

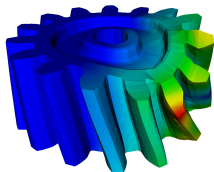
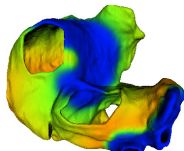
The FEniCS Project

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NOTUR 2011

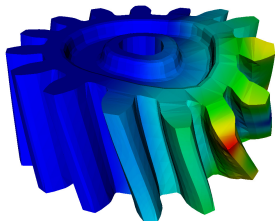
2011-05-23



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/Ubuntu GNU/Linux
- Licensed under the GNU LGPL



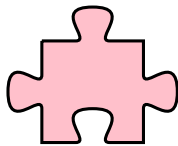
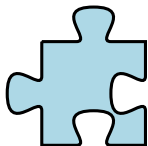
<http://www.fenicsproject.org/>

Collaborators

University of Chicago, Argonne National Laboratory, Delft University of Technology, Royal Institute of Technology KTH, Simula Research Laboratory, Texas Tech University, University of Cambridge, ...

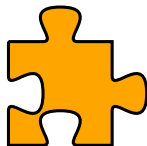
FEniCS is new technology combining generality, efficiency, simplicity and reliability

Generality



Code Generation

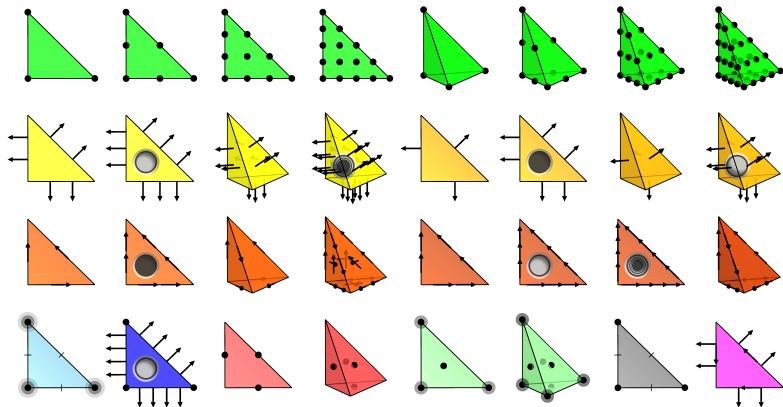
Efficiency



- Generality through *abstraction*
- Efficiency through *code generation, adaptivity, parallelism*
- Simplicity through *high level scripting*
- Reliability through *adaptive error control*

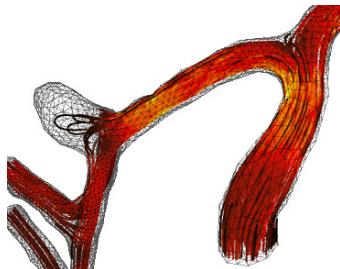
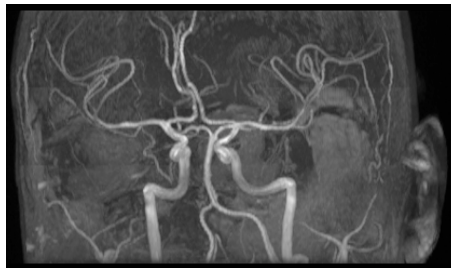
FEniCS is automated FEM

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



What has FEniCS been used for?

Computational hemodynamics



- Low wall shear stress may trigger aneurysm growth
- Solve the incompressible Navier–Stokes equations on patient-specific geometries

$$\begin{aligned}\dot{u} + \nabla u \cdot u - \nabla \cdot \sigma(u, p) &= f \\ \nabla \cdot u &= 0\end{aligned}$$

Computational hemodynamics (contd.)



```
# 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)

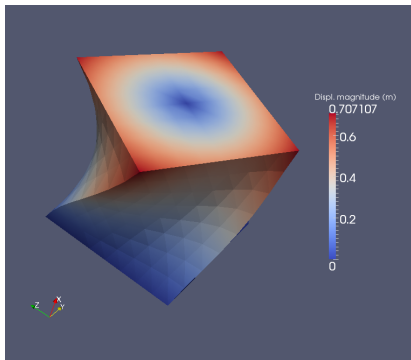
# Tentative velocity step (sigma formulation)
U = 0.5*(u0 + u)
F1 = rho*(1/k)*inner(v, u - u0)*dx +
rho*inner(v, grad(u0)*(u0 - w))*dx \
+ inner(epsilon(v), sigma(U, p0))*dx \
+ inner(v, p0*n)*ds - mu*inner(grad(U).T*n, v)*ds \
- inner(v, f)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# 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 the solver to be implemented in a minimal amount of code

Hyperelasticity



```
class Twist(StaticHyperelasticity):  
  
    def mesh(self):  
        n = 8  
        return UnitCube(n, n, n)  
  
    def dirichlet_conditions(self):  
        clamp = Expression(("0.0", "0.0", "0.0"))  
        twist = Expression(("0.0",  
            "y0 + (x[1]-y0)*cos(theta)  
            - (x[2]-z0)*sin(theta) - x[1]",  
            "z0 + (x[1]-y0)*sin(theta)  
            + (x[2]-z0)*cos(theta) - x[2]"))  
        twist.y0 = 0.5  
        twist.z0 = 0.5  
        twist.theta = pi/3  
        return [clamp, twist]  
  
    def dirichlet_boundaries(self):  
        return ["x[0] == 0.0", "x[0] == 1.0"]  
  
    def material_model(self):  
        mu = 3.8461  
        lmbda = Expression("x[0]*5.8+(1-x[0])*5.7")  
  
        material = StVenantKirchhoff([mu, lmbda])  
        return material  
  
    def __str__(self):  
        return "A cube twisted by 60 degrees"
```

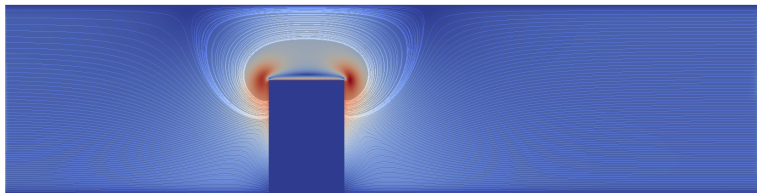
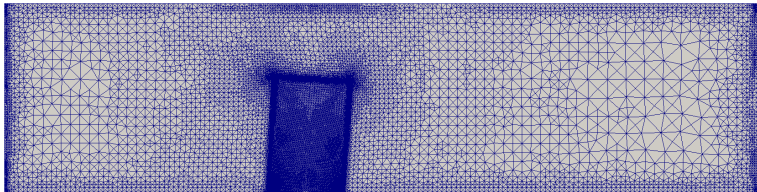
- CBC.Solve is a collection of FEniCS-based solvers developed at the CBC
- CBC.Twist, CBC.Flow, CBC.Swing, CBC.Beat, ...

Fluid–structure interaction



- The FSI problem is a computationally very expensive coupled multiphysics problem
- The FSI problem has many important applications in engineering and biomedicine

Fluid–structure interaction (contd.)



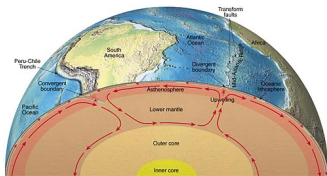
- Fluid governed by the incompressible Navier–Stokes equations
- Structure modeled by the St. Venant–Kirchhoff model
- Adaptive refinement in space and time

Computational geodynamics

$$-\operatorname{div} \sigma' - \nabla p = (Rb\phi - RaT) e$$
$$\operatorname{div} u = 0$$

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \Delta T$$

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = k_c \Delta \phi$$

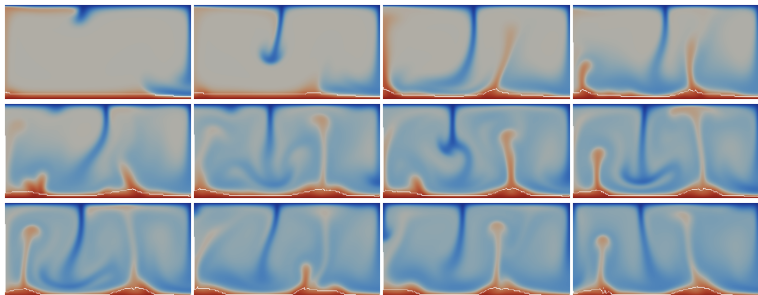


$$\sigma' = 2\eta \dot{\epsilon}(u)$$

$$\dot{\epsilon}(u) = \frac{1}{2} (\nabla u + \nabla u^T)$$

$$\eta = \eta_0 \exp(-bT/\Delta T + c(h - x_2)/h)$$

Computational geodynamics (contd.)



- The mantle convection simulator is implemented in Python/FEniCS
- Images show a sequence of snapshots of the temperature distribution

How to use FEniCS?

Installation



Official packages for Debian and Ubuntu



Drag and drop installation on Mac OS X



Binary installer for Windows

- Automated building from source for a multitude of platforms
- VirtualBox / VMWare + Ubuntu!

Hello World in FEniCS: problem formulation

Poisson's equation

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

Finite element formulation

Find $u \in V$ such that

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in \hat{V}$$

Hello World in FEniCS: problem formulation

Poisson's equation

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

Variational formulation

Find $u \in V$ such that

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

Hello World in FEniCS: implementation

```
from dolfin import *

mesh = UnitSquare(32, 32)

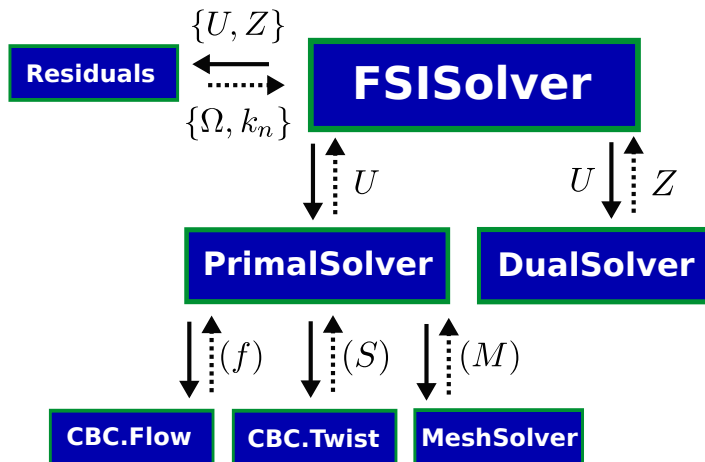
V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

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

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

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

Implementation of advanced solvers in FEniCS



Implementation of advanced solvers in FEniCS

```
# 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, lambda] = parameters
        return lambda/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
```

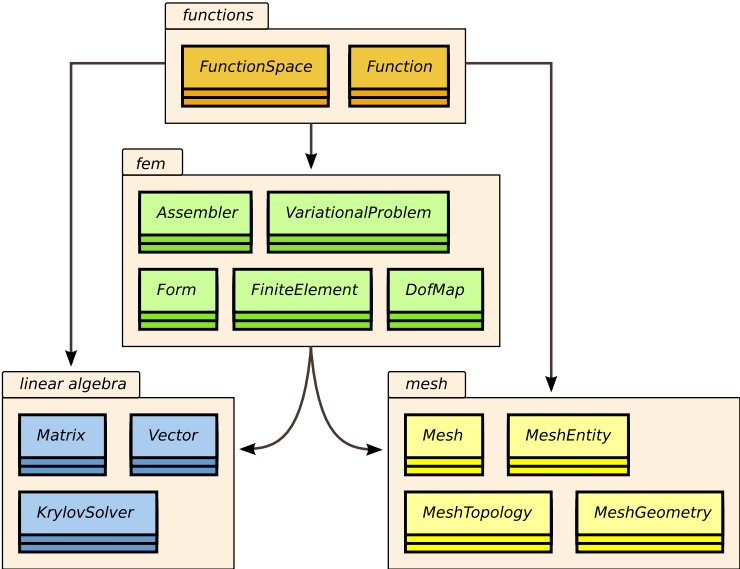
Key features

- Simple and intuitive object-oriented API, C++ or Python
- Automatic and efficient evaluation of variational forms
- Automatic and efficient assembly of linear systems
- Distributed (clusters) and shared memory (multicore) parallelism
- General families of finite elements, including arbitrary order continuous and discontinuous Lagrange elements, BDM, RT, Nédélec, ...
- 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 input/output formats
- Built-in plotting

Basic API

- Mesh, MeshEntity, Vertex, Edge, Face, Facet, Cell
 - FiniteElement, FunctionSpace
 - TrialFunction, TestFunction, Function
 - grad(), curl(), div(), ...
 - Matrix, Vector, KrylovSolver
 - assemble(), solve(), plot()
-
- Python interface generated semi-automatically by SWIG
 - C++ and Python interfaces almost identical

DOLFIN class diagram



FEniCS under the hood

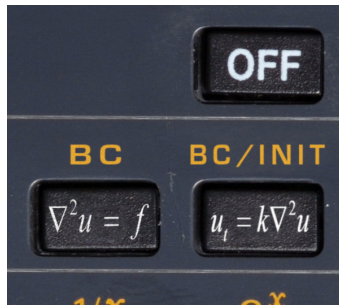
Automated Scientific Computing

Input

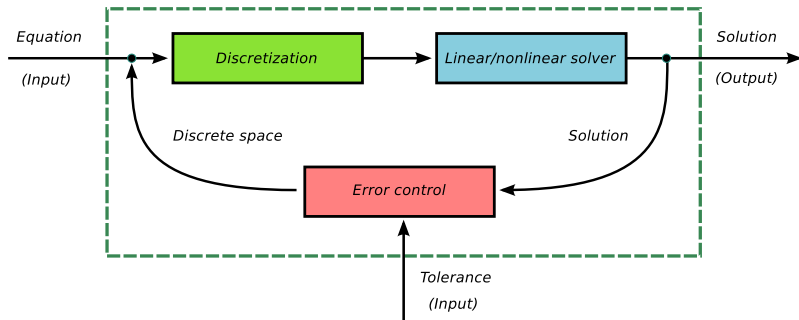
- $A(u) = f$
- $\epsilon > 0$

Output

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



Automated Scientific Computing: a blueprint



Automatic code generation

Input

Equation (variational problem)

Output

Efficient application-specific code

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

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

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

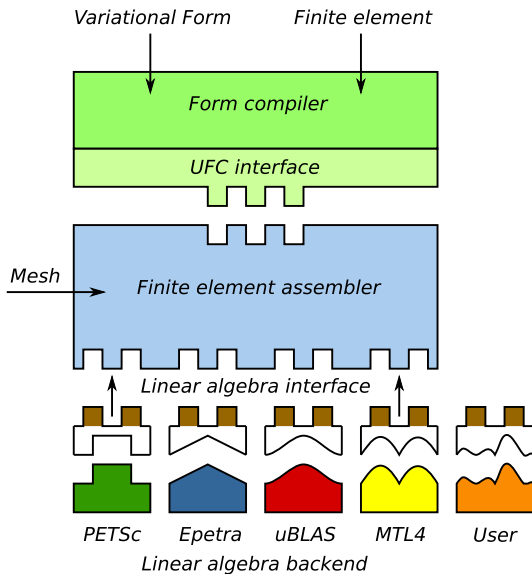
// Compute geometry tensors
const double G0_0_0 = det*(Jinv_00*Jinv_00 + Jinv_01*Jinv_01);
const double G0_0_1 = det*(Jinv_00*Jinv_10 + Jinv_01*Jinv_11);
const double G0_1_0 = det*(Jinv_10*Jinv_00 + Jinv_11*Jinv_01);
const double G0_1_1 = det*(Jinv_10*Jinv_10 + Jinv_11*Jinv_11);
```

Equation (variational form)

Form compiler

Application-specific code

Assembler interfaces



Linear algebra in DOLFIN

- Generic linear algebra interface to
 - PETSc
 - Trilinos/Epetra
 - uBLAS
 - MTL4
- Eigenvalue problems solved by SLEPc for PETSc matrix types
- Matrix-free solvers (“virtual matrices”)

Linear algebra backends

```
>>> from dolfin import *
>>> parameters["linear_algebra_backend"] = "PETSc"
>>> A = Matrix()
>>> parameters["linear_algebra_backend"] = "Epetra"
>>> B = Matrix()
```

Code generation system

```
from dolfin import *

mesh = UnitSquare(32, 32)

V = FunctionSpace(mesh, "CG", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("sin(x[0])*sin(x[1])")
a = (grad(u), grad(v)) + (u, v)
L = (f, v)

A = assemble(a, mesh)
b = assemble(L, mesh)

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

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

Code generation system

```
from dolfin import *

mesh = UnitSquare(32, 32)

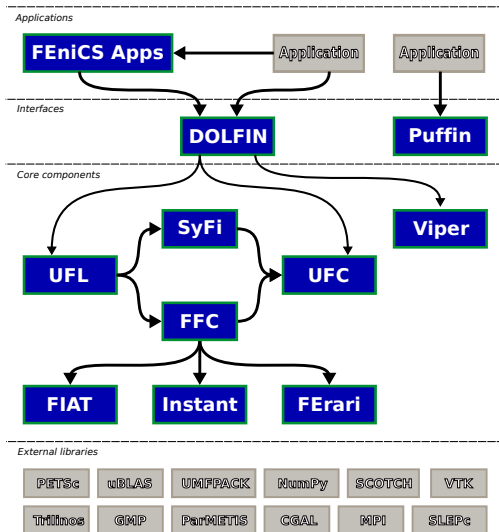
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a = (grad(u), grad(v)) + (u, v)
L = (f, v)

A = assemble(a, mesh)
b = assemble(L, mesh)























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

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

FEniCS software components

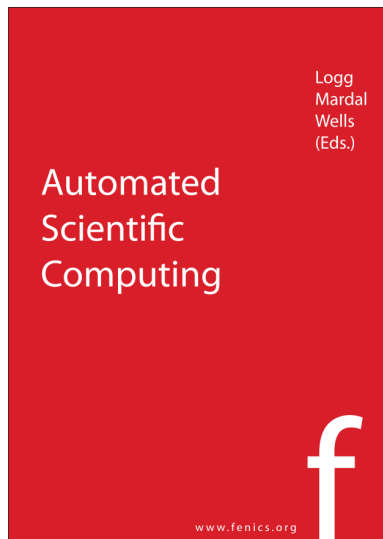


Quality assurance by continuous testing

	fenics-buildbot	lucid-amd64 	maverick-i386 	mac-osx 	linux64-exp 
		9 (9) / 9	9 (9) / 9	9 (9) / 9	9 (9) / 9
  ferari	Success	Success	Success	Success	
  fiat	Success	Success	Success	Success	
  ufc	Success	Success	Success	Success	
  instant	Success	Success	Success	Success	
  ufl	Success	Success	Success	Success	
  ffc	Success	Success	Success	building	
  viper	Success	Success	Success	Success	
  dolfin	Success	Success	Success	Success	
  syfi	Success	Success	Success	Success	
		9 (9) / 9	9 (9) / 9	9 (9) / 9	9 (9) / 9

Closing remarks

The state of FEniCS



- Parallelization (2009)
- Automated error control (2010)
- Debian/Ubuntu (2010)
- Documentation (2010)
- Latest release: 0.9.11 (May 2011)

- Release of 1.0 (2011)
- Book (2011)
- New web page (2011)

Summary

- Automated solution of differential equations
- Simple installation
- Simple scripting in Python
- Efficiency by automated code generation
- Free/open-source (LGPL)

Upcoming events

- Release of 1.0 (2011)
- Book (2011)
- New web page (2011)
- Mini courses / seminars (2011)

<http://www.fenicsproject.org/>

<http://www.simula.no/research/acdc/>

