

# Finite Element Code Generation: Simplicity, Generality, Efficiency

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# Solving differential equations

- ▶ Build a calculator
- ▶ One button for each equation?
- ▶ 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!

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

```
// Extract vertex coordinates
const double * const 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];

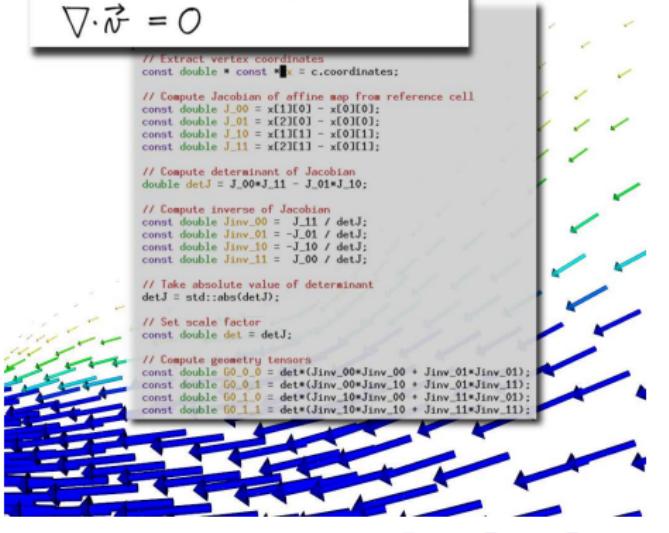
// Compute determinant of Jacobian
double detJ = J_00 * J_11 - J_01 * J_10;

// 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;

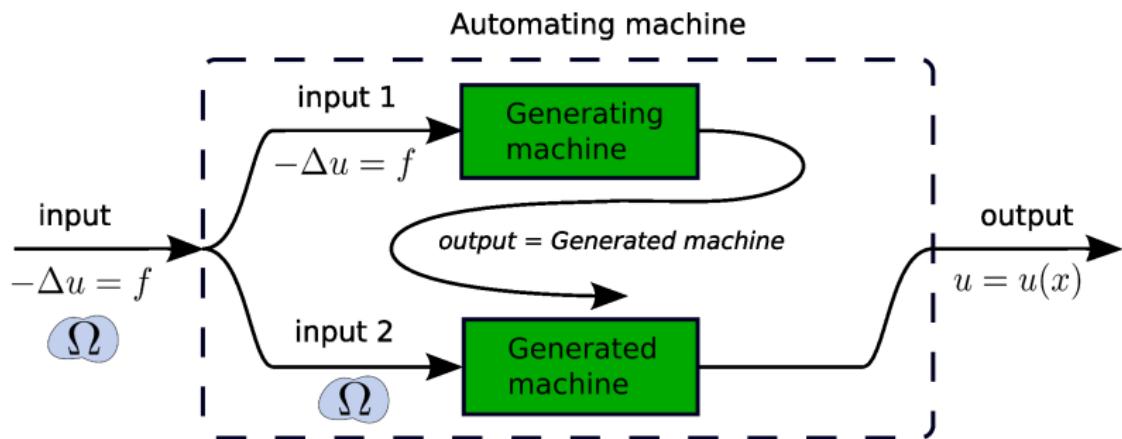
// Take absolute value of determinant
detJ = std::abs(detJ);

// Set scale factor
const double det = detJ;

// Compute geometry tensors
const double G0_00 = det*(Jinv_00 * Jinv_00 + Jinv_01 * Jinv_01);
const double G0_01 = det*(Jinv_00 * Jinv_10 + Jinv_01 * Jinv_11);
const double G0_10 = det*(Jinv_10 * Jinv_00 + Jinv_11 * Jinv_01);
const double G0_11 = det*(Jinv_10 * Jinv_10 + Jinv_11 * Jinv_11);
```



# Automate the solution of differential equations



# Simplicity

- ▶ Simple and intuitive user interface
  - ▶ Close to mathematical abstractions
  - ▶ Close to mathematical notation
  - ▶ But give users what they expect: Matrix, Vector, Mesh, Form (?)
- ▶ Simplicity of implementation
  - ▶ Simple components: each component does one thing and does it well
  - ▶ Simple components: independent development
  - ▶ Simplicity by (new) mathematical ideas
  - ▶ Simplicity by (new) programming techniques

## 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

...      (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
- ▶ Automation of Computational Mathematical Modeling (ACMM)
- ▶ [www.fenics.org](http://www.fenics.org)



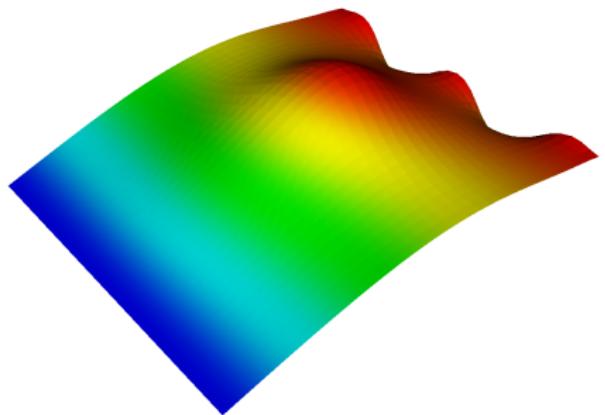
# Poisson's equation

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

$$a(v, u) = \int_{\Omega} \nabla v \cdot \nabla u \, dx$$

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

# 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

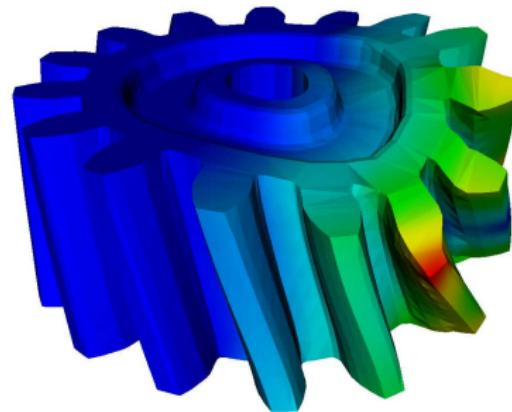
Differential equation:

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

where

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

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



- ▶ 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

$$\begin{aligned} a(v, u) &= \int_{\Omega} \nabla v : \sigma(u) \, dx \\ L(v) &= \int_{\Omega} v \cdot f \, dx \end{aligned}$$

# 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

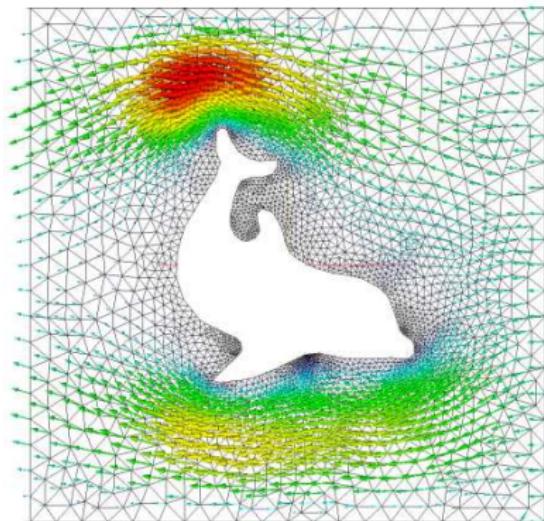
Differential equation

Differential equation:

$$-\Delta u + \nabla p = f$$

$$\nabla \cdot u = 0$$

- ▶ 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

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

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

# 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 $H(\text{div})$ elements

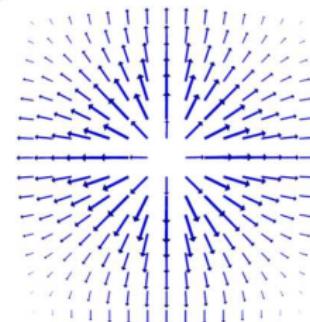
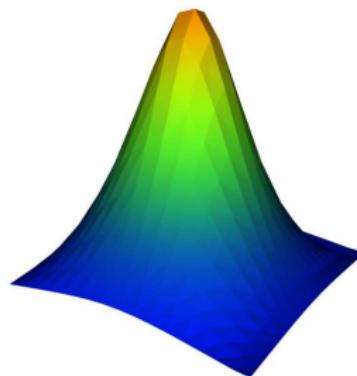
Differential equation

Differential equation:

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

$$\nabla \cdot \sigma = f$$

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



# Mixed Poisson with $H(\text{div})$ 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

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

# Mixed Poisson with $H(\text{div})$ 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
```

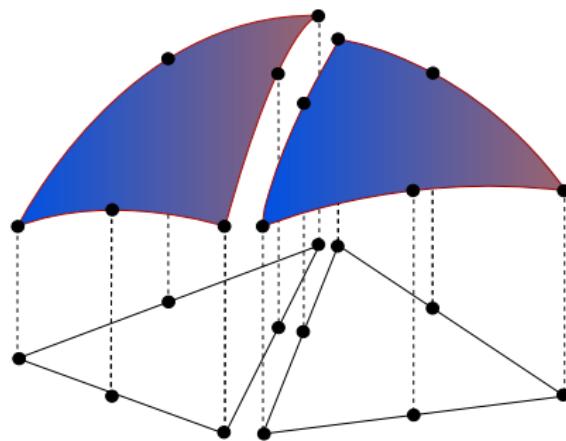
# Poisson's equation with DG elements

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

$$\begin{aligned} a(v, u) &= \int_{\Omega} \nabla v \cdot \nabla u \, dx \\ &\quad + \sum_S \int_S -\langle \nabla v \rangle \cdot [\![u]\!]_n - [\![v]\!]_n \cdot \langle \nabla u \rangle + (\alpha/h) [\![v]\!]_n \cdot [\![u]\!]_n \, dS \\ &\quad + \int_{\partial\Omega} -\nabla v \cdot [\![u]\!]_n - [\![v]\!]_n \cdot \nabla u + (\gamma/h) vu \, ds \\ L(v) &= \int_{\Omega} vf \, dx + \int_{\partial\Omega} vg \, ds \end{aligned}$$

# Poisson's equation with DG elements

## Implementation

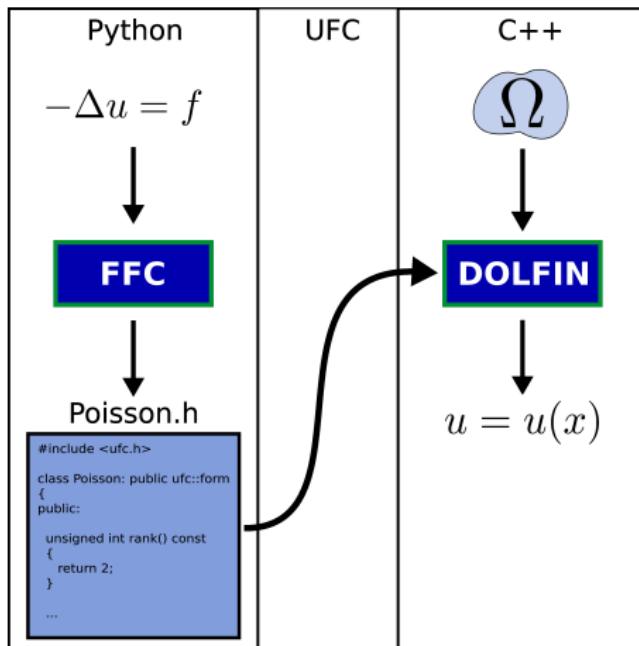
```
DG1 = FiniteElement("Discontinuous Lagrange", "triangle", 1)

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

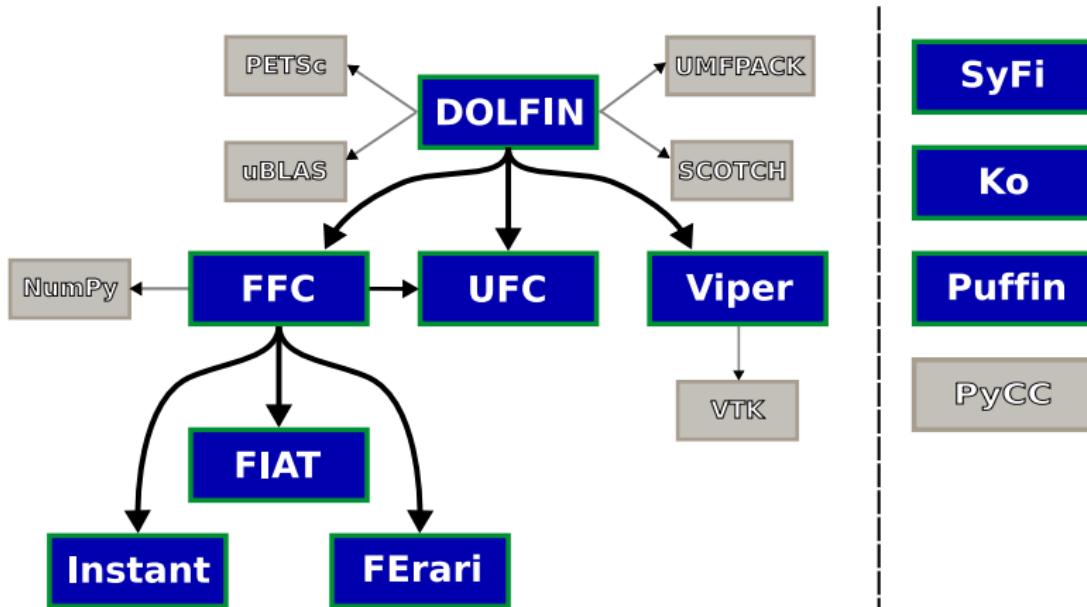
f = Function(DG1)
g = Function(DG1)
n = FacetNormal("triangle")
h = MeshSize("triangle")

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, ...

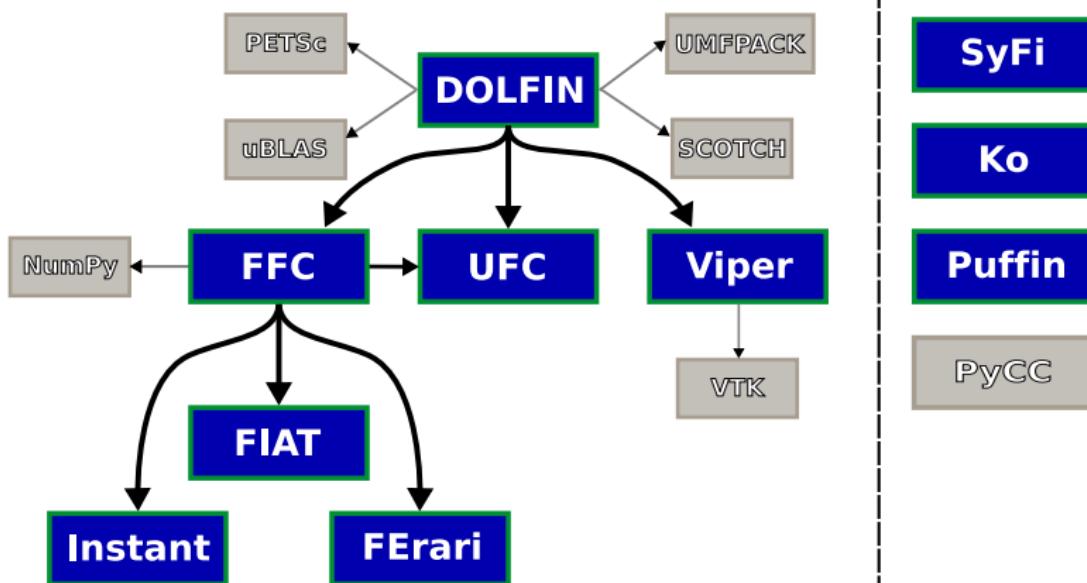
# Future plans (highlights)

- ▶ 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

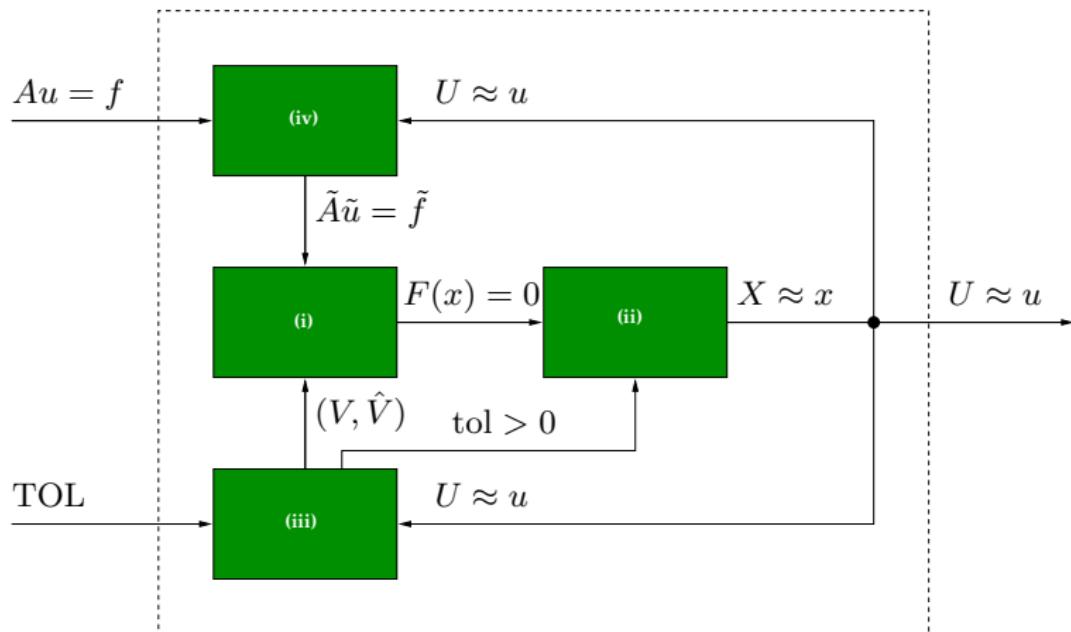
→ [www.fenics.org](http://www.fenics.org) ←

*Additional slides*

# Software components

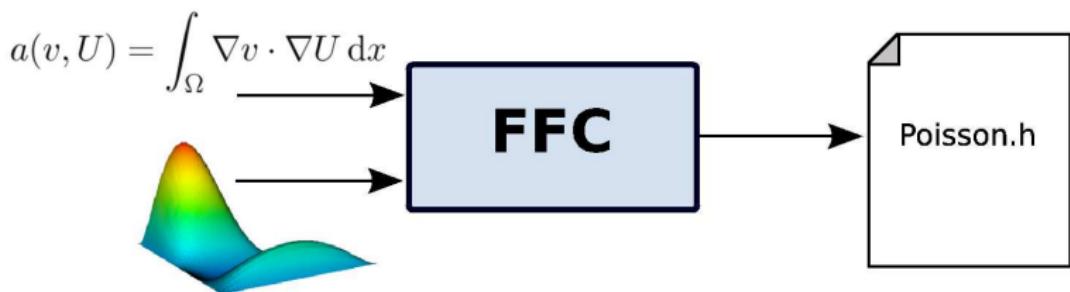


# Automation of CMM



# 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
- ▶  $\text{mcG}(q)/\text{mdG}(q)$  and  $\text{cG}(q)/\text{dG}(q)$  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”)