement('Discontinuous Lagrange', triangle, 1)

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

n = FacetNormal(triangle)
h = MeshSize(triangle)

alpha = 4.0
gamma = 8.0

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



Interfaces

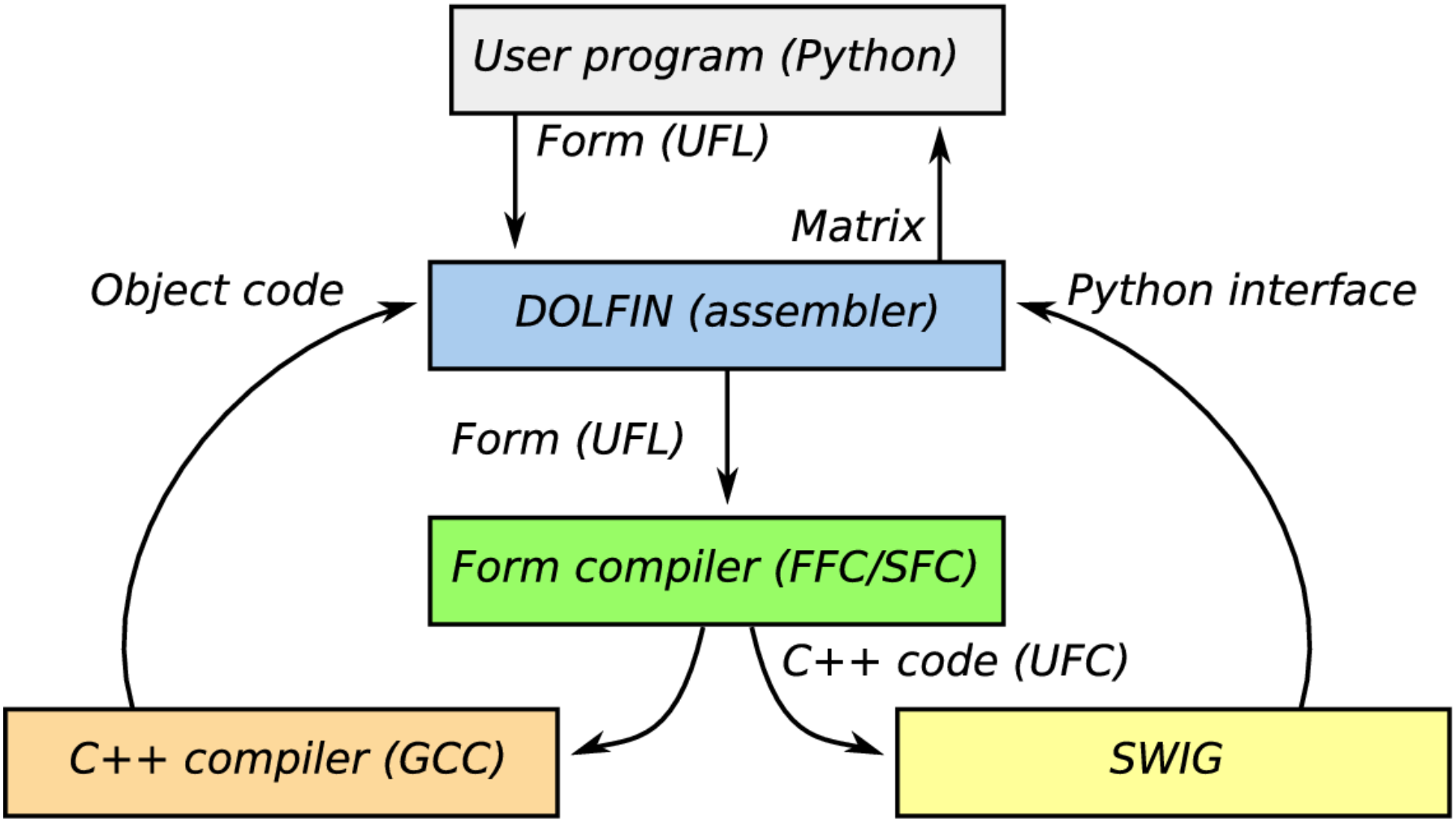
- C++ interface
  - C++ class library (`Matrix, Vector, Mesh, Function, ...`)
  - Forms expressed in separate form files (`.ufl`)
  - Call form compiler on command line (`ffc Poisson.ufl`)
  - Include generated code (`#include ''Poisson.h''`)

- Python interface
  - Python class library (`Matrix, Vector, Mesh, Function, ...`)
  - Integrated form language:

```
A = assemble(dot(grad(v), grad(u)))
```

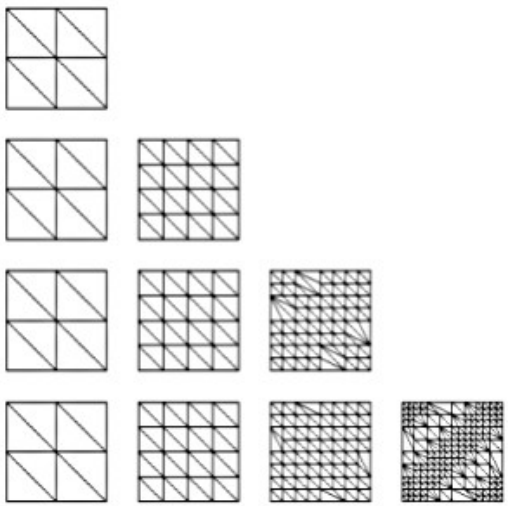
  - Automated code generation
  - Dynamic loading of generated code (JIT compilation)

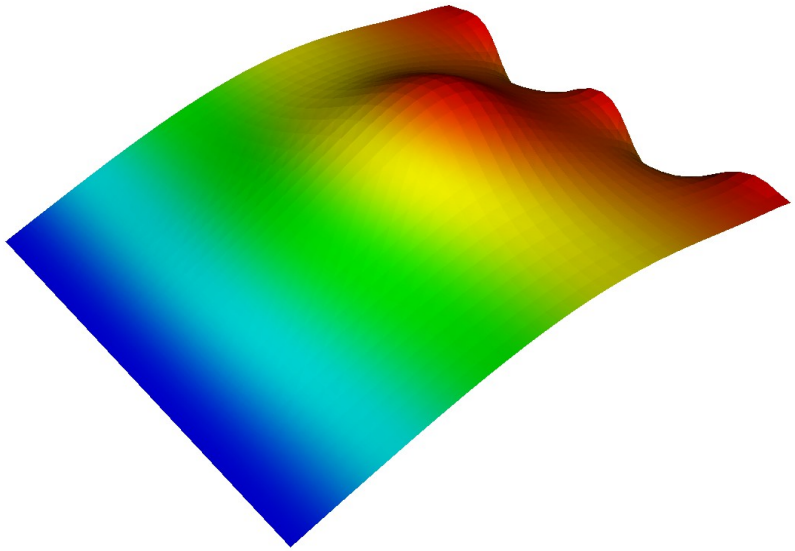
Just-In-Time Compilation (JIT)

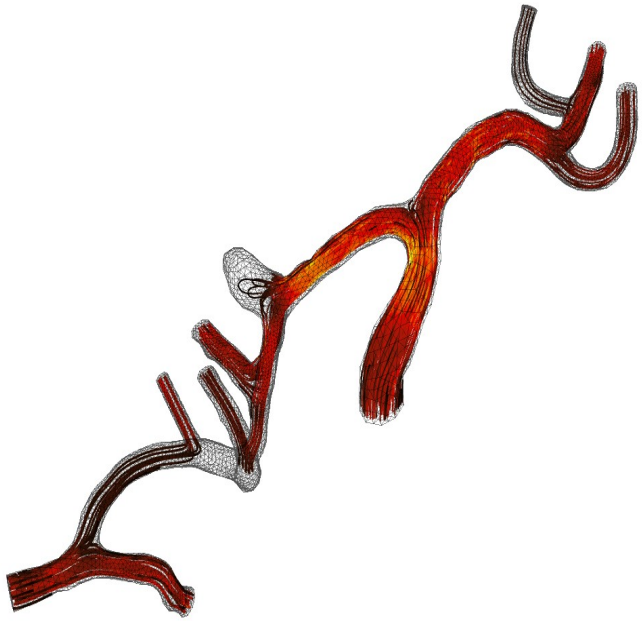


Examples

- Matrix assembly
- Mesh refinement
- Solving Poisson's equation
- User-defined operators
- Solving the Navier-Stokes equations







Matrix Assembly

```
mesh = UnitCube(16, 16, 16)
V = FunctionSpace(mesh, 'CG', 5)

v = TestFunction(V)
u = TrialFunction(V)
f = Function(V, 'sin(x[0]*x[1]*x[2])')
a = (grad(v), grad(u))
L = (v, f)

A = assemble(a)
b = assemble(L)
```


Mesh Refinement

```
mesh = Mesh('mesh.xml')

cell_markers = MeshFunction('bool', mesh, 3)
for cell in cells(mesh):
    if condition:
        cell_markers.set(cell, True)

mesh.refine(cell_markers)
mesh.smooth()
plot(mesh)
```

Solving Poisson's Equation (I)

```
a = (grad(v), grad(u))
L = (v, f)

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

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

# solve(A, u.vector(), b, cg, amg_hypre)
```

Solving Poisson's Equation (II)

```
a = (grad(v), grad(u))
L = (v, f)

problem = VariationalProblem(a, L, bc)
u = problem.solve()

plot(u)
plot(grad(u))
```


Linear Elasticity

Variational formulation (mathematical notation)

$$\epsilon(v) = \frac{1}{2}(\text{grad}(v) + (\text{grad}(v))^\top)$$

$$\sigma(v) = 2\mu\epsilon(v) + \lambda(\text{tr}\,\epsilon)I$$

$$a(v,u) = (\epsilon(v), \sigma(u))$$

$$L(v) = (v, f)$$

Linear Elasticity

Variational formulation (implementation)

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

def sigma(v):
    return 2*mu*epsilon(v) + l*tr(epsilon(v))*I

a = (epsilon(v), sigma(u))
L = (v, f)
```


Solving Navier-Stokes

```
def solve(self, problem, options=OPTIONS):

    # Get problem parameters
    mesh = problem.mesh
    shape = self.shape(mesh)

    # Set time step
    h = MeshSize(shape, mesh)
    dt = problem.dt or 0.25*h.min()

    # Create finite element spaces
    V = VectorElement("CG", shape, 1)
    Q = FiniteElement("CG", shape, 1)
    DG = FiniteElement("DG", shape, 0)

    # Test and trial functions
    v = TestFunction(V)
    q = TestFunction(Q)
    u = TrialFunction(V)
    p = TrialFunction(Q)

    # Functions
    u0 = Function(V, mesh, Vector())
    us = Function(V, mesh, Vector())
    u1 = Function(V, mesh, Vector())
    p1 = Function(Q, mesh, Vector())
    nu = Function(DG, mesh, problem.nu)
    k  = Function(DG, mesh, dt)
    f  = problem.f

    # Tentative velocity step
    a0 = dot(v, u)*dx + k*nu*dot(grad(v), grad(u))*dx
    L0 = dot(v, u0)*dx + k*dot(v, f)*dx - k*dot(v, mult(grad(u0), u0))*dx

    # Poisson problem for the pressure
    a1 = 1.0e-6*p*q*dx + dot(grad(q), grad(p))*dx
    L1 = -(1.0/k)*q*div(us)*dx

    # Velocity update
    a2 = dot(v, u)*dx
    L2 = dot(v, us)*dx - k*dot(v, grad(p1))*dx

    # Assemble matrices
    A0 = assemble(a0, mesh)
    A1 = assemble(a1, mesh)
    A2 = assemble(a2, mesh)
```

```
# Time loop
t = 0.0
while t < problem.T:

    # Propagate values to next time step
    t += dt
    u0.assign(u1)

    # Compute tentative velocity
    b = assemble(L0, mesh)
    [bc.apply(A0, b, a0) for bc in problem.bcv]
    solve(A0, us.vector(), b, gmres, ilu)

    # Compute p1
    b = assemble(L1, mesh)
    [bc.apply(A1, b, a1) for bc in problem.bcp]
    solve(A1, p1.vector(), b, gmres, amg)

    # Compute u1
    b = assemble(L2, mesh)
    [bc.apply(A2, b, a2) for bc in problem.bcv]
    solve(A2, u1.vector(), b, gmres, ilu)
```

Current Activities

- UFL: Unified Form Language
- Parallel assembly/solve
- Higher order meshes
- Finite element exterior calculus
- Automated error control / adaptivity

- FEniCS book project (Springer Verlag 2009)
- FEniCS'09 workshop June 11-12 2009

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