Software Components for Solving PDEs

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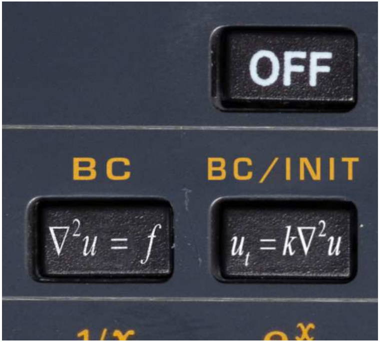
The FEniCS project

- Initiated in 2003
- Free software for the Automation of CMM
- Collaborators (in order of appearance):
  - University of Chicago
  - Argonne National Laboratory
  - Delft University of Technology
  - Royal Institute of Technology (KTH)
  - Simula Research Laboratory
  - Texas Tech
- Automate the solution of differential equations
- www.fenics.org

Automate the solution of differential equations

- Build a calculator
- One button for each equation?

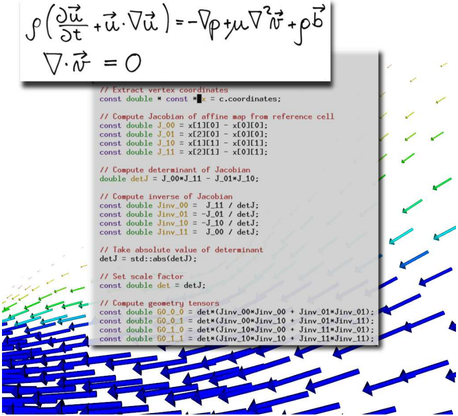
- Too many buttons!



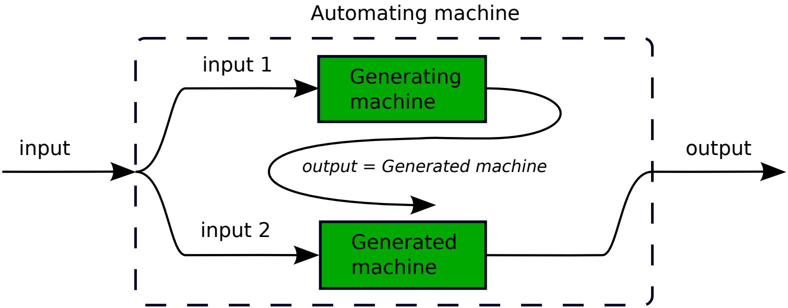
Automate the solution of differential equations

- Input: Differential equation
- Generate computer code
- Compute solution

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



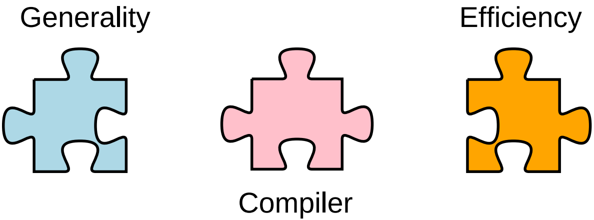
Automate the solution of differential equations



Generality *and* efficiency

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

Possible to combine generality with efficiency by generating code



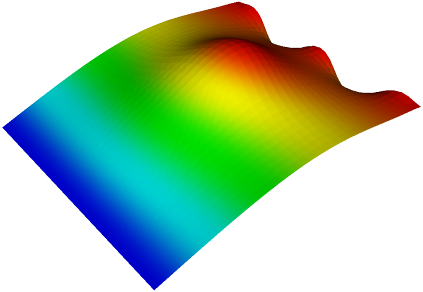
Poisson's equation

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

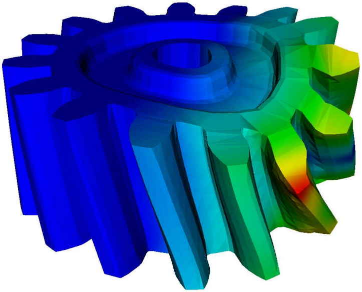
Differential equation:

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

where

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

- 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
```

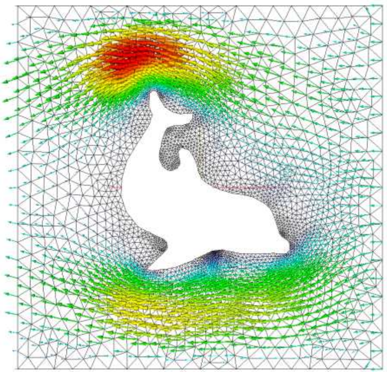
The Stokes equations

Differential equation

Differential equation:

$$-\Delta u + \nabla p = f$$
$$\nabla \cdot u = 0$$

- 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

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

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

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
```

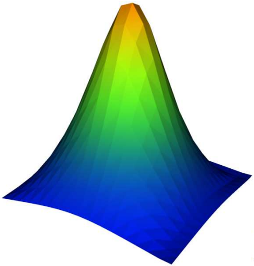
Mixed Poisson with $H(\mathrm{div})$ elements

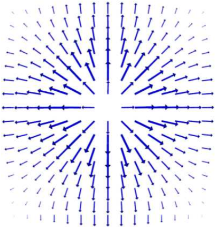
Differential equation

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

$$a((\tau, w), (\sigma, u)) = \int_\Omega \tau \cdot \sigma - \nabla \cdot \tau \, u + w \nabla \cdot \sigma \, \mathrm{d}x$$

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

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
```

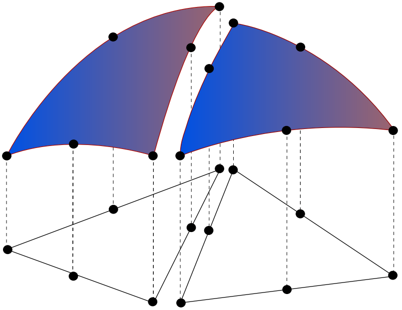
Poisson's equation with DG elements

Differential equation

Differential equation:

$$-\Delta u = f$$

- $u \in L_2$
- u discontinuous accross 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
```

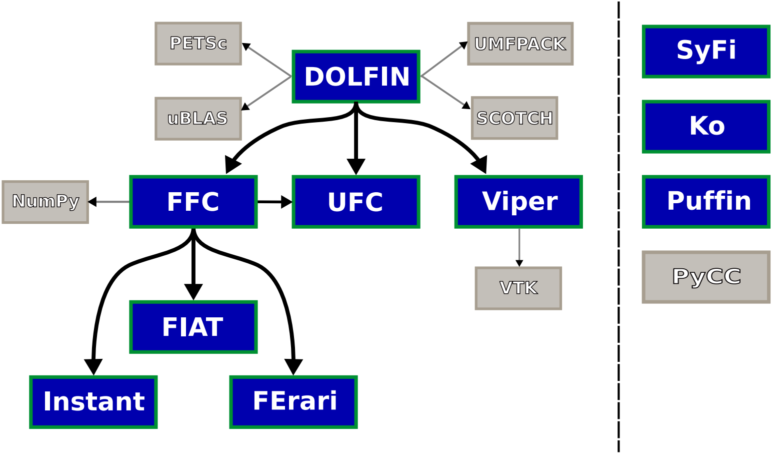
Journal papers (selection)

- *Automating the Finite Element Method*
  Logg, Arch. Comput. Methods Engrg. (2007)
- *Efficient Compilation of a Class of Variational Forms*
  Kirby, Logg, ACM Trans. Math. Software. (2007),
- *Geometric Optimization of the Evaluation of Finite Element Matrices*
  Kirby, Scott, SIAM J. Sci. Comput. (2007)
- *A Compiler for Variational Forms*
  Kirby, Logg, ACM Trans. Math. Software. (2006),
- *Optimizing FIAT with Level 3 BLAS*
  Kirby, ACM Trans. Math. Software. (2006)
- *Topological Optimization of the Evaluation of Finite Element Matrices*
  Kirby, Logg, Scott, Terrel, SIAM J. Sci. Comput. (2006)
- *Optimizing the Evaluation of Finite Element Matrices*
  Kirby, Knepley, Logg, Scott, SIAM J. Sci. Comput. (2005)
- *FIAT: A New Paradigm for Computing Finite Element Basis Functions*
  Kirby, ACM Trans. Math. Software. (2004)

Developer/user base

- 200–300 daily visits at `http://www.fenics.org/`
- 500 monthly downloads
- 10–15 active developers
- 50 registered users on the FEniCS wiki
- Workshops:
  - FEniCS'05 in Chicago
  - FEniCS'06 in Delft
  - FEniCS'07 (08) in Baton Rouge (LSU)
- Google page rank is 6/10 (Simula has 7/10)

Software components



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")

Recent updates

- UFC, a framework for finite element assembly
- Discontinuous Galerkin methods
- BDM and RT elements
- A new improved mesh library
- Mesh and graph partitioning
- Improved linear algebra supporting PETSc and uBLAS
- Optimized code generation (FErari)
- Improved ODE solvers
- PyDOLFIN, the Python interface of DOLFIN
- Bugzilla database, pkg-config
- Improved manual, compiler support, demos, matrix factory, file formats, . . .

PyCC

- Initiated in 2005
- In–house research tool for solving PDEs and ODEs
- PyCC aims at being a flexible and numerically efficient research tool for application scientists
- Fits together state–of–the–art libraries through Python:
  - DOLFIN (Mesh)
  - SyFi (Matrices)
  - Trilinos (AMG)
  - Hypre (AMG)

PyCC provides a Matlab-like environment for defining and solving PDEs in Python

- Focus on the (block) linear algebra level
- Matrices constructed through factory methods
- Support for generation of custom matrices
- Block preconditioning for optimal solution algorithms
- Numpy arrays used extensively for numerical efficiency in Python
- Live visualization through Viper (PyCC bi–product)
- Happy merge with DOLFIN/PyDOLFIN

Applications

PyCC development is application driven

- Cardiac computations
  - Mono- and bidomain equations
  - Cell modelling (ODEs/PDEs)
  - Inverse problems
- Flow problems
  - Stokes equation
  - Navier-Stokes equations
- Linear and non–linear elasticity

Publications (selection)

- *A linear system of partial differential equations modeling the resting potential of a heart with regional ischemia*
  MacLachlan, Sundnes, Skavhaug, Lysaker, Nielsen, Tveito, Math. Biosci. (2007)
- *Application of symbolic finite element tools to nonlinear hyperelasticity*
  Alnæs, Mardal, Sundnes, MekIT'07
- *SyFi - An Element Matrix Factory, with Emphasis on the Incompressible Navier-Stokes Equations*
  Mardal, Para'06
- *Using Python to Solve Partial Differential Equations*
  Mardal, Skavhaug, Lines, Staff, Ødegård, Computing in Science & Engineering (2007)

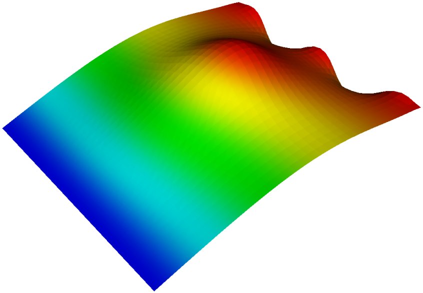
Poisson's equation

Differential equation

Differential equation:

$$-\Delta u = f \quad \text{in } \Omega$$

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



Poisson's equation

Implementation

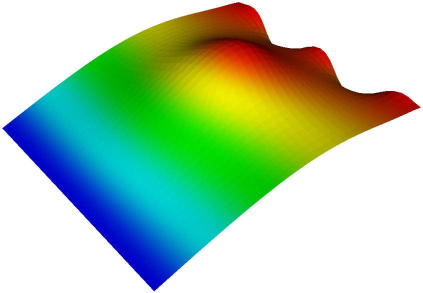
```
mesh = UnitSquare(100,100)
mfac = MatrixFactory(mesh)
L = mfac.computeStiffnessMatrix()
M = mfac.computeMassMatrix()
A = L
u = numpy.zeros(A.n)
b = M*f(mfac.x(), mfac.y())
ConjugateGradients.solve(A, u, b)
```

Heat equation

Differential equation

$$u_t = \Delta u + f \quad \text{in } \Omega, \quad t > 0$$
$$u(x,0) = u_0(x) \quad \text{in } \Omega \text{ at } t = 0$$

- Heat diffusion
- Particle diffusion
- Action potential propagation in nerve cells
- Financial processes
- etc.



Heat equation

Implementation

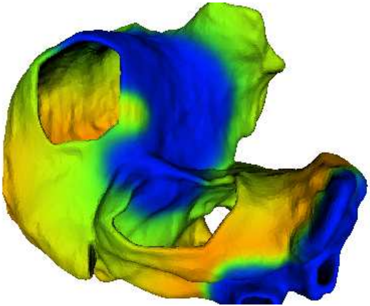
```
mesh = UnitSquare(100, 100)
mfac = MatrixFactory(mesh)
L = mfac.computeStiffnessMatrix()
M = mfac.computeMassMatrix()
A = M + dt*L
u = numpy.zeros(A.m)
for i in xrange(50):
    b = M*(u + f(mfac.x(),mfac.y(),t))
    ConjugateGradients.solve(A, u, b)
```

The Bidomain Equations

Differential Equation

$$\frac{\partial v}{\partial t} = \nabla \cdot (M_i \nabla v) + \nabla \cdot (M_i \nabla u) - I_{\text{ion}}(v, s),$$
$$0 = \nabla \cdot (M_i \nabla v) + \nabla \cdot ((M_i + M_e) \nabla u)$$

- v: Transmembrane potential
- u: Extra cellular potential
- I_{ion}: ODE system describing the ion flow across the cell membrane
- M_i and M_e: conductivity tensors



Bidomain equations

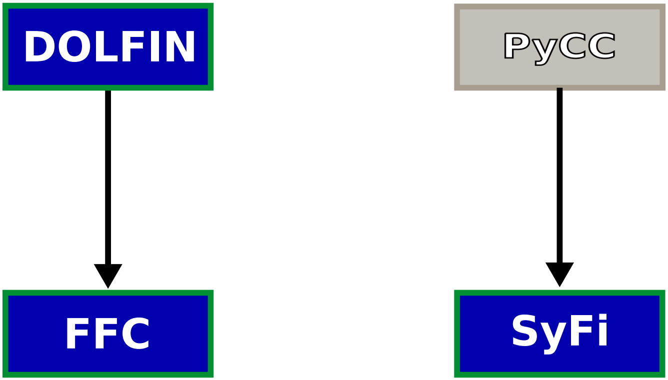
Implementation

```
mesh = Mesh("atria.xml.gz")
mfac = MatrixFactory(mesh)
M = mfac.computeMassMatrix()
Ai = mfac.computeStiffnessMatrix(tf_i)
Aie = mfac.computeStiffnessMatrix(tf_ie)
A = M + dt*Ai
B = dt*Ai
Bt = dt*Ai
C = dt*Aie
A_b = BlockMatrix((A,B),(Bt,C))
Ainv_b = DiagBlockMatrix((prec(A),prec(C)))
```

Future plans (highlights)

- UFL/UFC
- Automation of error control
  - Automatic generation of dual problems
  - Automatic generation of a posteriori error estimates
- Mesh algorithms
  - Adaptive mesh refinement
  - Mesh algorithms for ALE methods
- Improved geometry support
- Finite element exterior calculus
- Packaging, installation, testing
- Tighter integration (merge) between DOLFIN and PyCC

Happy merge



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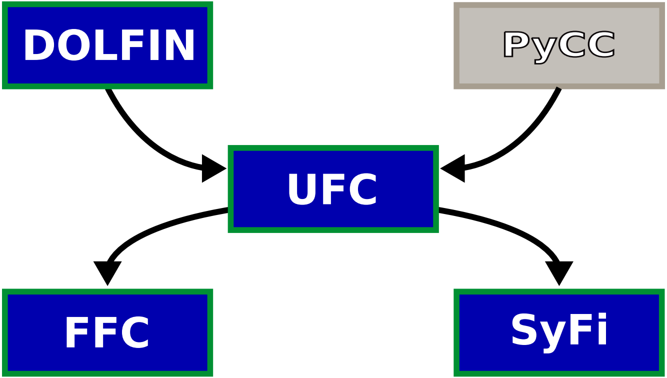

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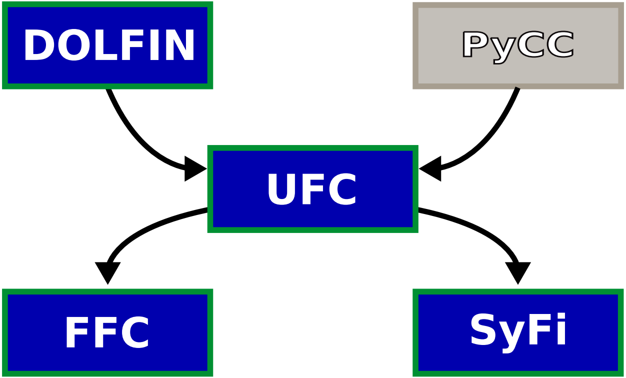

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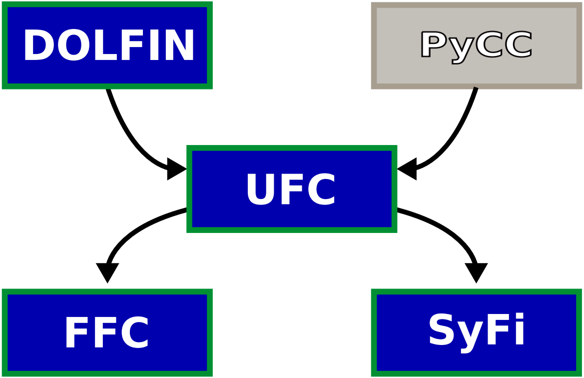

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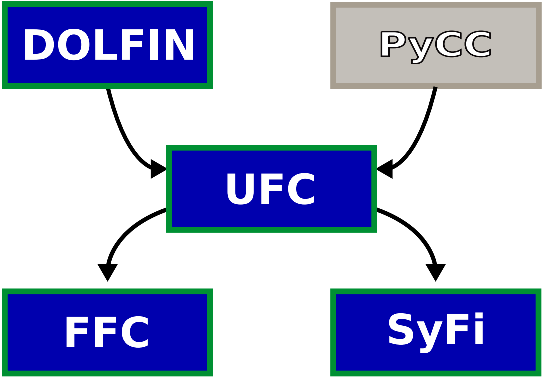

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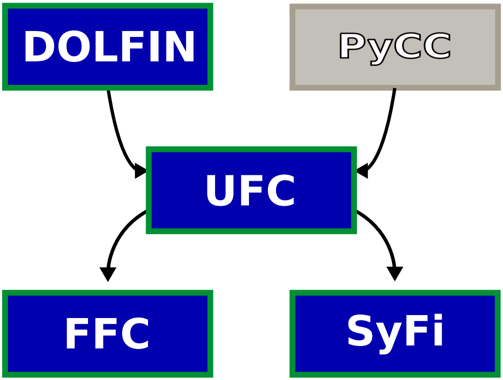

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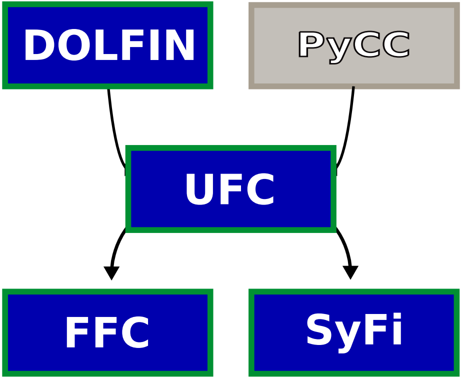

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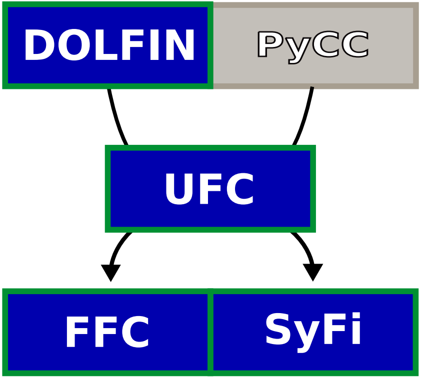

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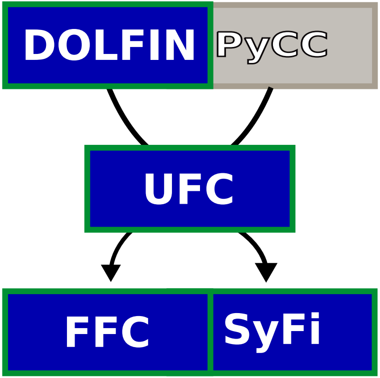

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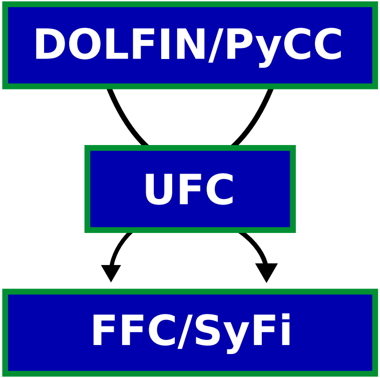

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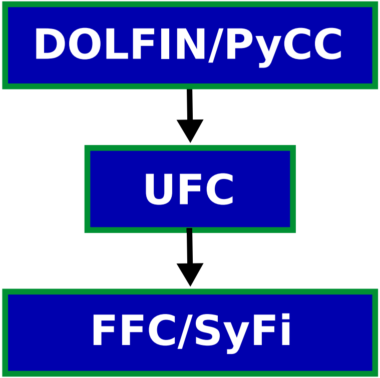
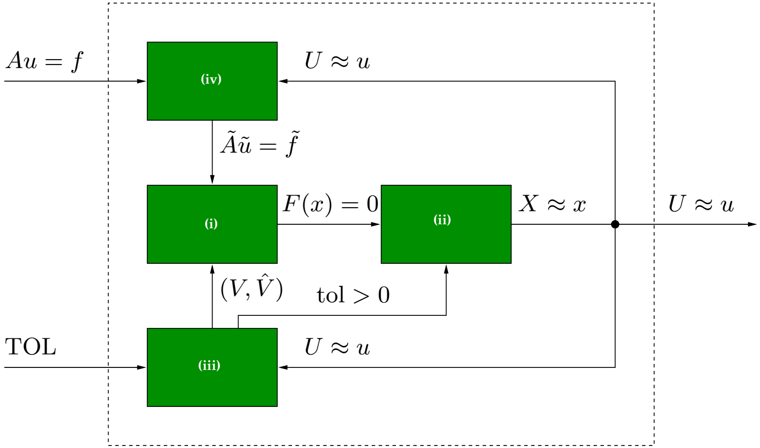


Additional slides

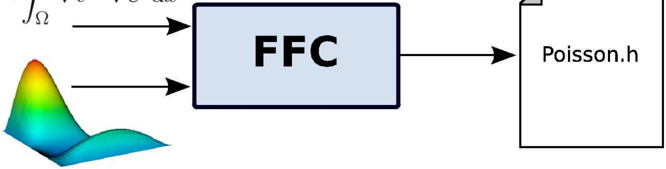
Automation of CMM



A common framework: UFL/UFC

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

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



Benchmarks

- Measure CPU time for the evaluation of the element tensor (the "element stiffness matrix")
- Code automatically generated by the form compiler FFC
- Compute speedup compared to a standard quadrature-based approach 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	—	—	—	—

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);
}
```