PDEs in FEniCS

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Ευρωπαϊκή Ένωση
Ευρωπαϊκό Κοινωνικό Ταμείο
ΕΠΙΧΕΙΡΗΣΙΑΚΟ ΠΡΟΓΡΑΜΜΑ
ΕΚΠΑΙΔΕΥΣΗ ΚΑΙ ΔΙΑ ΒΙΟΥ ΜΑΘΗΣΗ
επένδυση στην κοινωνία της γνώσης
ΥΠΟΥΡΓΕΙΟ ΠΑΙΔΕΙΑΣ ΚΑΙ ΘΡΗΣΚΕΥΜΑΤΩΝ
ΕΙΔΙΚΗ ΥΠΗΡΕΣΙΑ ΔΙΑΧΕΙΡΙΣΗΣ
ΕΣΠΑ 2007-2013
πρόγραμμα για την ανάπτυξη
ΕΥΡΩΠΑΪΚΟ ΚΟΙΝΩΝΙΚΟ ΤΑΜΕΙΟ
Με τη συγχρηματοδότηση της Ελλάδας και της Ευρωπαϊκής Ένωσης

What is FEniCS

"The FEniCS Project is a collection of free software with an extensive list of features for automated, efficient solution of differential equations."

http://fenicsproject.org/

FEniCS is a multi-institutional project

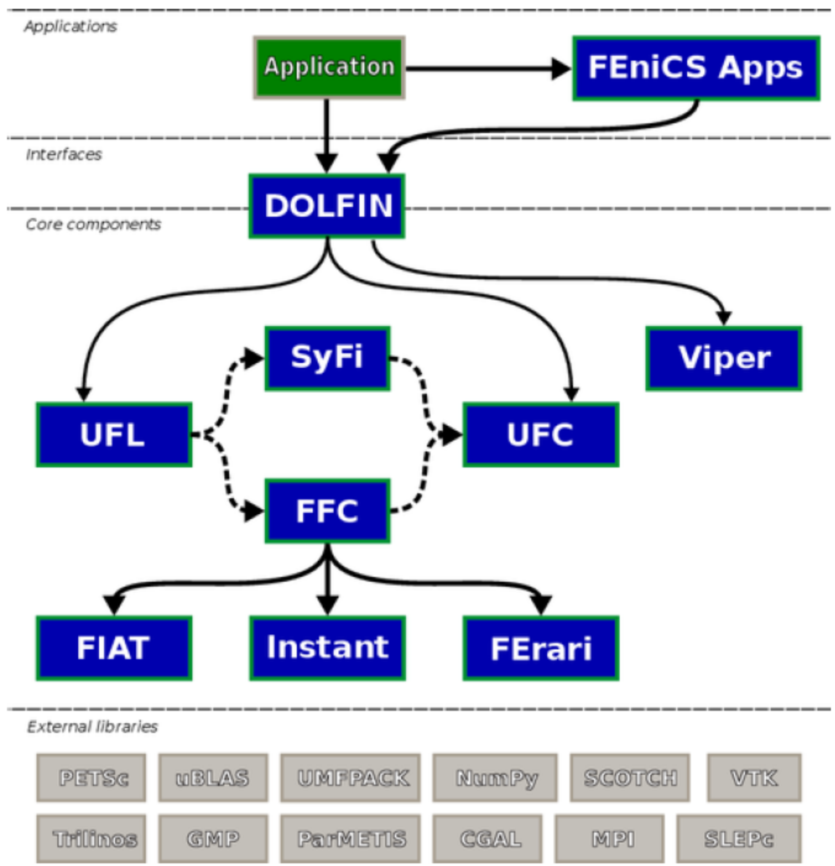
- Initiated 2003 by Univ. of Chicago and Chalmers Univ. of Technology (Ridgway Scott and Claes Johnson)
- Important contributions from
  - Univ.of Chicago (Rob Kirby, Andy Terrel, Matt Knepley, R. Scott)
  - Chalmers Univ. of Technology (Anders Logg, Johan Hoffman, Johan Janson)
  - Delft Univ. of Technology (Garth Wells, Kristian Oelgaard)
- Current key institutions:
  - Simula Research Laboratory (Anders Logg, Marie Rognes, Martin Alnæs, Johan Hake, Kent-Andre Mardal, ...)
  - Cambridge University (Garth Wells, ...)
- About 20 active developers
- Lots of application developers

FEniCS Features

- Automated solution of variational problems
- Automated error control and adaptivity
- An extensive library of finite elements
- High performance linear algebra: PETSc, Trilinos/Epetra, uBlas, MTL4
- Computational Meshes: adaptive refinement, mesh partitioning (parmetis, scotch)
- Visualization and plotting
- Extensive documentation: It has its own book!

FEniCS Components

- DOLFIN: Problem solving environment
- FFC: FEniCS Form compiler
- FIAT: FInite element Automatic Tabulator
- UFC: Unified Form-assembl Code Code generation interface
- UFL: the Unified Form-assembly Code
- JIT compiler: instant



FEniCS is easy to install

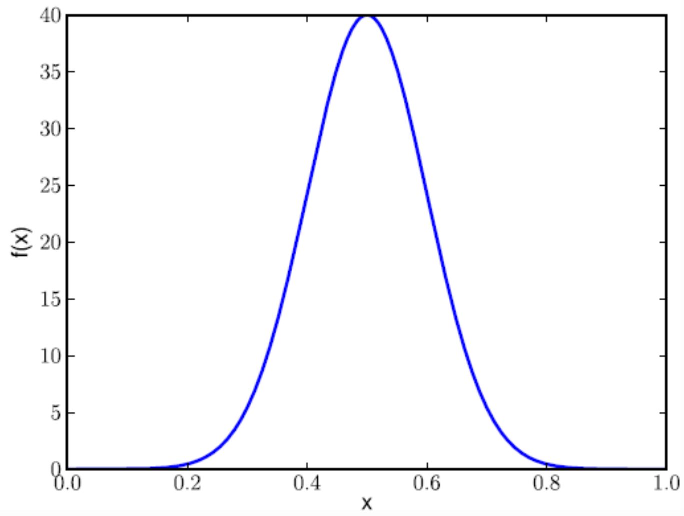
- Easiest on Ubuntu (Debian):
  `sudo apt-get install fenics`
- Mac OS X drag and drop installation (.dmg file)
- Windows binary installer
- Automated installation from source (compile & link)

We will first use FEniCS to solve a stationary diffusion problem, the Poisson equation on the unit interval

Poisson

$$-u'' = f(x); \quad u'(0) = 4; \quad u(1) = 0$$

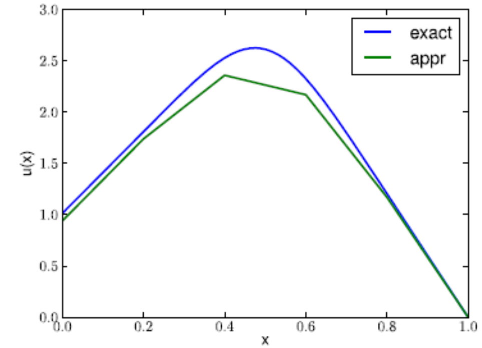
Source, $f(x)$



The problem can be stated, solved and plotted, using a **PyDOLFIN** script written in 16 lines

```
>>> from dolfin import *
>>>
>>> mesh = UnitInterval(5)
>>> V = FunctionSpace(mesh, "CG", 1)
>>>
>>> def right(x, on_boundary):
...     return x > 1-DOLFIN_EPS
...
>>> g = Constant(0)
>>> bc = DirichletBC(V, g, right)
>>>
>>> f = Expression("A*exp(-pow(x[0]-0.5,2)/(2*pow(sigma,2)))")
>>> f.A, f.sigma = 40, 0.1
>>>
>>> u = TrialFunction(V)
>>> v = TestFunction(V)
>>>
>>> a = inner(grad(v),grad(u))*dx
>>> L = f*v*dx - 4*v*ds
>>>
>>> problem = VariationalProblem(a, L, bc)
>>> u = problem.solve()
>>>
>>> plot(u)
```

$$
\begin{aligned}
-u'' &= f \\
u'(0) &= 4 \\
u(1) &= 0
\end{aligned}
$$



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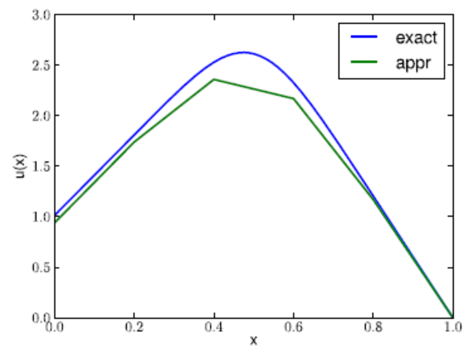
```

Domain
Solution space

$$
\begin{aligned}
-u'' &= f \\
u'(0) &= 4 \\
u(1) &= 0
\end{aligned}
$$



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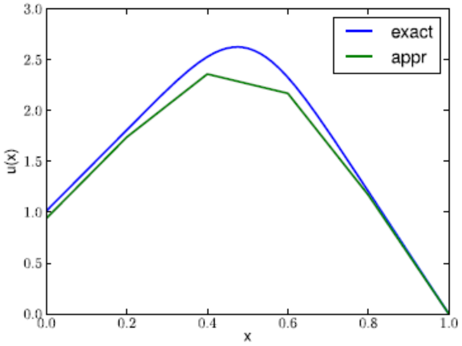
```

Boundary condition

$$
\begin{aligned}
-u'' &= f \\
u'(0) &= 4 \\
u(1) &= 0
\end{aligned}
$$



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```

Source term

$$
\begin{aligned}
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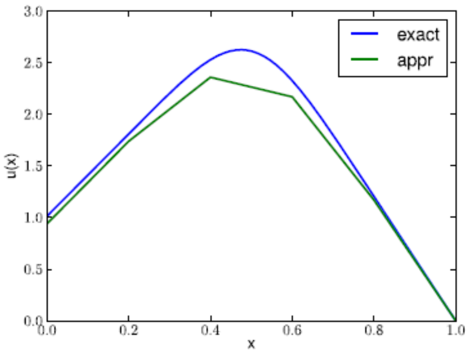
u'(0) &= 4 \\
u(1) &= 0
\end{aligned}
$$



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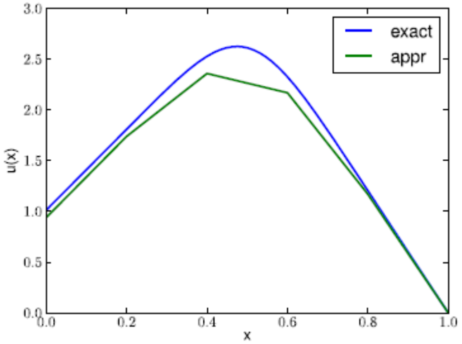
Variational formulation

$$\begin{aligned} -u'' &= f \\ u'(0) &= 4 \\ u(1) &= 0 \end{aligned}$$



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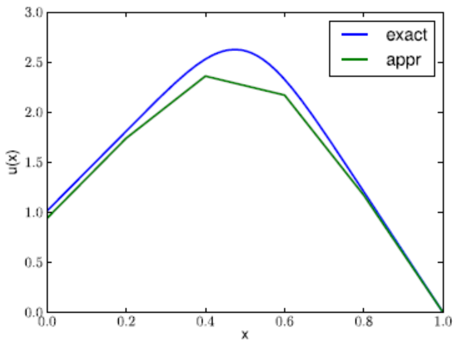
>>> u = problem.solve()
>>>
>>> plot(u)
```

Solve and plot

$$\begin{aligned} -u'' &= f \\ u'(0) &= 4 \\ u(1) &= 0 \end{aligned}$$



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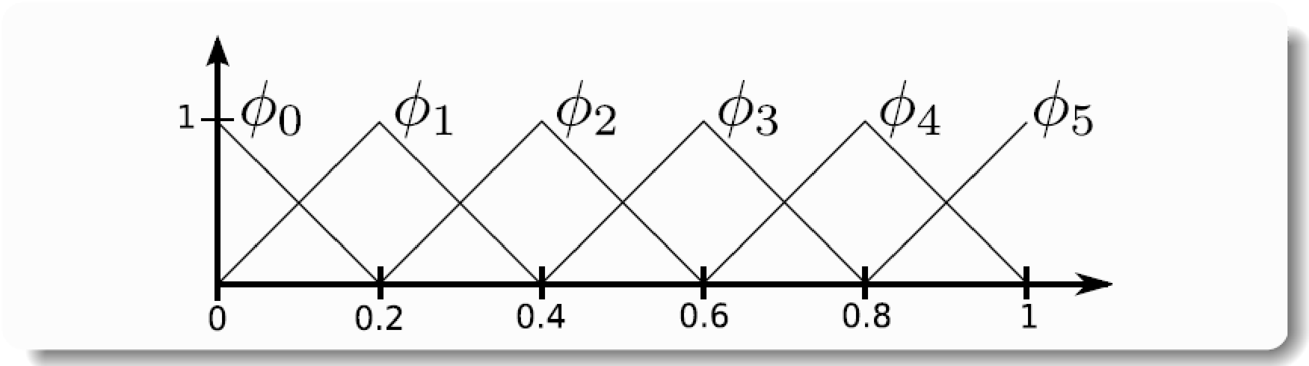


A **FunctionSpace** in PyDOLFIN takes a mesh and a *finite element* as arguments.

```
>>> mesh = UnitInterval(5)
>>> V = FunctionSpace(mesh, "Lagrange", 1)
```

Any scalar function on the domain can be approximated using a linear combination of the basis functions in the **FunctionSpace**

Discrete **Function**

$$u(x) \simeq \sum_{j=0}^{5} u_j \phi_j(x)$$
$$= u_0\phi_0 + u_1\phi_1 + u_2\phi_2 + u_3\phi_3 + u_4\phi_4 + u_5\phi_5$$
$$U = [u_0, u_1, u_2, u_3, u_4, u_5]$$

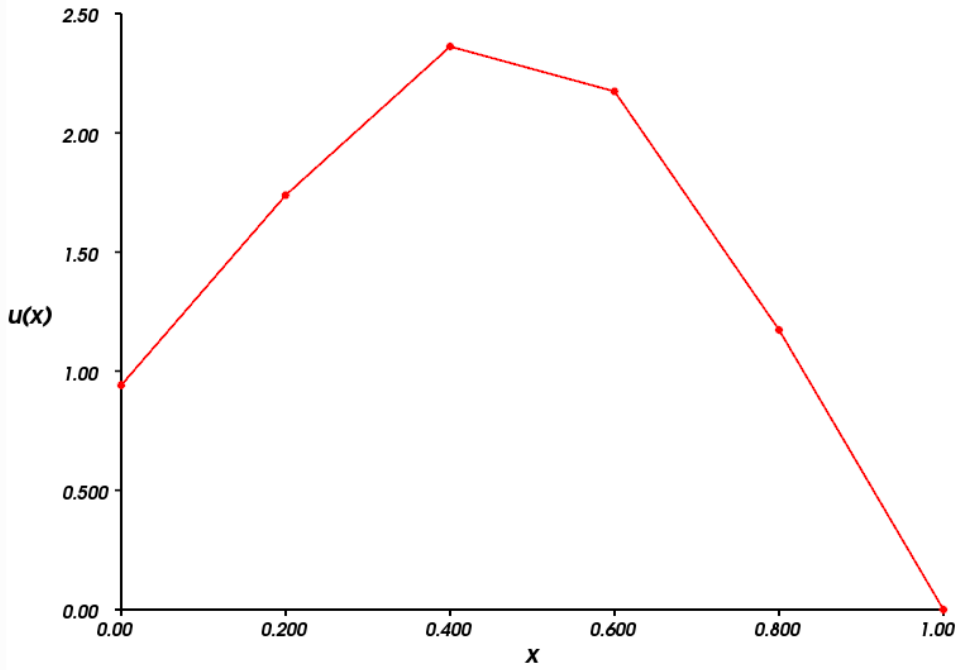
Evaluation is done by interpolation

```
>>> u = Function(V)
>>> u.vector().array()
[ 0.,  0.,  0.,  0.,  0.,  0.]
>>> u(0.1)
0.0
>>> u.vector()[0] = 1
>>> u(0.1)
0.49999999999999967
```

- U is called the vector of *expansion coefficients*

The solution of our problem is a discrete **Function**

Solution: $u(x)$




```
>>> plot(u)
>>> u.vector().array()
array([ 0.94,  1.74,  2.36,  2.17,  1.17,  0.  ])
```

The PDE can be re-written using the *discrete weak* formulation, which eventually will let us describe our problem as a *linear algebraic system*: $Ax = b$

Strong formulation

$$-u'' = f$$

- Should be true for every point (*strong*) in space

Discrete weak formulation

$$\begin{aligned} u(x) &= \sum_{j=0}^{5} u_j \phi_j(x) \\ -\int_0^1 u'' \phi_i dx &= \int_0^1 f \phi_i dx, \ i = 0, ..., 5 \end{aligned}$$

- By weighting the equation with ϕ_i and taking the integral over the whole domain, we solve an approximation of u (*weak*)

Before we simplify the *weak form*, we treat the *dirichlet* boundary condition: $u(1) = 0$

- The *dirichlet* boundary conditions at x=1, is treated by letting $\phi_i(1) = 0$ ($\Rightarrow \phi_5 = 0$)
- Then adding a function $g(x)$ to our *function space* which equals 0 at x=1

$$u(x) = \sum_{j=0}^{5} u_j \phi_j(x) + g(x)$$

```
>>> def right(x, on_boundary):
...     return x > 1-DOLFIN_EPS
...
>>> g = Constant(0)
>>> bc = DirichletBC(V, g, right)
```

To be able to use piecewise linear basis functions, we need to partial integrate the left hand side of the (discrete) weak form as, $\int_0^1 u''\phi_i dx = 0$

Integration by parts

$$-\int_0^1 u'v\,dx = \int_0^1 uv'\,dx - [uv]_0^1$$

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Integration by parts

$$
\begin{aligned}
-\int_0^1 u'v\,dx &= \int_0^1 uv'\,dx - [uv]_0^1 \\
-\int_0^1 u''\phi_i dx &= \int_0^1 u'\phi_i' dx + u'(0)\phi_i(0) - u'(1)\phi_i(1)
\end{aligned}
$$

- This includes the derivatives at the boundaries!

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Integration by parts

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\begin{aligned}
-\int_0^1 u' v \, dx &= \int_0^1 u v' \, dx - [uv]_0^1 \\
-\int_0^1 u'' \phi_i dx &= \int_0^1 u' \phi_i' dx + u'(0)\phi_i(0) - u'(1)\phi_i(1)
\end{aligned}
$$

- This includes the derivatives at the boundaries!
- Recall that our *boundary conditions* implies that $\phi_i(1) = 0$ and $u'(0) = 4$, which gives us:

$$\int_0^1 u' \phi_i' dx = \int_0^1 f \phi_i dx - 4\phi_i(1), \; i = 0, \ldots, 5$$

We are now ready to describe the *weak form* as a *linear algebraic system*: $Ax = b$

$$\text{LHS: } \int_0^1 u'\phi_i' dx = \int_0^1 \left(\sum_{j=0}^{5} u_j \phi_j \right)' \phi_i' dx$$

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$$\sum_{j=0}^{5} \left(\int_0^1 \phi_j' \phi_i' dx \right) u_j = \int_0^1 f \phi_i dx - 4\phi_i(0), \; i = 0, \ldots, 5$$

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$$Ax = b, \text{ where :}$$

$$A_{ij} = \int_0^1 \phi_j' \phi_i' dx, \, x_j = u_j \text{ and } b_i = \int_0^1 f \phi_i dx - 4\phi_i(0)$$

PyDOLFIN provides functionality to assemble the *matrix A* and the *vector b* (using numerical integration), and to solve the linear system

Recall that after integration by part we had:

$$\int_0^1 u' \phi_i' dx = \int_0^1 f \phi_i dx - 4\phi_i(0), \; i = 0, \ldots, 5$$

PyDOLFIN provides functionality to assemble the *matrix A* and the *vector b* (using numerical integration), and to solve the linear system

Recall that after integration by part we had:

$$\int_0^1 u'\phi_i' dx = \int_0^1 f\phi_i dx - 4\phi_i(0),\ i = 0, ..., 5$$

We use v instead of ϕ_i and we can write our problem as: find $u \in V$ such that

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

$$a(u,v) = \int_\Omega u'v'dx \quad \text{and} \quad L(v) = \int_\Omega f\,v\,dx - \int_{\partial\Omega} 4v\,ds$$

The *variational formulation*

UFL in **FEniCS** can be used to describe variational forms, and **PyDOLFIN** can be used to solve **VariationalProblems**

Mathematical notation:

find $u \in V$ such that

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

where:

$$a(u, v) = \int_\Omega u' v' dx$$

$$L(v) = \int_\Omega f\, v\, dx - \int_{\partial\Omega} 4v\, ds$$

PyDOLFIN notation:

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```
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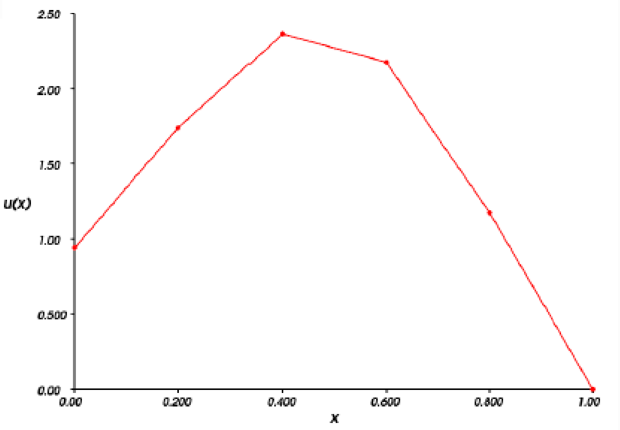
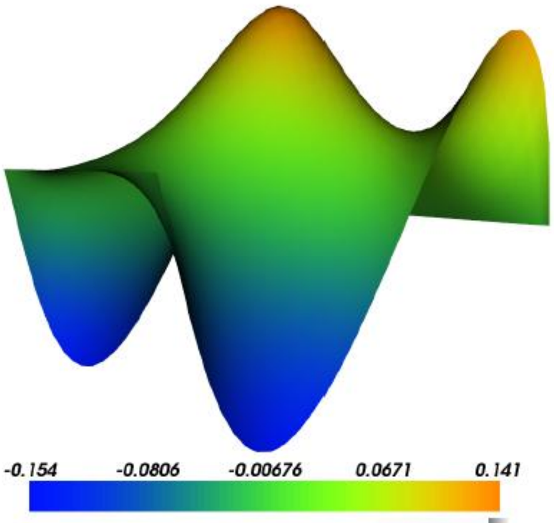


$$-\nabla^2 u = f; \ \frac{\partial u}{\partial n}(:, [0,1]) = g; \ u([0,1], :) = 0$$

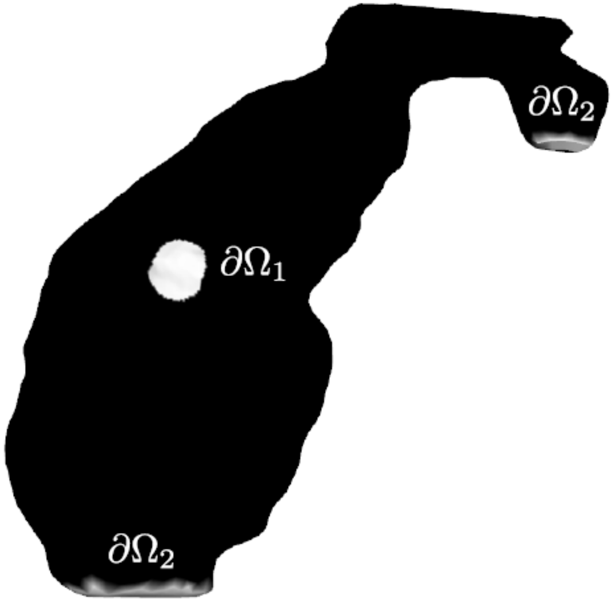
```
>>> from dolfin import *
>>>
>>> mesh = UnitSquare(32, 32)
>>> V = FunctionSpace(mesh, "CG", 1)
>>>
>>> def boundary(x):
...     return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EP
...
>>> u0 = Constant(0.0)
>>> bc = DirichletBC(V, u0, boundary)
>>>
>>> v = TestFunction(V)
>>> u = TrialFunction(V)
>>> f = Expression("10*exp(-(pow(x[0] - 0.5, 2) + pow(x[1] - 0.5, 2)) / 0.02)")
>>> g = Expression("-sin(5*x[0])")
>>> a = inner(grad(v), grad(u))*dx
>>> L = v*f*dx + v*g*ds
>>>
>>> problem = VariationalProblem(a, L, bc)
>>> u = problem.solve()
>>> plot(u, interactive=True)
```



Time dependent system, like the diffusion equation, can be solved using the same framework

PDE

$$
\begin{aligned}
\dot{u} &= D\nabla^2 u && \text{in } \Omega \\
D\frac{\partial u}{\partial n} &= J(t) && \text{on } \partial\Omega_1 \\
u &= 1 && \text{on } \partial\Omega_2 \\
u(0,:) &= 1 \\
J(t) &= \begin{cases} 100 & : t \leq J_{stop} \\ 0 & : t > J_{stop} \end{cases}
\end{aligned}
$$



Diffusion equation solved using **PyDOLFIN** (Domain declarations)

```
>>> from dolfin import *
>>>
>>> mesh = Mesh("single-TT.xml.gz")
>>> subdomains = MeshFunction("uint", mesh, 2)
>>> V = FunctionSpace(mesh, "CG", 1)
>>>
>>> tstop = 3.0; J_stop = 2.0; dt = 0.02; u0 = 1; J0 = 100; D = 100
>>>
>>> class Outflow(SubDomain):
...     def inside(self, x, on_boundary):
...         return (on_boundary and -110 < x[0] and x[0] < -50 and \
...                 70 < x[1] and x[1] < 130 and \
...                 22 < x[2] and x[2] < 82) or (5 < x[0] and x[0] < 75 and \
...                 -105 < x[1] and x[1] < -35 and \
...                 -210 < x[2] and x[2] < -140)
...
>>> class Inflow(SubDomain):
...     def inside(self, x, on_boundary):
...         return on_boundary and ((x[0]-65)**2+(x[1]+30)**2+x[2]**2 < 16**2)
...
>>> outflow = Outflow()
>>> inflow = Inflow()
>>>
>>> inflow.mark(subdomains, 2)
>>>
>>> out_values = Constant(1)
>>> bc = DirichletBC(V, out_values, outflow)
```

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Domain, Subdomains & Solution space

Diffusion equation solved using **PyDOLFIN** (Domain declarations)

Model parameters

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>>> class Outflow(SubDomain):
...     def inside(self, x, on_boundary):
...         return (on_boundary and -110 < x[0] and x[0] < -50 and \
...                 70 < x[1] and x[1] < 130 and \
...                 22 < x[2] and x[2] < 82) or (5 < x[0] and x[0] < 75 and \
...                 -105 < x[1] and x[1] < -35 and \
...                 -210 < x[2] and x[2] < -140)
...
>>> class Inflow(SubDomain):
...     def inside(self, x, on_boundary):
...         return on_boundary and ((x[0]-65)**2+(x[1]+30)**2+x[2]**2 < 16**2)
...
>>> outflow = Outflow()
>>> inflow = Inflow()
>>>
>>> inflow.mark(subdomains, 2)
>>>
>>> out_values = Constant(1)
>>> bc = DirichletBC(V, out_values, outflow)
```

Diffusion equation solved using **PyDOLFIN** (Domain declarations)

```
>>> from dolfin import *
>>>
>>> mesh = Mesh("single-TT.xml.gz")
>>> subdomains = MeshFunction("uint", mesh, 2)
>>> V = FunctionSpace(mesh, "CG", 1)
>>>
>>> tstop = 3.0; J_stop = 2.0; dt = 0.02; u0 = 1; J0 = 100; D = 100
>>>
>>> class Outflow(SubDomain):
...     def inside(self, x, on_boundary):
...         return (on_boundary and -110 < x[0] and x[0] < -50 and \
...                 70 < x[1] and x[1] < 130 and \
...                 22 < x[2] and x[2] < 82) or (5 < x[0] and x[0] < 75 and \
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>>> outflow = Outflow()
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>>>
>>> inflow.mark(subdomains, 2)
>>>
>>> out_values = Constant(1)
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```

Define boundaries

Diffusion equation solved using **PyDOLFIN** (linear algebra initialization)

```
>>> u = TrialFunction(V)
>>> v = TestFunction(V)
>>>
>>> K = assemble(inner(grad(u),grad(v))*dx)
>>> M = assemble(u*v*dx)
>>> source = assemble(v*ds(2), exterior_facet_domains=subdomains)
>>>
>>> u_n = Function(V)
>>>
>>> A = K.copy()
>>> b = Vector(A.size(1))
>>> b[:] = 0.0
>>> x = u_n.vector()
>>> x[:] = u0
```

Diffusion equation solved using **PyDOLFIN** (linear algebra initialization)

```
>>> u = TrialFunction(V)
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>>>
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>>> A = K.copy()
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>>> b[:] = 0.0
>>> x = u_n.vector()
>>> x[:] = u0
```

Basis functions

Diffusion equation solved using **PyDOLFIN** (linear algebra initialization)

Assemble tensors

```
>>> u = TrialFunction(V)
>>> v = TestFunction(V)
>>>
>>> K = assemble(inner(grad(u),grad(v))*dx)
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```

Diffusion equation solved using **PyDOLFIN** (linear algebra initialization)

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>>> u_n = Function(V)
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>>> b[:] = 0.0
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>>> x[:] = u0
```

Initialise linear algebra

The diffusion equation on *weak form*, using *backward Euler* for the time discretization

Strong form

$$\dot{u} = D\nabla^2 u \text{ in } \Omega; \qquad D\frac{\partial u}{\partial n} = J(t) \text{ on } \partial\Omega_1; \qquad u = 1 \text{ on } \partial\Omega_2$$

Weak form

$$\begin{aligned}
\int_\Omega \dot{u} v \, dx &= \int_\Omega D\nabla^2 u v \, dx \\
\int_\Omega \dot{u} v \, dx &= -D \int_\Omega \nabla u \nabla v \, dx + \int_{\partial\Omega_1} D\frac{\partial u}{\partial n} v \, ds \\
\int_\Omega \frac{u^n - u^{n-1}}{\Delta t} v \, dx &= -D \int_\Omega \nabla u^n \nabla v \, dx + \int_{\partial\Omega_1} J v \, ds \\
\int_\Omega u^n v + \Delta t D \nabla u^n \nabla v \, dx &= \int_\Omega u^{n-1} v \, dx + \Delta t J \int_{\partial\Omega_1} v \, ds
\end{aligned}$$

Instead of using the *variational form*, it is convenient to express the *weak form* on *matrix form*

Matrix form

$$(\mathbf{M} + \Delta t\, D\, \mathbf{K})\, U^n \quad = \quad \mathbf{M}\, U^{n-1} + \Delta t\, J(t)\, source$$

where U^n is the vector of *expansion coefficients* and

$$\left.\begin{aligned} M_{ij} &= \int_\Omega \phi_i \phi_j dx \\ K_{ij} &= \int_\Omega \nabla\phi_i \nabla\phi_j dx; \\ source_i &= \int_{\partial\Omega_1} \phi_i ds \end{aligned}\right\} \text{ for all } \phi_i \text{ and } \phi_j \text{ in } V$$

Assemble of tensors in **PyDOLFIN**

```
>>> K = assemble(inner(grad(u),grad(v))*dx)
>>> M = assemble(u*v*dx)
>>> source = assemble(v*ds(2), exterior_facet_domains=subdomains)
```

Each time step we need to solve a *linear system*

Weak form on *Matrix form*

$$(\mathbf{M} + \Delta t\, D\, \mathbf{K})\, U^n \quad = \quad \mathbf{M}\, U^{n-1} + \Delta t\, J(t)\, source$$

Each time step we need to solve a *linear system*

Weak form on *Matrix form*

$$(\mathbf{M} + \Delta t\, D\, \mathbf{K})\, U^n \quad = \quad \mathbf{M}\, U^{n-1} + \Delta t\, J(t)\, source$$

Time stepping in **PyDOLFIN**

```
>>> t = 0.0
>>> plot(u_n, vmin=1, vmax=5, rescale=False)
>>> while t < tstop:
...     t += float(dt)
...
...     A.assign(K)
...     A *= D*dt
...     A += M
...
...     b[:] = 0.0
...     if t <= J_stop:
...         b[:] = source
...         b *= dt*J0
...
...     b+= M*x
...
...     bc.apply(A, b)
...
...     solve(A, x, b)
...     plot(u_n)
```

```
>>> tstop = 3.0; J_stop = 2.0; dt = 0.02; u0 = 1; J0 = 100; D = 100
```