

Hans Petter Langtangen*, Anders Logg†

The FEniCS Tutorial – Writing State-of-the-Art Finite Element Solvers in Minutes

Apr 19, 2016

Springer

Email: hpl@simula.no. Center for Biomedical Computing, Simula Research Laboratory and Department of Informatics, University of Oslo.

†Email: logg@chalmers.se. Department of Mathematics, Chalmers University of Technology and Center for Biomedical Computing, Simula Research Laboratory.

Contents

Preface	1
1 Preliminaries	3
1.1 The FEniCS Project	3
1.2 What you will learn	4
1.3 Working with this tutorial	4
1.4 Obtaining the software	5
1.4.1 Installation using Docker containers	5
1.4.2 Installation using Ubuntu packages	6
1.4.3 Testing your installation	7
1.5 Obtaining the tutorial examples	7
1.6 Background knowledge	8
1.6.1 Programming in Python	8
1.6.2 The finite element method	8
2 Fundamentals: Solving the Poisson equation	11
2.1 Mathematical problem formulation	11
2.1.1 Finite element variational formulation	12
2.1.2 Abstract finite element variational formulation	14
2.1.3 Choosing a test problem	15
2.1.4 FEniCS implementation	16
2.1.5 Running the program	17
2.1.6 Dissection of the program	19
2.1.7 Degrees of freedom and vertex values	26
2.2 Deflection of a membrane	27
2.2.1 Scaling	27
2.2.2 Defining the mesh	28
2.2.3 Defining the load	28
2.2.4 Variational form	29
2.2.5 Visualization	29
2.2.6 Curve plots through the domain	30

2.2.7	Running ParaView	31
2.2.8	Using the built-in visualization tool	33
3	A Gallery of finite element solvers	35
3.1	The time-dependent diffusion equation	35
3.1.1	Variational formulation	35
3.1.2	A simple implementation	38
3.1.3	Diffusion of a Gaussian function	41
3.2	A nonlinear Poisson equation	43
3.2.1	Variational formulation	43
3.2.2	A simple implementation	44
3.3	The equations of linear elasticity	47
3.3.1	Variational formulation	47
3.3.2	A simple implementation	49
3.4	The Navier–Stokes equations	51
3.4.1	Variational formulation	51
3.4.2	A simple implementation	51
4	Mesh generation, subdomains and boundary conditions	53
4.1	Physical problem formulation	53
4.2	Mathematical problem formulation	54
4.3	Scaling the equation	54
4.4	Finite element variational formulation	56
4.5	Mesh generation	56
4.6	Subdomain markers	56
4.7	The complete program	56
5	Python programming and PDE solver design	59
5.1	Refactored implementation	59
5.1.1	A general solver function	59
5.1.2	Verification and unit tests	61
5.2	Useful extensions	63
5.2.1	Controlling the solution process	63
5.2.2	Linear solvers and preconditioners	68
5.2.3	Linear variational problem and solver objects	69
5.2.4	Writing out the discrete solution	69
5.2.5	Parameterizing the number of space dimensions	73
5.2.6	Computing derivatives	74
5.2.7	A variable-coefficient Poisson problem	78
5.2.8	Creating the linear system explicitly	95
5.2.9	Taking advantage of structured mesh data	98
5.3	Postprocessing computations	104
5.3.1	Computing functionals	104
5.3.2	Computing convergence rates	105
5.4	Multiple domains and boundaries	111

Contents	vii
5.4.1 Combining Dirichlet and Neumann conditions	111
5.4.2 Multiple Dirichlet conditions	114
5.4.3 Working with subdomains	115
5.4.4 Multiple Neumann, Robin, and Dirichlet condition	120
5.4.5 Refactoring of a solver function into solver and problem classes	129
References	137
Index	139

Preface

This book gives a concise and gentle introduction to finite element programming in Python based on the popular FEniCS software library. FEniCS can be programmed in both C++ and Python, but this tutorial focuses exclusively on Python programming, since this is the simplest and most effective approach for beginners. It will also deliver high performance since FEniCS automatically delegates compute-intensive tasks to C++ by help of code generation. After having digested the examples in this tutorial, the reader should be able to learn more from the FEniCS documentation, the numerous demo programs that come with the software, and the comprehensive FEniCS book *Automated Solution of Differential Equations by the Finite element Method* [21]. This tutorial is a further development of the opening chapter in [21].

We thank Johan Hake, Kent-Andre Mardal, and Kristian Valen-Sendstad for many helpful discussions during the preparation of the first version of this tutorial for the FEniCS book [21]. We are particularly thankful to Professor Douglas Arnold for very valuable feedback on early versions of the text. Øystein Sørensen pointed out a lot of typos and contributed with many helpful comments. Many errors and typos were also reported by Mauricio Angeles, Ida Drøsdal, Miroslav Kuchta, Hans Ekkehard Plessner, Marie Rognes, and Hans Joachim Scroll. Ekkehard Ellmann as well as two anonymous reviewers provided a series of suggestions and improvements.

Oslo, May 2016

Hans Petter Langtangen, Anders Logg

Watch out for shortcomings!

This book is still in an initial state so the reader is encouraged to send email to the authors on `logg@chalmers.se`^a about typos, errors, and suggestions for improvements.

^a<mailto:logg@chalmers.se>

Chapter 1

Preliminaries

1.1 The FEniCS Project

The FEniCS Project is a research and software project aiming at creating mathematical methods and software for automated computational mathematical modeling. This means creating easy, intuitive, efficient and flexible software for solving partial differential equations (PDEs) using finite element methods. FEniCS was initially created in 2003 and is developed in collaboration between researchers from a number of universities and research institutes around the world. For more information about FEniCS and the latest updates of the FEniCS software and this tutorial, visit the FEniCS web page at <http://fenicsproject.org>.

FEniCS consists of a number of building blocks (software components) that together form the FEniCS software: DOLFIN, FFC, FIAT, UFL, and a few others. FEniCS users rarely need to think about this internal organization of FEniCS, but since even casual users may sometimes encounter the names of various FEniCS components, we briefly list the components and their main roles in FEniCS. DOLFIN is the computational high-performance C++ backend of FEniCS. DOLFIN implements data structures such as meshes, function spaces and functions, compute-intensive algorithms such as finite element assembly and mesh refinement, and interfaces to linear algebra solvers and data structures such as PETSc. DOLFIN also implements the FEniCS problem-solving environment in both C++ and Python. FFC is the code generation engine of FEniCS (the form compiler), responsible for generating efficient C++ from high-level mathematical abstractions. FIAT is the finite element backend of FEniCS, responsible for generating finite element basis functions, and UFL implements the abstract mathematical language by which users may express variational problems.

1.2 What you will learn

The goal of this tutorial is introduce the concept of programming finite element solvers for PDEs and get you started with FEniCS through a series of simple examples that demonstrate

- how to define a PDE problem as a finite element variational problem,
- how to create (mesh) simple domains,
- how to deal with Dirichlet, Neumann, and Robin conditions,
- how to deal with variable coefficients,
- how to deal with domains built of several materials (subdomains),
- how to compute derived quantities like the flux vector field or a functional of the solution,
- how to quickly visualize the mesh, the solution, the flux, etc.,
- how to solve nonlinear PDEs,
- how to solve time-dependent PDEs,
- how to set parameters governing solution methods for linear systems,
- how to create domains of more complex shape.

1.3 Working with this tutorial

The mathematics of the illustrations is kept simple to better focus on FEniCS functionality and syntax. This means that we mostly use the Poisson equation and the time-dependent diffusion equation as model problems, often with input data adjusted such that we get a very simple solution that can be exactly reproduced by any standard finite element method over a uniform, structured mesh. This latter property greatly simplifies the verification of the implementations. Occasionally we insert a physically more relevant example to remind the reader that the step from solving a simple model problem to a challenging real-world problem is often quite easy with FEniCS.

Using FEniCS to solve PDEs may seem to require a thorough understanding of the abstract mathematical framework of the finite element method as well as expertise in Python programming. Nevertheless, it turns out that many users are able to pick up the fundamentals of finite elements *and* Python programming as they go along with this tutorial. Simply keep on reading and try out the examples. You will be amazed of how easy it is to solve PDEs with FEniCS!

1.4 Obtaining the software

Reading this tutorial obviously requires access to FEniCS. FEniCS is a complex software library, both in itself and due to its many dependencies to state-of-the-art open-source scientific software libraries. Manually building FEniCS and all its dependencies from source can thus be a daunting task. Even for an expert who knows exactly how to configure and build each component, a full build can literally take hours! In addition to the complexity of the software itself, there is an additional layer of complexity in how many different kinds of operating systems (GNU/Linux, Mac OS X, Windows) that may be running on a user’s laptop or compute server, with different requirements for how to configure and build software.

For this reason, the FEniCS Project provides prebuilt packages to make the installation easy, fast and foolproof.

FEniCS download and installation

In this tutorial, we highlight the two main options for installing the FEniCS software: Docker containers and Ubuntu packages. While the Docker containers work on all operating systems, the Ubuntu packages only work on Ubuntu-based systems. For more installation options, such as building FEniCS from source, check out the official FEniCS installation instructions at <http://fenicsproject.org/download>.

1.4.1 Installation using Docker containers

A modern solution to the challenge of software installation on diverse software platforms is to use so-called *containers*. The FEniCS Project provides custom-made containers that are controlled, consistent and high-performance software environments for FEniCS programming. FEniCS containers work equally well¹ on all operating systems, including Linux, Mac and Windows.

To use FEniCS containers, you must first install the Docker platform. Docker installation is simple, just follow the instructions from the Docker web page². Once you have installed Docker, just copy the following line into a terminal window:

¹Running Docker containers on Mac and Windows involves a small performance overhead compared to running Docker containers on Linux. However, this performance penalty is typically small and is often compensated for by using the highly tuned and optimized version of FEniCS that comes with the official FEniCS containers, compared to building FEniCS and its dependencies from source on Mac or Windows.

²<https://www.docker.com>

Terminal

```
Terminal> curl -s http://get.fenicsproject.org | sh
```

Mac and Windows users should make sure to run this command inside the Docker Quickstart Terminal!

The command above will install the program `fenicsproject` on your system. This command lets you easily create FEniCS sessions (containers) on your system:

Terminal

```
Terminal> fenicsproject run
```

This command has several useful options, such as easily switching between the latest release of FEniCS, the latest development version and many more. To learn more, type `fenicsproject help`.

Sharing files with FEniCS containers

When you run a FEniCS session using `fenicsproject run`, it will automatically share your current working directory (the directory from which you run the `fenicsproject` command) with the FEniCS session. When the FEniCS session starts, it will automatically enter into a directory named `shared` which will be identical with your current working directory on your host system. This means that you can easily edit files and write data inside the FEniCS session, and the files will be directly accessible on your host system. It is recommended that you edit your programs using your favorite editor (such as Emacs or Vim) on your host system and use the FEniCS session only to run your program(s).

1.4.2 Installation using Ubuntu packages

For users of Ubuntu GNU/Linux, FEniCS can also be installed easily via the standard Ubuntu package manager `apt-get`. Just copy the following lines into a terminal window:

Terminal

```
Terminal> sudo add-apt-repository ppa:fenics-packages/fenics
Terminal> sudo apt-get update
Terminal> sudo apt-get install fenics
Terminal> sudo apt-get dist-upgrade
```

This will add the FEniCS package archive (PPA) to your Ubuntu computer’s list of software sources and then install FEniCS. This step will also automatically install packages for dependencies of FEniCS.

Watch out for old packages!

In addition to being available from the FEniCS PPA, the FEniCS software is also part of the official Ubuntu repositories. However, depending on which release of Ubuntu you are running, and when this release was created in relation to the latest FEniCS release, the official Ubuntu repositories might contain an outdated version of FEniCS. For this reason, it is better to install from the FEniCS PPA.

1.4.3 Testing your installation

Once you have installed FEniCS, you should make a quick test to see that your installation works properly. To do this, type the following command in a FEniCS-enabled³ terminal:

```
Terminal> python -c 'import fenics'
```

If all goes well, you should be able to run this command without any error message (or any other output).

1.5 Obtaining the tutorial examples

In this tutorial, you will learn finite element and FEniCS programming through a number of example programs that demonstrate both how to solve particular PDEs using the finite element method, how to program solvers in FEniCS, and how to create well-designed Python codes that can later be extended to solve more complex problems. All example programs are available from the web page of this book at <http://fenicsproject.org/tutorial>. The programs as well as the source code for this text can also be accessed directly from the Git repository⁴ for this book.

³For users of FEniCS containers, this means first running the command `fenicsproject run`.

⁴<https://github.com/hplgit/fenics-tutorial/>

1.6 Background knowledge

1.6.1 Programming in Python

While you can likely pick up basic Python programming by working through the examples in this tutorial, you may want to have some additional material on the language. A natural starting point for beginners is the classical *Python Tutorial* [10], or a tutorial geared towards scientific computing [18]. In the latter, you will also find lots of pointers to other tutorials for scientific computing in Python. Among ordinary books we recommend the general introduction *Dive into Python* [22] as well as texts that focus on scientific computing with Python [13–17].

Python versions

Python comes in two versions, 2 and 3, and these are not compatible. FEniCS has a code base that runs under both versions. All the programs in this tutorial are also developed such that they can be run under both Python 2 and 3. Programs that need to print must then start with

```
from __future__ import print_function
```

to enable the `print` function from Python 3 in Python 2. All use of `print` in the programs in this tutorial consists of function calls, like `print('a:', a)`. Almost all other constructions are of a form that looks the same in Python 2 and 3.

To start a FEniCS Python 3 session, users of FEniCS containers should run the command `fenicsproject run stable-py3`.

1.6.2 The finite element method

There are a large number of books on the finite element method. The books typically fall in either of two categories: the abstract mathematical version of the method and the engineering “structural analysis” formulation. FEniCS builds heavily on concepts from the abstract mathematical exposition. The first author has in development a book⁵ that explains all details of the finite element method in an intuitive way, though with the abstract mathematical formulations that FEniCS employ.

The finite element text by Larson and Bengzon [20] is our recommended introduction to the finite element method, with a mathematical notation

⁵<http://hplgit.github.io/fem-book/doc/web/index.html>

that goes well with FEniCS. An easy-to-read book, which also provides a good general background for using FEniCS, is Gockenbach [11]. The book by Donea and Huerta [7] has a similar style, but aims at readers with interest in fluid flow problems. Hughes [12] is also recommended, especially for those interested in solid mechanics and heat transfer applications.

Readers with a background in the engineering “structural analysis” version of the finite element method may find Bickford [3] as an attractive bridge over to the abstract mathematical formulation that FEniCS builds upon. Those who have a weak background in differential equations in general should consult a more fundamental book, and Eriksson *et al* [8] is a very good choice. On the other hand, FEniCS users with a strong background in mathematics and interest in the mathematical properties of the finite element method, will appreciate the texts by Brenner and Scott [5], Braess [4], Ern and Guermond [9], Quarteroni and Valli [23], or Ciarlet [6].

Chapter 2

Fundamentals: Solving the Poisson equation

The goal of this chapter is to show how the Poisson equation, the most basic of all PDEs, can be quickly solved with a few lines of FEniCS code. We introduce the most fundamental FEniCS objects such as `Mesh`, `Function`, `FunctionSpace`, `TrialFunction`, and `TestFunction`, and learn how to write a basic PDE solver, including the specification of the mathematical variational problem, applying boundary conditions, calling the FEniCS solver, and plotting the solution.

2.1 Mathematical problem formulation

Let us start by writing a “Hello, World!” program. In the world of PDEs, this must be a program that solves the Poisson equation:

$$-\nabla^2 u(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \text{ in } \Omega, \tag{2.1}$$

$$u(\mathbf{x}) = u_0(\mathbf{x}), \quad \mathbf{x} \text{ on } \partial\Omega. \tag{2.2}$$

Here, $u = u(\mathbf{x})$ is the unknown function, $f = f(\mathbf{x})$ is a prescribed function, ∇^2 is the Laplace operator (also often written as Δ), Ω is the spatial domain, and $\partial\Omega$ is the boundary of Ω . A stationary PDE like this, together with a complete set of boundary conditions, constitute a *boundary-value problem*, which must be precisely stated before it makes sense to start solving it with FEniCS.

In two space dimensions with coordinates x and y , we can write out the Poisson equation as

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f(x, y). \tag{2.3}$$

The unknown u is now a function of two variables, $u = u(x, y)$, defined over a two-dimensional domain Ω .

The Poisson equation arises in numerous physical contexts, including heat conduction, electrostatics, diffusion of substances, twisting of elastic rods, inviscid fluid flow, and water waves. Moreover, the equation appears in numerical splitting strategies of more complicated systems of PDEs, in particular the Navier–Stokes equations.

Solving a PDE such as the Poisson equation in FEniCS consists of the following steps:

1. Identify the computational domain (Ω), the PDE, its boundary conditions, and source terms (f).
2. Reformulate the PDE as a finite element variational problem.
3. Write a Python program which defines the computational domain, the variational problem, the boundary conditions, and source terms, using the corresponding FEniCS abstractions.
4. Call FEniCS to solve the PDE and, optionally, extend the program to compute derived quantities such as fluxes and averages, and visualize the results.

We shall now go through steps 2–4 in detail. The key feature of FEniCS is that steps 3 and 4 result in fairly short code, while most other software frameworks for PDEs require much more code and more technically difficult programming.

2.1.1 Finite element variational formulation

FEniCS is based on the finite element method, which is a general and efficient mathematical machinery for numerical solution of PDEs. The starting point for the finite element methods is a PDE expressed in *variational form*. Readers who are not familiar with variational problems will get a brief introduction to the topic in this tutorial, but getting and reading a proper book on the finite element method in addition is encouraged. Section 1.6.2 contains a list of some suitable books.

The basic recipe for turning a PDE into a variational problem is to multiply the PDE by a function v , integrate the resulting equation over the domain Ω , and perform integration by parts of terms with second-order derivatives. The function v which multiplies the PDE is called a *test function*. The unknown function u to be approximated is referred to as a *trial function*. The terms test and trial function are used in FEniCS programs too. Suitable function spaces must be specified for the test and trial functions. For standard PDEs arising in physics and mechanics such spaces are well known.

In the present case, we first multiply the Poisson equation by the test function v and integrate over Ω :

$$-\int_{\Omega} (\nabla^2 u)v \, dx = \int_{\Omega} fv \, dx. \quad (2.4)$$

We then apply integration by parts to the integrand with second-order derivatives. We find that

$$-\int_{\Omega} (\nabla^2 u)v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} \frac{\partial u}{\partial n} v \, ds, \quad (2.5)$$

where $\frac{\partial u}{\partial n} = \nabla u \cdot n$ is the derivative of u in the outward normal direction n on the boundary. The test function v is required to vanish on the parts of the boundary where the solution u is known, which in the present problem implies that $v = 0$ on the whole boundary $\partial\Omega$. The second term on the right-hand side of (2.5) therefore vanishes. From (2.4) and (2.5) it follows that

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} fv \, dx. \quad (2.6)$$

If we require that this equation holds for all test functions v in some suitable space \hat{V} , the so-called *test space*, we obtain a well-defined mathematical problem that uniquely determines the solution u which lies in some (possibly different) function space V , the so-called *trial space*. We refer to (2.6) as the *weak form* or *variational form* of the original boundary-value problem (2.1)–(2.2).

The proper statement of our variational problem now goes as follows: Find $u \in V$ such that

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} fv \, dx \quad \forall v \in \hat{V}. \quad (2.7)$$

The trial and test spaces V and \hat{V} are in the present problem defined as

$$\begin{aligned} V &= \{v \in H^1(\Omega) : v = u_0 \text{ on } \partial\Omega\}, \\ \hat{V} &= \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}. \end{aligned}$$

In short, $H^1(\Omega)$ is the mathematically well-known Sobolev space containing functions v such that v^2 and $|\nabla v|^2$ have finite integrals over Ω (essentially meaning that the functions are continuous). The solution of the underlying PDE must lie in a function space where also the derivatives are continuous, but the Sobolev space $H^1(\Omega)$ allows functions with discontinuous derivatives. This weaker continuity requirement of u in the variational statement (2.7), as a result of the integration by parts, has great practical consequences when it comes to constructing finite element function spaces. In particular, it allows the use of piecewise polynomial function spaces; i.e., function spaces constructed by stitching together polynomial functions on simple domains such as intervals, triangles, or tetrahedrons.

The variational problem (2.7) is a *continuous problem*: it defines the solution u in the infinite-dimensional function space V . The finite element method for the Poisson equation finds an approximate solution of the variational problem (2.7) by replacing the infinite-dimensional function spaces V and \hat{V} by *discrete* (finite-dimensional) trial and test spaces $V_h \subset V$ and $\hat{V}_h \subset \hat{V}$. The discrete variational problem reads: Find $u_h \in V_h \subset V$ such that

$$\int_{\Omega} \nabla u_h \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in \hat{V}_h \subset \hat{V}. \quad (2.8)$$

This variational problem, together with a suitable definition of the function spaces V_h and \hat{V}_h , uniquely defines our approximate numerical solution of Poisson's equation (2.1). The mathematical framework may seem complicated at first glance, but the good news is the finite element variational problem (2.8) looks the same as the continuous variational problem (2.7), and FEniCS can automatically solve variational problems like (2.8)!

What we mean by the notation u and V

The mathematics literature on variational problems writes u_h for the solution of the discrete problem and u for the solution of the continuous problem. To obtain (almost) a one-to-one relationship between the mathematical formulation of a problem and the corresponding FEniCS program, we shall drop the subscript $_h$ and use u for the solution of the discrete problem and u_e for the exact solution of the continuous problem, *if* we need to explicitly distinguish between the two. Similarly, we will let V denote the discrete finite element function space in which we seek our solution.

2.1.2 Abstract finite element variational formulation

It turns out to be convenient to introduce the following canonical notation for variational problems:

$$a(u, v) = L(v). \quad (2.9)$$

For the Poisson equation, we have:

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (2.10)$$

$$L(v) = \int_{\Omega} f v \, dx. \quad (2.11)$$

From the mathematics literature, $a(u, v)$ is known as a *bilinear form* and $L(v)$ as a *linear form*. We shall in every linear problem we solve identify the terms with the unknown u and collect them in $a(u, v)$, and similarly collect all terms with only known functions in $L(v)$. The formulas for a and L are then coded directly in the program.

FEniCS provides all the necessary mathematical notation needed to express the variational problem $a(u, v) = L(v)$. To solve a linear PDE in FEniCS, such as the Poisson equation, a user thus needs to perform only two steps:

- Express the PDE as a (discrete) variational problem: find $u \in V$ such that $a(u, v) = L(v)$ for all $v \in \hat{V}$.
- Choose the finite element spaces V and \hat{V} by specifying the domain (the mesh) and the type of function space (polynomial degree and type).

2.1.3 Choosing a test problem

The Poisson equation (2.1) has so far featured a general domain Ω and general functions u_0 and f . For our first implementation, we must decide on specific choices of Ω , u_0 , and f . It will be wise to construct a specific problem where we can easily check that the computed solution is correct. Solutions that are lower-order polynomials are primary candidates. Standard finite element function spaces of degree r will exactly reproduce polynomials of degree r . And piecewise linear elements ($r = 1$) are able to exactly reproduce a quadratic polynomial on a uniformly partitioned mesh. This important result can be used to verify our implementation. We just manufacture some quadratic function in 2D as the exact solution, say

$$u_e(x, y) = 1 + x^2 + 2y^2. \quad (2.12)$$

By inserting (2.12) into the Poisson equation (2.1), we find that $u_e(x, y)$ is a solution if

$$f(x, y) = -6, \quad u_0(x, y) = u_e(x, y) = 1 + x^2 + 2y^2,$$

regardless of the shape of the domain as long as u_e is prescribed along the boundary. We choose here, for simplicity, the domain to be the unit square,

$$\Omega = [0, 1] \times [0, 1].$$

This simple but very powerful method for constructing test problems is called the *method of manufactured solutions*: pick a simple expression for the exact solution, plug it into the equation to obtain the right-hand side (source term f), then solve the equation with this right-hand side and try to reproduce the exact solution.

Tip: Try to verify your code with exact numerical solutions!

A common approach to testing the implementation of a numerical method is to compare the numerical solution with an exact analytical solution of the test problem and conclude that the program works if the error is “small enough”. Unfortunately, it is impossible to tell if an error of size 10^{-5} on a 20×20 mesh of linear elements is the expected (in)accuracy of the numerical approximation or if the error also contains the effect of a bug in the code. All we usually know about the numerical error is its *asymptotic properties*, for instance that it is proportional to h^2 if h is the size of a cell in the mesh. Then we can compare the error on meshes with different h values to see if the asymptotic behavior is correct. This is a very powerful verification technique and is explained in detail in Section 5.3.2. However, if we have a test problem for which we know that there should be no approximation errors, we know that the analytical solution of the PDE problem should be reproduced to machine precision by the program. That is why we emphasize this kind of test problems throughout this tutorial. Typically, elements of degree r can reproduce polynomials of degree r exactly, so this is the starting point for constructing a solution without numerical approximation errors.

2.1.4 FEniCS implementation

A FEniCS program for solving our test problem for the Poisson equation in 2D with the given choices of u_0 , f , and Ω may look as follows:

```
from fenics import *

# Create mesh and define function space
mesh = UnitSquareMesh(8, 8)
V = FunctionSpace(mesh, 'P', 1)

# Define boundary conditions
u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]', degree=2)

def u0_boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, u0_boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Constant(-6.0)
```

```

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

# Compute solution
u = Function(V)
solve(a == L, u, bc)

# Plot solution on the screen
u.rename('u', 'solution')
plot(u)
plot(mesh)

# Dump solution to file in VTK format
vtkfile = File('poisson.pvd')
vtkfile << u

# Compute error in L2 norm
error_L2norm = errornorm(u0, u, 'L2')

# Compute maximum error at vertices
vertex_values_u0 = u0.compute_vertex_values(mesh)
vertex_values_u = u.compute_vertex_values(mesh)
import numpy as np
error_vertices = np.max(np.abs(vertex_values_u0 - vertex_values_u))

# Print errors
print('error_L2norm = ', error_L2norm)
print('error_vertices = ', error_vertices)

# Hold plot
interactive()

```

The complete code can be found in the file `ft01_poisson_flat.py`.

2.1.5 Running the program

The FEniCS program must be available in a plain text file, written with a text editor such as Atom, Sublime Text, Emacs, Vim, or similar.

There are several ways to run a Python program like `ft01_poisson_flat.py`:

- Use a terminal window
- Use an intergrated development environment (IDE), e.g., Spyder
- Use a Jupyter notebook

Terminal window. Open a terminal window, move to the directory containing the program and type the following command:

	Terminal	
--	----------	--

Terminal> `python ft01_poisson_flat.py`

Note that this command must be run in a FEniCS-enabled terminal. For users of the FEniCS Docker containers, this means that you must type this command after you have started a FEniCS session using `fenicsproject run`.

When running the above command, FEniCS will run the program to compute the approximate solution u . The approximate solution u will be compared to the exact solution u_e and the error in the maximum norm will be printed. Since we know that our approximate solution should reproduce the exact solution to within machine precision, this error should be small, something on the order of 10^{-15} .

AL 1: Add text here discussing what to expect in terms of plotting.
Perhaps we have seamless notebook plotting working soon...

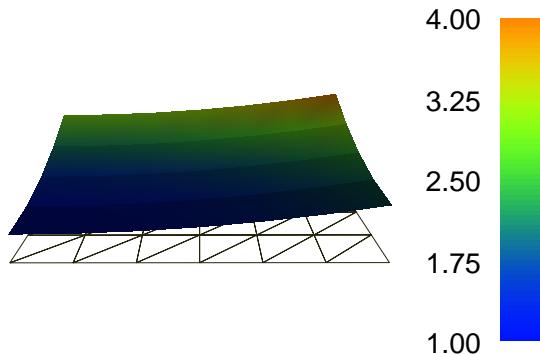


Fig. 2.1 Plot of the solution in the first FEniCS example.

Spyder. Many prefer to work in an integrated development environment where there is an editor for programming, a window for executing code, a window for inspecting objects, etc. The Spyder tool comes with all major Python installations. Just open the file `ft01_poisson_flat.py` and press the play button to run it. We refer to the Spyder tutorial to learn more about working in the Spyder environment. Spyder is highly recommended if you are used to working in the *graphical* MATLAB environment.

Jupyter notebooks. Notebooks make it possible to mix text and executable code in the same document, but you can also just use it to run programs in a web browser. Start `jupyter notebook` from a terminal window, find the **New** pulldown menu in the upper right part of the GUI, choose a new notebook in Python 2 or 3, write `%load ft01_poisson_flat.py` in the blank cell of this notebook, then write Shift+Enter to execute the cell. The file

`ft01_poisson_flat.py` will be loaded into the notebook. Re-execute the cell (Shift+Enter) to run the program. You may divide the entire program into several cells to examine intermediate results: place the cursor where you want to split the cell and choose **Edit - Split Cell**.

hpl 2: Need to describe this with more care. The first program seems to have some problems with printing the error to the notebook unless we drop the plot commands. Anyway, there should be in-browser plot commands.

2.1.6 Dissection of the program

We shall now dissect this FEniCS program in detail. The program is written in the Python programming language. You may either take a quick look at the official Python tutorial¹ to pick up the basics of Python if you are unfamiliar with the language, or you may learn enough Python as you go along with the examples in the present tutorial. The latter strategy has proven to work for many newcomers to FEniCS. This is because both the amount of abstract mathematical formalism and the amount of Python expertise that is actually needed to be productive with FEniCS is quite limited. And Python is an easy-to-learn language that you will certainly come to love and use far beyond FEniCS programming. Section 1.6.1 lists some relevant Python books.

The listed FEniCS program defines a finite element mesh, a finite element function space V on this mesh, boundary conditions for u (the function u_0), and the bilinear and linear forms $a(u, v)$ and $L(v)$. Thereafter, the unknown trial function u is computed. Then we can compare the numerical and exact solution as well as visualize the computed solution u .

The important first line. The first line in the program,

```
from fenics import *
```

imports the key classes `UnitSquareMesh`, `FunctionSpace`, `Function`, and so forth, from the FEniCS library. All FEniCS programs for solving PDEs by the finite element method normally start with this line.

Generating simple meshes. The statement

```
mesh = UnitSquareMesh(8, 8)
```

defines a uniform finite element mesh over the unit square $[0, 1] \times [0, 1]$. The mesh consists of *cells*, which in 2D are triangles with straight sides. The parameters 8 and 8 specify that the square should be divided into 8×8 rectangles, each divided into a pair of triangles. The total number of triangles (cells) thus becomes 128. The total number of vertices in the mesh is $9 \cdot 9 = 81$. In later chapters, you will learn how to generate more complex meshes.

¹<http://docs.python.org/tutorial/>

hpl 3: Note that plot was made by the old partitioning 6×4 . Probably no issue.

Defining the finite element function space. Having a mesh, we can define a finite element function space V over this mesh:

```
V = FunctionSpace(mesh, 'P', 1)
```

The second argument '`P`' specifies the type of element, while the third argument is the degree of the basis functions of the element. The type of element is here "`P`", implying the standard Lagrange family of elements. You may also use '`Lagrange`' to specify this type of element. FEniCS supports all simplex element families and the notation defined in the Periodic Table of the Finite Elements² [2].

The third argument 1 specifies the degree of the finite element. In this case, the standard P_1 linear Lagrange element, which is a triangle with nodes at the three vertices. Some finite element practitioners refer to this element as the "linear triangle". The computed solution u will be continuous and linearly varying in x and y over each cell in the mesh. Higher-degree polynomial approximations over each cell are trivially obtained by increasing the third parameter to `FunctionSpace`, which will then generate function spaces of type P_2 , P_3 , and so forth. Changing the second parameter to '`DP`' creates a function space for discontinuous Galerkin methods.

Defining the trial and test functions. In mathematics, we distinguish between the trial and test spaces V and \hat{V} . The only difference in the present problem is the boundary conditions. In FEniCS we do not specify the boundary conditions as part of the function space, so it is sufficient to work with one common space V for the trial and test functions in the program:

```
u = TrialFunction(V)
v = TestFunction(V)
```

Defining the boundary and the boundary conditions. The next step is to specify the boundary condition: $u = u_0$ on $\partial\Omega$. This is done by

```
bc = DirichletBC(V, u0, u0_boundary)
```

where u_0 is an expression defining the solution values on the boundary, and $u0_boundary$ is a function (or object) defining which points belong to the boundary.

Boundary conditions of the type $u = u_0$ are known as *Dirichlet conditions*. For the present finite element method for the Poisson problem, they are also called *essential boundary conditions*, as they need to be imposed explicitly as part of the trial space (in contrast to being defined implicitly as part of the variational formulation). Naturally, the FEniCS class used to define Dirichlet boundary conditions is named `DirichletBC`.

²<http://femtable.org>

The variable `u0` refers to an `Expression` object, which is used to represent a mathematical function. The typical construction is

```
u0 = Expression(formula, degree=1)
```

where `formula` is a string containing the mathematical expression. This formula is written with C++ syntax. The expression is automatically turned into an efficient, compiled C++ function. The second argument `degree` is a parameter that specifies how the expression should be treated in computations. FEniCS will interpolate the expression into some finite element space. It is usually a good choice to interpolate expressions into the same space V that is used for the trial and test functions, but in certain cases, one may want to use a more accurate (higher degree) representation of expressions.

The expression may depend on the variables `x[0]` and `x[1]` corresponding to the x and y coordinates. In 3D, the expression may also depend on the variable `x[2]` corresponding to the z coordinate. With our choice of $u_0(x,y) = 1 + x^2 + 2y^2$, the formula string can be written as `1 + x[0]*x[0] + 2*x[1]*x[1]`:

```
u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]', degree=1)
```

String expressions must have valid C++ syntax!

The string argument to an `Expression` object must obey C++ syntax. Most Python syntax for mathematical expressions are also valid C++ syntax, but power expressions make an exception: `p**a` must be written as `pow(p,a)` in C++ (this is also an alternative Python syntax). The following mathematical functions can be used directly in C++ expressions when defining `Expression` objects: `cos`, `sin`, `tan`, `acos`, `asin`, `atan`, `atan2`, `cosh`, `sinh`, `tanh`, `exp`, `frexp`, `ldexp`, `log`, `log10`, `modf`, `pow`, `sqrt`, `ceil`, `fabs`, `floor`, and `fmod`. Moreover, the number π is available as the symbol `pi`. All the listed functions are taken from the `cmath` C++ header file, and one may hence consult the documentation of `cmath` for more information on the various functions.

If/else tests are possible using the C syntax for inline branching. The function

$$f(x,y) = \begin{cases} x^2, & x,y \geq 0 \\ 2, & \text{otherwise} \end{cases}$$

is implemented as

```
f = Expression('x[0] >= 0 && x[1] >= 0? pow(x[0], 2) : 2', degree=1)
```

Parameters in expression strings are allowed, but must be initialized via keyword arguments when creating the `Expression` object. For example, the function $f(x) = e^{-\kappa\pi^2 t} \sin(\pi kx)$ can be coded as

```
f = Expression('exp(-kappa*pow(pi,2)*t)*sin(pi*k*x[0])', degree=1,
               kappa=1.0, t=0, k=4)
```

At any time, parameters can be updated:

```
f.t += dt
f.k = 10
```

The function `u0_boundary` specifies which points that belong to the part of the boundary where the boundary condition should be applied:

```
def u0_boundary(x, on_boundary):
    return on_boundary
```

A function like `u0_boundary` for marking the boundary must return a boolean value: `True` if the given point `x` lies on the Dirichlet boundary and `False` otherwise. The argument `on_boundary` is `True` if `x` is on the physical boundary of the mesh, so in the present case, where we are supposed to return `True` for all points on the boundary, we can just return the supplied value of `on_boundary`. The `u0_boundary` function will be called for every discrete point in the mesh, which allows us to have boundaries where u are known also inside the domain, if desired.

One way to think about the specification of boundaries in FEniCS is that FEniCS will ask you (or rather the function `u0_boundary` which you have implemented) whether or not a specific point `x` is part of the boundary. FEniCS already knows whether the point belongs to the *actual* boundary (the mathematical boundary of the domain) and kindly shares this information with you in the variable `on_boundary`. You may choose to use this information (as we do here), or ignore it completely.

The argument `on_boundary` may also be omitted, but in that case we need to test on the value of the coordinates in `x`:

```
def u0_boundary(x):
    return x[0] == 0 or x[1] == 0 or x[0] == 1 or x[1] == 1
```

Comparing floating-point values using an exact match test with `==` is not good programming practice, because small round-off errors in the computations of the `x` values could make a test `x[0] == 1` become false even though `x` lies on the boundary. A better test is to check for equality with a tolerance, either explicitly

```
def u0_boundary(x):
    return abs(x[0]) < tol or abs(x[1]) < tol \
        or abs((x[0] - 1) < tol or abs(x[1] - 1) < tol
```

or with the `near` command in FEniCS:

```
def u0_boundary(x):
    return near(x[0], 0, tol) or near(x[1], 0, tol) \
        or near(x[0], 1, tol) or near(x[1], 1, tol)
```

Defining the source term. Before defining the bilinear and linear forms $a(u, v)$ and $L(v)$ we have to specify the source term f :

```
f = Expression('-6', degree=1)
```

When f is constant over the domain, f can be more efficiently represented as a `Constant`:

```
f = Constant(-6)
```

Defining the variational problem. We now have all the ingredients we need to define the variational problem:

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

In essence, these two lines specify the PDE to be solved. Note the very close correspondence between the Python syntax and the mathematical formulas $\nabla u \cdot \nabla v dx$ and $f v dx$. This is a key strength of FEniCS: the formulas in the variational formulation translate directly to very similar Python code, a feature that makes it easy to specify and solve complicated PDE problems. The language used to express weak forms is called UFL (Unified Form Language) [1, 21] and is an integral part of FEniCS.

Forming and solving the linear system. Having defined the finite element variational problem and boundary condition, we can now ask FEniCS to compute the solution:

```
u = Function(V)
solve(a == L, u, bc)
```

Note that we first defined the variable u as a `TrialFunction` and used it to represent the unknown in the form a . Thereafter, we redefined u to be a `Function` object representing the solution; i.e., the computed finite element function u . This redefinition of the variable u is possible in Python and often done in FEniCS applications for linear problems. The two types of objects that u refers to are equal from a mathematical point of view, and hence it is natural to use the same variable name for both objects.

Plotting the solution. Once the solution has been computed, it can be visualized by the `plot()` command:

```
plot(u)
plot(mesh)
interactive()
```

Clicking on **Help** or typing **h** in the plot windows brings up a list of commands. For example, typing **m** brings up the mesh. With the left, middle, and right mouse buttons you can rotate, translate, and zoom (respectively) the plotted surface to better examine what the solution looks like. You must click **Ctrl+q** to kill the plot window and continue execution beyond the command `interactive()`. In the example program, we have therefore placed the call to `interactive()` at the very end. Alternatively, one may use the command `plot(u, interactive=True)` which again means you can interact with the plot window and that execution will be halted until the plot window is closed.

Figure 2.1 displays the resulting u function.

Exporting and post-processing the solution. It is also possible to dump the computed solution to file for post-processing, e.g., in VTK format:

```
vtkfile = File('poisson.pvd')
vtkfile << u
```

The `poisson.pvd` file can now be loaded into any front-end to VTK, in particular ParaView or VisIt. The `plot()` function is intended for quick examination of the solution during program development. More in-depth visual investigations of finite element solutions will normally benefit from using highly professional tools such as ParaView and VisIt.

Prior to plotting and storing solutions to file it is wise to give `u` a proper name by `u.rename('u', 'solution')`. Then `u` will be used as name in plots (rather than the more cryptic default names like `f_7`).

Once the solution has been stored to file, it can be opened in Paraview by choosing **File - Open**. Find the file `poisson.pvd`, and click the green **Apply** button to the left in the GUI. A 2D color plot of $u(x, y)$ is then shown. You can save the figure to file by **File - Export Scene...** and choosing a suitable filename. For more information about how to install and use Paraview, see the <http://www.paraview.org/>.

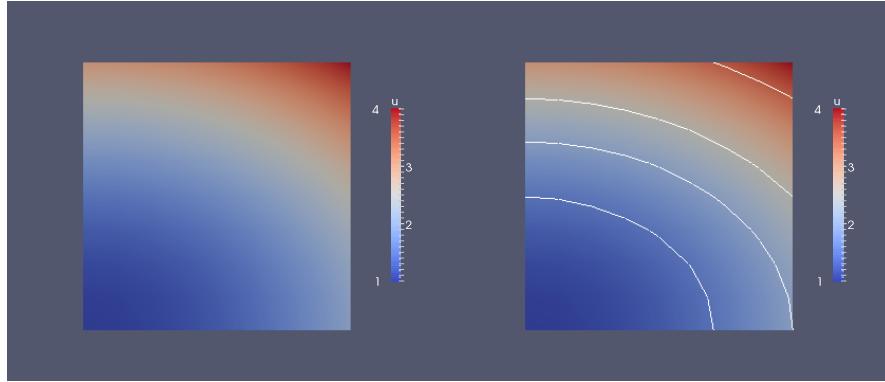


Fig. 2.2 Visualization of test problem in ParaView, with contour lines added in the right plot.

Computing the error. Finally, we compute the error to check the accuracy of the solution. We do this by comparing the finite element solution u with the exact solution u_0 , which in this example happens to be the same as the `Expression` used to set the boundary conditions. We compute the error in two different ways. First, we compute the L^2 norm of the error, defined by

$$E = \sqrt{\int_{\Omega} (u_0 - u)^2 dx}.$$

Since the exact solution is quadratic and the finite element solution is piecewise linear, this error will be nonzero. To compute this error in FEniCS, we simply write

```
error_L2norm = errornorm(u0, u, 'L2')
```

The `errornorm()` function can also compute other error norms such as the H^1 norm. Type `pydoc fenics.errornorm` in a terminal window for details.

We also compute the maximum value of the error at all the vertices of the finite element mesh. As mentioned above, we expect this error to be zero to within machine precision for this particular example. To compute the error at the vertices, we first ask FEniCS to compute the value of both u_0 and u at all vertices, and then subtract the results:

```
vertex_values_u0 = u0.compute_vertex_values(mesh)
vertex_values_u  = u.compute_vertex_values(mesh)
import numpy as np
error_vertices = np.max(np.abs(vertex_values_u0 - vertex_values_u))
```

We have here used maximum and absolute value functions from `numpy`, because these are much more efficient for large arrays (a factor of 30) than Python's built-in `max` and `abs` functions.

How to check that the error vanishes?

With inexact arithmetics, as we always have on a computer, the maximum error at the vertices is not zero, but should be a small number. The machine precision is about 10^{-16} , but in finite element calculations, rounding errors of this size may accumulate, to produce an error larger than 10^{-16} . Experiments show that increasing the number of elements and increasing the degree of the finite element polynomials increases the error. For a mesh with $2 \times (20 \times 20)$ cubic Lagrange elements (degree 3) the error is about $2 \cdot 10^{-12}$, while for 81 linear elements the error is about $2 \cdot 10^{-15}$.

2.1.7 Degrees of freedom and vertex values

A finite element function like u is expressed as a linear combination of basis functions ϕ_j , spanning the space V :

$$u = \sum_{j=1}^N U_j \phi_j. \quad (2.13)$$

By writing `solve(a == L, u, bc)` in the program, a linear system will be formed from a and L , and this system is solved for the U_1, \dots, U_N values. The U_1, \dots, U_N values are known as the *degrees of freedom* (“dofs”) or *nodal values* of u . For Lagrange elements (and many other element types) U_j is simply the value of u at the node with global number j . The location of the nodes and cell vertices coincide for linear Lagrange elements, while for higher-order elements there are additional nodes associated with the facets, edges and sometimes also the interior of cells.

Having u represented as a `Function` object, we can either evaluate $u(x)$ at any point x in the mesh (expensive operation!), or we can grab all the degrees of freedom values U directly by

```
u_nodal_values = u.vector()
```

The result is a `Vector` object, which is basically an encapsulation of the vector object used in the linear algebra package that is used to solve the linear system arising from the variational problem. Since we program in Python it is convenient to convert the `Vector` object to a standard `numpy` array for further processing:

```
u_array = u_nodal_values.array()
```

With `numpy` arrays we can write MATLAB-like code to analyze the data. Indexing is done with square brackets: `u_array[j]`, where the index j always starts at 0. If the solution is computed with piecewise linear Lagrange elements (P_1), then the size of the array `u_array` is equal to the number of vertices, and each `u[j]` is the value at some vertex in the mesh. However, the degrees of freedom are not necessarily numbered in the same way as the vertices of the mesh, see Section 5.2.4 for details. If we therefore want to know the values at the vertices, we need to call the function `u.compute_vertex_values()`. This function returns the values at all the vertices of the mesh as a `numpy` array with the same numbering as for the vertices of the mesh, for example:

```
u_vertex_values = u.compute_vertex_values()
```

Note that `u_array` and `u_vertex_values` are arrays of the same length and containing the same values, albeit in different order.

2.2 Deflection of a membrane

AL 4: I AM HERE

The previous problem and code targeted a simple test problem where we can easily verify the implementation. Now we turn the attention to a more physically relevant problem, in a non-trivial geometry, and that results in solutions of somewhat more exciting shape.

We want to compute the deflection $D(x,y)$ of a two-dimensional, circular membrane, subject to a load p over the membrane. The appropriate PDE model is

$$-T\nabla^2 D = p(x,y) \quad \text{in } \Omega = \{(x,y) | x^2 + y^2 \leq R\}. \quad (2.14)$$

Here, T is the tension in the membrane (constant), and p is the external pressure load. The boundary of the membrane has no deflection, implying $D = 0$ as boundary condition. A localized load can be modeled as a Gaussian function:

$$p(x,y) = \frac{A}{2\pi\sigma} \exp\left(-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2 - \frac{1}{2}\left(\frac{y-y_0}{\sigma}\right)^2\right). \quad (2.15)$$

The parameter A is the amplitude of the pressure, (x_0, y_0) the localization of the maximum point of the load, and σ the “width” of p .

2.2.1 Scaling

The localization of the pressure, (x_0, y_0) , is for simplicity set to $(0, R_0)$. There are many physical parameters in this problem, and we can benefit from grouping them by means of scaling. Let us introduce dimensionless coordinates $\bar{x} = x/R$, $\bar{y} = y/R$, and a dimensionless deflection $w = D/D_c$, where D_c is a characteristic size of the deflection. Introducing $\bar{R}_0 = R_0/R$, we get

$$\frac{\partial^2 w}{\partial \bar{x}^2} + \frac{\partial^2 w}{\partial \bar{y}^2} = \alpha \exp(-\beta^2(\bar{x}^2 + (\bar{y} - \bar{R}_0)^2)) \quad \text{for } \bar{x}^2 + \bar{y}^2 < 1,$$

where

$$\alpha = \frac{R^2 A}{2\pi T D_c \sigma}, \quad \beta = \frac{R}{\sqrt{2}\sigma}.$$

With an appropriate scaling, \bar{w} and its derivatives are of size unity, so the left-hand side of the scaled PDE is about unity in size, while the right-hand side has α as its characteristic size. This suggest choosing α to be unity, or around unit. We shall in particular choose $\alpha = 4$. With this value, the solution is $w(\bar{x}, \bar{y}) = 1 - \bar{x}^2 - \bar{y}^2$. (One can also find the analytical solution in scaled

coordinates and show that the maximum deflection $D(0,0)$ is D_c if we choose $\alpha = 4$ to determine D_c .) With $D_c = AR^2/(8\pi\sigma T)$ and dropping the bars we get the scaled problem

$$\nabla^2 w = 4 \exp(-\beta^2(x^2 + (y - R_0)^2)), \quad (2.16)$$

to be solved over the unit circle with $w = 0$ on the boundary. Now there are only two parameters to vary: the dimensionless extent of the pressure, β , and the localization of the pressure peak, $R_0 \in [0, 1]$. As $\beta \rightarrow 0$, we have a special case with solution $w = 1 - x^2 - y^2$.

Given a computed w , the physical deflection is given by

$$D = \frac{AR^2}{8\pi\sigma T} w.$$

Just a few modifications are necessary in our previous program to solve this new problem.

2.2.2 Defining the mesh

A mesh over the unit circle can be created by the `mshr` tool in FEniCS:

```
from mshr import *
domain = Circle(Point(0.0, 0.0), 1.0)
n = 20
mesh = generate_mesh(domain, n)
plot(mesh, interactive=True)
```

The `Circle` shape from `mshr` takes the center and radius of the circle as the two first arguments, while `n` is the resolution, here the suggested number of cells per radius.

2.2.3 Defining the load

The right-hand side pressure function is represented by an `Expression` object. There are two physical parameters in the formula for f that enter the expression string and these parameters must have their values set by keyword arguments:

```
beta = 8
R0 = 0.6
p = Expression(
    '4*exp(-pow(beta,2)*(pow(x[0], 2) + pow(x[1]-R0, 2)))',
    beta=beta, R0=R0)
```

The coordinates in `Expression` objects *must* be a vector with indices 0, 1, and 2, and with the name `x`. Otherwise we are free to introduce names of parameters as long as these are given default values by keyword arguments. All the parameters initialized by keyword arguments can at any time have their values modified. For example, we may set

```
p.beta = 12
p.R0 = 0.3
```

2.2.4 Variational form

We may introduce `w` instead of `u` as primary unknown and `p` instead of `f` as right-hand side function:

```
w = TrialFunction(V)
v = TestFunction(V)
a = dot(grad(w), grad(v))*dx
L = p*v*dx

w = Function(V)
solve(a == L, w, bc)
```

2.2.5 Visualization

It would be of interest to visualize `p` along with `w` so that we can examine the pressure force and the membrane's response. We must then transform the formula (`Expression`) to a finite element function (`Function`). The most natural approach is to construct a finite element function whose degrees of freedom are calculated from `p`. That is, we interpolate `p`:

```
p = interpolate(p, V)
```

Note that the assignment to `p` destroys the previous `Expression` object `p`, so if it is of interest to still have access to this object, another name must be used for the `Function` object returned by `interpolate`.

We can now plot `w` and `p` on the screen as well as dump the fields to file in VTK format:

```
plot(w, title='Deflection')
plot(p, title='Load')

vtkfile1 = File('membrane_deflection.pvd')
vtkfile1 << w
vtkfile2 = File('membrane_load.pvd')
vtkfile2 << p
```

Figure 2.3 shows the result of the `plot` commands.

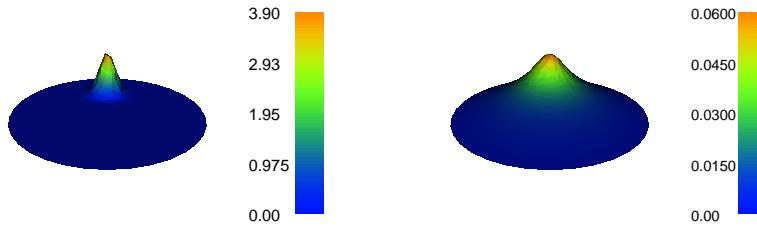


Fig. 2.3 Load (left) and resulting deflection (right) of a circular membrane.

2.2.6 Curve plots through the domain

The best way to compare the load and the deflection is to make a curve plot along the line $x = 0$. This is just a matter of defining a set of points along the line and evaluating the finite element functions w and p at these points:

```
# Curve plot along x=0 comparing p and w
import numpy as np
import matplotlib.pyplot as plt
tol = 1E-8 # Avoid hitting points outside the domain
y = np.linspace(-1+tol, 1-tol, 101)
points = [(0, y_) for y_ in y] # 2D points
w_line = np.array([w(point) for point in points])
p_line = np.array([p(point) for point in points])
plt.plot(y, 100*w_line, 'r', y, p_line, 'b--') # magnify w
plt.legend(['100 x deflection', 'load'], loc='upper left')
plt.xlabel('y'); plt.ylabel('$p$ and $100u$')
```

(Remember a `plt.show()` at the end to show the plot on the screen.) The resulting curve plot appears in Figure 2.4. It is seen how the localized input (p) is heavily damped and smoothed in the output (w). This reflects a typical property of the Poisson equation.

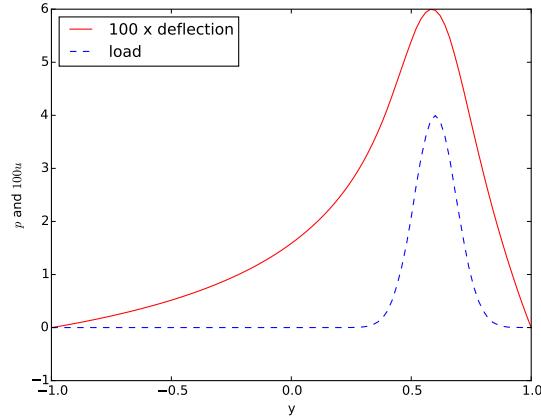


Fig. 2.4 Comparison of membrane load and deflection.

2.2.7 Running ParaView

ParaView³ is a very strong and well-developed tool for visualizing scalar and vector fields, including those computed by FEniCS.

Our program file writes w and p to file as finite element functions. The default filenames are `membrane_deflection.pvd` for w and `membrane_load.vtu` for p . These files are in VTK format and their data can be visualized in ParaView.

1. Start the ParaView application.
2. Open a file with **File - Open....** You will see a list of .pvd and .vtu files. More specifically you see `membrane_deflection.pvd`. Choose this file.
3. Click on **Apply** to the left (*Properties* pane) in the GUI, and ParaView will visualize the contents of the file, here as a color image.
4. To get rid of the axis in the lower left corner of the plot area and axis cross in the middle of the circle, find the *Show Orientation Axis* and *Show Center* buttons to the right in the second row of buttons at the top of the GUI. Click on these buttons to toggle axis information on/off.
5. If you want a color bar to explain the mapping between w values and colors, go to the *Color Map Editor* in the right of the GUI and use the *Show/hide color legend* button. Alternatively, find *Coloring* in the lower left part of the GUI, and toggle the *Show* button.
6. The color map, by default going from blue (low values) to red (high values), can easily be changed. Find the *Coloring* menu in the left part of the GUI, click *Edit*, then in the *Color Map Editor* double click at the left end of the

³<http://www.paraview.org>

color spectrum and choose another color, say yellow, then double click at the right end of the spectrum and choose pink, scroll down to the bottom of the dialog and click *Update*. The color map now goes from yellow to pink.

7. To save the plot to file, click on **File - Export Scene...**, fill in a filename, and save. See Figure 2.5 (middle).
8. To change the background color of plots, choose **Edit - Settings..., Color tab**, click on **Background Color**, and choose it to be, e.g., white. Then choose **Foreground Color** to be something different.
9. To plot the mesh with colors reflecting the size of w , find the *Representation* drop down menu in the left part of the GUI, and replace *Surface* by *Wireframe*.
10. To overlay a surface plot with a wireframe plot, load w and plot as surface, then load w again and plot as wireframe. Make sure both icons in the *Pipeline Browser* in the left part of the GUI are *on* for the `membrane_deflection.pvd` files you want to display. See Figure 2.5 (left).
11. Redo the surface plot. Then we can add some contour lines. Press the semi-sphere icon in the third row of buttons at the top of the GUI (the so-called *filters*). A set of contour values can now be specified at in a dialog box in the left part of the GUI. Remove the default contour (0.578808) and add 0.01, 0.02, 0.03, 0.04, 0.05. Click *Apply* and see an overlay of white contour lines. In the *Pipeline Browser* you can click on the icons to turn a filter on or off.
12. Divide the plot window into two, say horizontally, using the top right small icon. Choose the **3D View** button. Open a new file and load `membrane_load.pvd`. Click on **Apply** to see a plot of the load.

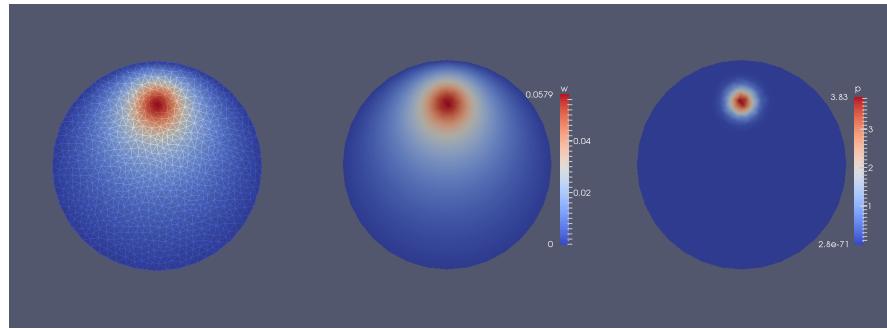


Fig. 2.5 Default visualizations in ParaView: deflection (left, middle) and pressure load (right).

A particularly useful feature of ParaView is that you can record GUI clicks (**Tools - Start/Stop Trace**) and get them translated to Python code. This

allows you automate the visualization process. You can also make curve plots along lines through the domain, etc.

For more information, we refer to The ParaView Guide [24] (free PDF available) and to the ParaView tutorial⁴ as well as an instruction video⁵.

2.2.8 Using the built-in visualization tool

This section explains some useful visualization features of the built-in visualization tool in FEniCS. The `plot` command applies the VTK package to visualize finite element functions in a very quick and simple way. The command is ideal for debugging, teaching, and initial scientific investigations. The visualization can be interactive, or you can steer and automate it through program statements. More advanced and professional visualizations are usually better created with advanced tools like Mayavi, ParaView, or VisIt.

The `plot` function can take additional arguments, such as a title of the plot, or a specification of a wireframe plot (elevated mesh) instead of a colored surface plot:

```
plot(mesh, title='Finite element mesh')
plot(w, wireframe=True, title='Solution')
```

Axes can be turned on by the `axes=True` argument, while `interactive=True` makes the program hang at the `plot` command - you have to type `q` in the plot window to terminate the plot and continue execution.

The left mouse button is used to rotate the surface, while the right button can zoom the image in and out. Point the mouse to the `Help` text down in the lower left corner to get a list of all the keyboard commands that are available.

The plots created by pressing `p` or `P` are stored in filenames having the form `dolfin_plot_X.png` or `dolfin_plot_X.pdf`, where `X` is an integer that is increased by one from the last plot that was made. The file stem `dolfin_plot_` can be set to something more suitable through the `hardcopy_prefix` keyword argument to the `plot` function, for instance, `plot(f, hardcopy_prefix='pressure')`.

Plots stored in PDF format need to be rotated 90 degrees before inclusion in documents. This can be done by the `convert -rotate 90` command (from the ImageMagick utility), but the resulting file has then no more high-resolution PDF vector graphics. A better solution is therefore to use `pdftk` to preserve the vector graphics:

Terminal

```
Terminal> pdftk dolfin_plot_1.pdf cat 1-endnorth output out.pdf
```

⁴http://www.paraview.org/Wiki/The_ParaView_Tutorial

⁵<https://vimeo.com/34037236>

For making plots in batch, we can do the following:

```
viz_w = plot(w, interactive=False)
viz_w.elevate(-10) # adjust (lift) camera from the default view
viz_w.plot(w)      # bring new settings into action
viz_w.write_png('deflection') # make deflection.png
viz_w.write_pdf('deflection') # make deflection.pdf
# Rotate pdf file (right) from landscape to portrait
import os
os.system('pdftk deflection.pdf cat 1-endnorth output w.pdf')
```

The ranges of the color scale can be set by the `range_min` and `range_max` keyword arguments to `plot`. The values must be `float` objects. These arguments are important to keep fixed for animations in time-dependent problems.

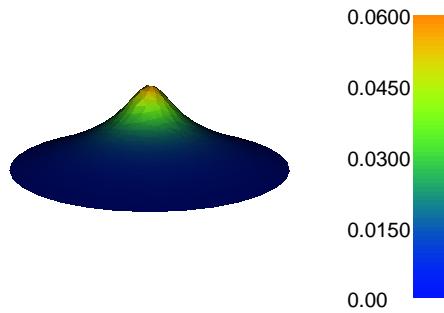


Fig. 2.6 Plot of the deflection of a membrane.

Chapter 3

A Gallery of finite element solvers

The goal of this chapter is to show how a range of important PDEs from science and engineering can be quickly solved with a few lines of FEniCS code. We start with the time-dependent diffusion equation and continue with a nonlinear Poisson equation, the vector PDE for linear elasticity, and the Navier-Stokes equations.

We derive the variational formulation and put together basic objects such as `Mesh`, `Function`, `FunctionSpace`, `TrialFunction`, and `TestFunction` to express in variational formulation in Python code in a way that closely resembles the mathematics.

3.1 The time-dependent diffusion equation

The examples in Section 2.1.4 illustrate that solving linear, stationary PDE problems with the aid of FEniCS is easy and requires little programming. FEniCS clearly automates the spatial discretization by the finite element method. One can use a separate, one-dimensional finite element method in the domain as well, but very often, it is easier to just use a finite difference method, or to formulate the problem as an ODE system and leave the time-stepping to an ODE solver.

hpl 5: Should exemplify all three approaches? With emphasis on simple finite differences?

3.1.1 Variational formulation

Our model problem for time-dependent PDEs reads

$$\frac{\partial u}{\partial t} = \nabla^2 u + f \text{ in } \Omega, \quad (3.1)$$

$$u = u_0 \text{ on } \partial\Omega, \quad (3.2)$$

$$u = I \text{ at } t = 0. \quad (3.3)$$

Here, u varies with space and time, e.g., $u = u(x, y, t)$ if the spatial domain Ω is two-dimensional. The source function f and the boundary values u_0 may also vary with space and time. The initial condition I is a function of space only.

A straightforward approach to solving time-dependent PDEs by the finite element method is to first discretize the time derivative by a finite difference approximation, which yields a recursive set of stationary problems, and then turn each stationary problem into a variational formulation.

Let superscript k denote a quantity at time t_k , where k is an integer counting time levels. For example, u^k means u at time level k . A finite difference discretization in time first consists in sampling the PDE at some time level, say k :

$$\frac{\partial}{\partial t} u^k = \nabla^2 u^k + f^k. \quad (3.4)$$

The time-derivative can be approximated by a finite difference. For simplicity and stability reasons we choose a simple backward difference:

$$\frac{\partial}{\partial t} u^k \approx \frac{u^k - u^{k-1}}{\Delta t}, \quad (3.5)$$

where Δt is the time discretization parameter. Inserting (3.5) in (3.4) yields

$$\frac{u^k - u^{k-1}}{\Delta t} = \nabla^2 u^k + f^k. \quad (3.6)$$

This is our time-discrete version of the diffusion PDE (3.1).

We may reorder (3.6) so that the left-hand side contains the terms with the unknown u^k and the right-hand side contains computed terms only. The result is a recursive set of spatial (stationary) problems for u^k (assuming u^{k-1} is known from computations at the previous time level):

$$u^0 = I, \quad (3.7)$$

$$u^k - \Delta t \nabla^2 u^k = u^{k-1} + \Delta t f^k, \quad k = 1, 2, \dots \quad (3.8)$$

Given I , we can solve for u^0 , u^1 , u^2 , and so on.

An alternative to (3.8), which can be convenient in implementations, is to collect all terms on one side of the equality sign:

$$F(u; v) = u^k - \Delta t \nabla^2 u^k - u^{k-1} - \Delta t f^k = 0, \quad k = 1, 2, \dots \quad (3.9)$$

We use a finite element method to solve (3.7) and either of the equations (3.8) or (3.9). This requires turning the equations into weak forms. As usual, we multiply by a test function $v \in \hat{V}$ and integrate second-derivatives by parts. Introducing the symbol u for u^k (which is natural in the program), the resulting weak form arising from formulation (3.8) can be conveniently written in the standard notation:

$$a(u, v) = L(v),$$

where

$$a(u, v) = \int_{\Omega} (uv + \Delta t \nabla u \cdot \nabla v) dx, \quad (3.10)$$

$$L(v) = \int_{\Omega} \left(u^{k-1} + \Delta t f^k \right) v dx. \quad (3.11)$$

The alternative form (3.9) has an abstract formulation

$$F(u; v) = 0,$$

where

$$F = \int_{\Omega} \left(uv + \Delta t \nabla u \cdot \nabla v - \left(u^{k-1} - \Delta t f^k \right) v \right) dx. \quad (3.12)$$

The initial condition (3.7) can also be turned into a weak form,

$$a_0(u, v) = L_0(v),$$

with

$$a_0(u, v) = \int_{\Omega} uv dx, \quad (3.13)$$

$$L_0(v) = \int_{\Omega} Iv dx. \quad (3.14)$$

The alternative is to construct u_0 by just interpolating I (which is also a much cheaper operation since no linear system is involved).

The continuous variational problem is to find $u^0 \in V$ such that $a_0(u^0, v) = L_0(v)$ holds for all $v \in \hat{V}$, and then find $u^k \in V$ such that $a(u^k, v) = L(v)$ for all $v \in \hat{V}$, or alternatively, $F(u^k, v) = 0$ for all $v \in \hat{V}$, $k = 1, 2, \dots$.

Approximate solutions in space are found by restricting the functional spaces V and \hat{V} to finite-dimensional spaces, exactly as we have done in the Poisson problems. We shall use the symbol u for the finite element approximation at time t_k . In case we need to distinguish this space-time discrete approximation from the exact solution of the continuous diffusion problem,

we use u_e for the latter. By u^{k-1} we mean the finite element approximation of the solution at time t_{k-1} .

Instead of solving (3.7) by a finite element method, i.e., projecting I onto V via the problem $a_0(u, v) = L_0(v)$, we could simply interpolate u^0 from I . That is, if $u^0 = \sum_{j=1}^N U_j^0 \phi_j$, we simply set $U_j = I(x_j, y_j)$, where (x_j, y_j) are the coordinates of node number j . We refer to these two strategies as computing the initial condition by either projecting I or interpolating I . Both operations are easy to compute through one statement, using either the `project` or `interpolate` function.

3.1.2 A simple implementation

Our program needs to implement the time stepping explicitly, but can rely on FEniCS to easily compute a_0 , L_0 , F , a , and L , and solve the linear systems for the unknowns.

Test problem. Before starting the coding, we shall construct a problem where it is easy to determine if the calculations are correct. The simple backward time difference is exact for linear functions, so we decide to have a linear variation in time. Combining a second-degree polynomial in space with a linear term in time,

$$u = 1 + x^2 + \alpha y^2 + \beta t, \quad (3.15)$$

yields a function whose computed values at the nodes will be exact, regardless of the size of the elements and Δt , as long as the mesh is uniformly partitioned. By inserting (3.15) in the PDE problem (3.1), it follows that u_0 must be given as (3.15) and that $f(x, y, t) = \beta - 2 - 2\alpha$ and $I(x, y) = 1 + x^2 + \alpha y^2$.

The code. A new programming issue is how to deal with functions that vary in space *and time*, such as the boundary condition u_0 given by (3.15). A natural solution is to apply an `Expression` object with time t as a parameter, in addition to the parameters α and β :

```
alpha = 3; beta = 1.2
u0 = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                alpha=alpha, beta=beta, t=0)
```

This function expression has the components of `x` as independent variables, while `alpha`, `beta`, and `t` are parameters. The parameters can later be updated as in

```
u0.t = t
```

The essential boundary conditions, along the entire boundary in this case, are set in the usual way,

```
def boundary(x, on_boundary): # define the Dirichlet boundary
    return on_boundary

bc = DirichletBC(V, u0, boundary)
```

We shall use u for the unknown u at the new time level and u_{-1} for u at the previous time level. The initial value of u_{-1} , implied by the initial condition on u , can be computed by either projecting or interpolating I . The $I(x,y)$ function is available in the program through $u0$, as long as $u0.t$ is zero. We can then do

```
u_1 = interpolate(u0, V)
# or
u_1 = project(u0, V)
```

Projecting versus interpolating the initial condition

To actually recover the exact solution (3.15) to machine precision, it is important not to compute the discrete initial condition by projecting I , but by interpolating I so that the degrees of freedom have exact values at $t = 0$ (projection results in approximative values at the nodes).

We may either define a or L according to the formulas above, or we may just define F and ask FEniCS to figure out which terms that go into the bilinear form a and which that go into the linear form L . The latter is convenient, especially in more complicated problems, so we illustrate that construction:

```
dt = 0.3      # time step

u = TrialFunction(V)
v = TestFunction(V)
f = Constant(beta - 2 - 2*alpha)

F = u*v*dx + dt*dot(grad(u), grad(v))*dx - (u_1 + dt*f)*v*dx
a, L = lhs(F), rhs(F)
```

Finally, we perform the time stepping in a loop:

```
u = Function(V)    # the unknown at a new time level
T = 2             # total simulation time
t = dt

while t <= T:
    u0.t = t
    solve(a == L, u, bc)

    t += dt
    u_1.assign(u)
```

Remember to update expression objects with the current time!

Inside the time loop, observe that `u0.t` must be updated before the `solve` statement to enforce computation of Dirichlet conditions at the current time level. (The Dirichlet conditions look up the `u0` object for values.)

The time loop above does not contain any comparison of the numerical and the exact solution, which we must include in order to verify the implementation. As in the Poisson equation example in Section 2.1.6, we compute the difference between the array of nodal values of `u` and the array of the interpolated exact solution. The following code is to be included inside the loop, after `u` is found:

```
u_e = interpolate(u0, V)
error = np.abs(u_e.vector().array() -
               u.vector().array()).max()
print('error, t=% .2f: %-10.3g' % (t, max_error))
```

The complete program code for this time-dependent case goes as follows:

```
from fenics import *
import numpy as np

# Create mesh and define function space
nx = ny = 4
mesh = UnitSquareMesh(nx, ny)
V = FunctionSpace(mesh, 'P', 1)

# Define boundary conditions
alpha = 3; beta = 1.2
u0 = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                alpha=alpha, beta=beta, t=0)

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, boundary)

# Initial condition
u_1 = interpolate(u0, V)
#project(u0, V) will not result in exact solution at the nodes!

dt = 0.3      # time step

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Constant(beta - 2 - 2*alpha)

F = u*v*dx + dt*dot(grad(u), grad(v))*dx - (u_1 + dt*f)*v*dx
```

```

a, L = lhs(F), rhs(F)

# Compute solution
u = Function(V)    # the unknown at a new time level
T = 1.9             # total simulation time
t = dt
while t <= T:
    print('time =', t)
    u0.t = t
    solve(a == L, u, bc)

    # Verify
    u_e = interpolate(u0, V)
    error = np.abs(u_e.vector().array() -
                    u.vector().array()).max()
    print('error, t=% .2f: %10.3g' % (t, error))

    t += dt
    u_1.assign(u)

```

The code is available in the file `ft02_diffusion_flat1.py`.

3.1.3 Diffusion of a Gaussian function

The mathematical problem. Now we want to solve a more physical problem, namely the diffusion of a Gaussian hill. It means that the initial condition is given by

$$I(x, y) = e^{-ax^2 - ay^2}$$

on a domain $[-2, 2] \times [2, 2]$. A possible value of a is 5.

Implementation. What are the necessary changes to the previous program?

1. The domain is not the unit square and it needs much higher resolution:
`mesh = RectangleMesh(Point(-2, -2), Point(2, 2), 30, 30).`
2. The boundary condition is zero everywhere: `DirichletBC(V, Constant(0), boundary)`.
3. The initial condition is different: `I = Expression('exp(...)').`
4. The time step should be sufficiently small: `dt = 0.01` or `dt = 0.05`.
5. The right-hand side function `f` is zero: `f = Constant(0)` (just 0 will give an error as functions in FEniCS must be `Expression`, `Function` (over a mesh) or `Constant`).
6. The end time for the simulation must be longer: `T = 0.8`.
7. The initial condition and the solution inside the time loop should be stored to file in VTK format for visualization: `vtkfile << (u, t)`.
8. We can add a `plot(u)` command inside the time loop as well.

The complete program appears below.

```

from fenics import *
import time

# Create mesh and define function space
nx = ny = 30
mesh = RectangleMesh(Point(-2,-2), Point(2,2), nx, ny)
V = FunctionSpace(mesh, 'P', 1)

# Define boundary conditions
def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, Constant(0), boundary)

# Initial condition
I = Expression('exp(-a*pow(x[0],2)-a*pow(x[1],2))', a=5)
u_1 = interpolate(I, V)
u_1.rename('u', 'initial condition')
vtkfile = File('diffusion.pvd')
vtkfile << (u_1, 0.0)
#project(u0, V) will not result in exact solution at the nodes!

dt = 0.01      # time step

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Constant(0)

F = u*v*dx + dt*dot(grad(u), grad(v))*dx - (u_1 + dt*f)*v*dx
a, L = lhs(F), rhs(F)

# Compute solution
u = Function(V)          # the unknown at a new time level
u.rename('u', 'solution') # name and label for u
T = 0.5                  # total simulation time
t = dt
while t <= T:
    print('time =', t)
    solve(a == L, u, bc)
    vtkfile << (u, float(t))
    plot(u)
    time.sleep(0.3)

    t += dt
    u_1.assign(u)

```

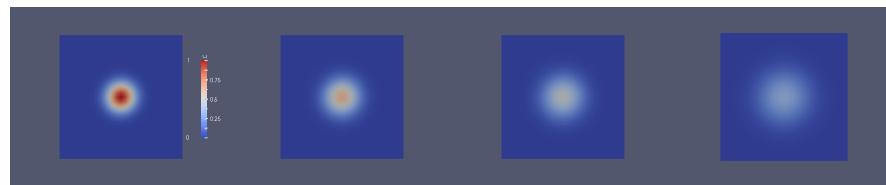
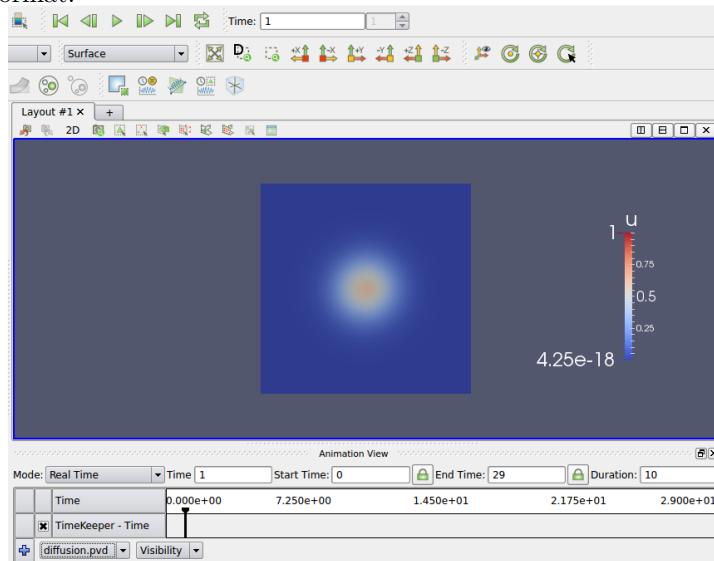
Visualization in ParaView. Start ParaView, choose **File - Open**, open the file `diffusion.pvd`, click the green **Apply** button on the left to see the initial condition being plotting. Choose **View - Animation View**. Click on the play button or (better) the next frame button in the row of buttons at the top of the GUI to see the evolution of the scalar field you just have computed:



The cross in the middle of the plot can be turned off by the **Show Center** button:



Choose **File - Save Animation...** to save the animation to the OGG video format.



3.2 A nonlinear Poisson equation

3.2.1 Variational formulation

Now we shall address how to solve nonlinear PDEs in FEniCS. Our sample PDE for implementation is taken as a nonlinear Poisson equation:

$$-\nabla \cdot (q(u) \nabla u) = f, \quad (3.16)$$

in Ω , with $u = u_0$ on the boundary $\partial\Omega$. The coefficient $q(u)$ makes the equation nonlinear (unless $q(u)$ is constant in u).

The variational formulation of our model problem reads: Find $u \in V$ such that

$$F(u; v) = 0 \quad \forall v \in \hat{V}, \quad (3.17)$$

where

$$F(u; v) = \int_{\Omega} (q(u) \nabla u \cdot \nabla v + fv) dx, \quad (3.18)$$

and

$$\begin{aligned} \hat{V} &= \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}, \\ V &= \{v \in H^1(\Omega) : v = u_0 \text{ on } \partial\Omega\}. \end{aligned}$$

The discrete problem arises as usual by restricting V and \hat{V} to a pair of discrete spaces. As usual, we omit any subscript on discrete spaces and simply say V and \hat{V} are chosen finite dimensional according to some mesh with some element type. Similarly, we let u from now on be the discrete solution.

The discrete nonlinear problem is then written as: find $u \in V$ such that

$$F(u; v) = 0 \quad \forall v \in \hat{V}, \quad (3.19)$$

with $u = \sum_{j=1}^N U_j \phi_j$. Since F is a nonlinear function of u , the variational statement gives rise to a system of nonlinear algebraic equations in the unknowns U_1, \dots, U_N .

3.2.2 A simple implementation

Overview. A working solver for the nonlinear Poisson equation is as easy to implement as a solver for the corresponding linear problem. All we need to do is the state the formula for F and call `solve(F == 0, u, bc)` instead of `solve(a == L, u, bc)` as we did in the linear case. Here is a minimalistic code:

```
from fenics import *

def q(u):
    """Nonlinear coefficient in the PDE."""
    return 1 + u**2
```

```

mesh = UnitSquareMesh(60, 40)
V = FunctionSpace(mesh, 'P', 1)
u0 = Expression(...)

def u0_boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, u0_boundary)

# Define variational problem
u = Function(V)
v = TestFunction(V)
f = Expression(...)
F = dot(q(u)*grad(u), grad(v))*dx - f*v*dx

# Compute solution
solve(F == 0, u, bc)

```

The major difference from a linear problem is that the unknown function `u` in the variational form is in the nonlinear case a `Function`, not a `TrialFunction`.

The `solve` function takes the nonlinear equations and derives symbolically the Jacobian matrix and runs a Newton method.

Constructing a test problem with SymPy. Let us do a specific computation. We then need choices for f and u_0 . Previously, we have worked with manufactured solutions that can be reproduced without approximation errors. This is more difficult in nonlinear problems, and the algebra is more tedious. However, we may utilize SymPy for symbolic computing and integrate such computations in the FEniCS solver. This allows us to easily experiment with different manufactured solutions. The forthcoming code with SymPy requires some basic familiarity with this package (here, defining symbols, `diff` for differentiation, `ccode` for C/C++ code generation).

We try out a two-dimensional manufactured solution that is linear in the unknowns:

```

# Warning: from fenics import * imports f, q, and sym
# (which overwrites our own f and q (function) objects
# and also sym if we do import sympy as sym).
# Therefore, do fenics import first and then overwrite
from fenics import *

def q(u):
    """Nonlinear coefficient in the PDE."""
    return 1 + u**2

# Use sympy to compute f given manufactured solution u
import sympy as sym
x, y = sym.symbols('x[0] x[1]')
u = 1 + x + 2*y
f = - sym.diff(q(u)*sym.diff(u, x), x) - \

```

```

    sym.diff(q(u)*sym.diff(u, y), y)
f = sym.simplify(f)

```

Define symbolic coordinates as required in Expression objects

Note that we would normally write `x, y = sym.symbols('x y')`, but if we want the resulting expressions to be have valid syntax for `Expression` objects, and then `x` reads `x[0]` and `y` must be `x[1]`. This is easily accomplished with `sympy` by defining the names of `x` and `y` as `x[0]` and `x[1]: x, y = sym.symbols('x[0] x[1]')`.

Turning the expressions for `u` and `f` into C or C++ syntax for `Expression` objects needs two steps. First we ask for the C code of the expressions,

```

u_code = sym.printing.ccode(u)
f_code = sym.printing.ccode(f)

```

Sometimes we need some editing of the result to match the required syntax of `Expression` objects, but not in this case. (The primary example is that `M_PI` for π in C/C++ must be replaced by `pi` for `Expression` objects.) In our case here, the output of `c_code` and `f_code` is

```

x[0] + 2*x[1] + 1
-10*x[0] - 20*x[1] - 10

```

After having defined the mesh, the function space, and the boundary, we define the boundary values, `u0`, as

```

u0 = Expression(u_code)

```

Similarly, we define the right-hand side function as

```

f = Expression(f_code)

```

The complete code is found in the file `ft03_poisson_flat_nonlinear.py`.

Name clash between `fenics` and program variables

In a program like the one above, strange errors may occur due to name clashes. If you define `sym`, `q`, and `f` prior to doing `from fenics import *`, the latter statement will also import variables with the names `sym`, `q`, and `f` and overwrite the objects you had! This may lead to strange errors. The best solution is to do `import fenics as fe` and prefix all FEniCS object names by `fe`. The next best solution is to do the `from fenics import *` first and then define our own variables that overwrite those imported from `fenics`. This is acceptable if we do not need `f`, `q`, and `sym` from `fenics`.

Running the code gives output that tells how the Newton iteration progresses. With $2(6 \times 4)$ cells we get convergence in 7 iterations with a tolerance of 10^{-9} , and the error in the numerical solution is about 10^{-11} . Using more elements, e.g., $2(16 \times 14)$, brings the error down to about 10^{-15} , which provides evidence for a correct implementation.

The current example shows how easy it is to solve a nonlinear problem in FEniCS. However, experts on numerical solution of nonlinear PDEs know very well that automated procedures may fail in nonlinear problems, and that it is often necessary to have much more manual control of the solution process than what we have in the current case. Therefore, we return to this problem in Chapter ?? in [19] and show how we can implement our own solution algorithms for nonlinear equations and also how we can steer the parameters in the automated Newton method used above. You will then realize how easy it is to implement tailored solution strategies for nonlinear problems in FEniCS.

3.3 The equations of linear elasticity

Analysis of structures is one of the major activities in modern engineering, thus making the PDEs for deformation of elastic bodies most likely the most popular PDE model in the world. It just takes a page of code to solve the equations of 2D or 3D elasticity in FEniCS, and the details follows below.

3.3.1 Variational formulation

The equations governing small elastic deformations of a body Ω can be written as

$$\nabla \cdot \sigma = \varrho f \text{ in } \Omega, \quad (3.20)$$

$$\sigma = \lambda \operatorname{tr} \varepsilon I + 2\mu \varepsilon, \quad (3.21)$$

$$\varepsilon = \frac{1}{2} \left(\nabla u + (\nabla u)^T \right), \quad (3.22)$$

where σ is the stress tensor, ϱ is the density of the material, f is the body force, λ and μ are Lame's elasticity coefficients for the material in Ω I is the identity tensor, tr is the trace operator on a tensor, ε is the strain tensor, and u is the displacement vector field.

We shall combine (3.21) and (3.22) to

$$\sigma = \lambda \nabla \cdot u I + \mu (\nabla u + (\nabla u)^T). \quad (3.23)$$

Note that (3.20)-(3.22) can easily be transformed to a vector PDE for u , which is the governing PDE for the unknown u . In the derivation of the variational formulation, however, the splitting of the equations as done above is convenient.

The variational formulation of (3.20)-(3.22) consists of forming the inner product of (3.20) and a *vector* test function $v \in \hat{V}$, where \hat{V} is a test vector function space, and integrating over the domain Ω :

$$\int_{\Omega} (\nabla \cdot \sigma) \cdot v \, dx = \int_{\Omega} \varrho f \cdot v \, dx.$$

Since $\nabla \cdot \sigma$ contains second-order derivatives of the primary unknown u , we integrate this term by parts:

$$\int_{\Omega} (\nabla \cdot \sigma) \cdot \nabla v \, dx - \int_{\Omega} \sigma : \nabla v \, dx + \int_{\partial\Omega} (\sigma \cdot n) \cdot v \, ds,$$

where the colon operator is the inner product between tensors, and n is the outward unit normal at the boundary. The quantity $\sigma \cdot n$ is known as the *traction* or stress vector at the boundary, and is often prescribed as a boundary condition. We assume that it is prescribed at a part $\partial\Omega_T$ of the boundary and set $T = \sigma \cdot n$. We then have

$$\int_{\Omega} (\sigma : \nabla v + \varrho f \cdot v) = \int_{\partial\Omega_T} T \cdot v \, ds.$$

Inserting (3.23) for σ gives the variational form with u as unknown.

We can now summarize the variational formulation as find $u \in V$ such that

$$a(u, v) = L(v) \quad \forall v \in \hat{V}, \tag{3.24}$$

where

$$a(u, v) = \int_{\Omega} \sigma(u) : \nabla v \, dx, \tag{3.25}$$

$$\sigma(u) = \lambda \nabla \cdot u I + \mu (\nabla u + (\nabla u)^T), \tag{3.26}$$

$$L(v) = - \int_{\Omega} \varrho f \cdot v \, dx + \int_{\partial\Omega_T} T \cdot v \, ds. \tag{3.27}$$

One can show that the inner product of a symmetric tensor A and a non-symmetric tensor B vanishes. If we express ∇v as a sum of its symmetric and non-symmetric parts, only the symmetric part will survive in the product $\sigma : \nabla v$ since σ is a symmetric tensor. This gives rise to the slightly different variational form

$$a(u, v) = \int_{\Omega} \sigma(u) : \varepsilon(v) \, dx, \tag{3.28}$$

where $\varepsilon(v)$ is the symmetric part of v :

$$\varepsilon(v) = \frac{1}{2}(\nabla v + (\nabla v)^T).$$

3.3.2 A simple implementation

Test problem. As test example, we may look at a clamped beam deformed under its own weight. Then $f = (0, 0, -g)$ is the body force with g as the acceleration of gravity. The beam is box-shaped with length L and square cross section of width W . We set $u = (0, 0, 0)$ at the clamped end, $x = 0$. The rest of the boundaries is traction free.

Let us scale the problem. **hpl 6:** This was meant to simplify the problem so we don't need values for λ , μ , ϱ , etc for a specific material, but the scaling requires some care. In the equation for u , arising from inserting (3.21) and (3.22) in (3.20),

$$\nabla \cdot (\lambda \nabla \cdot u) + \mu \nabla^2 u = \varrho f,$$

we insert coordinates made dimensionless by L , and $\bar{u} = u/u_c$, which results in the dimensionless governing equation

$$\bar{\nabla} \cdot (\bar{\nabla} \cdot \bar{u}) + \beta \bar{\nabla}^2 \bar{u} = \bar{f}, \quad \bar{f} = (0, 0, \gamma),$$

where $\beta = \mu/\lambda$ is a dimensionless elasticity parameter and

$$\gamma = \frac{\varrho g L^2}{u_c \lambda}.$$

Sometimes, one will argue to chose u_c to make γ unity ($u_c = \varrho g L^2 / \lambda$). This is often the reasoning for getting a \bar{u} that is of order unity. However, in elasticity, this leads us to displacements of the size of the geometry, which looks very strange in plots. We therefore want the characteristic displacement to be a small fraction of the characteristic length of the geometry. Actually, for a clamped beam, one has a deflection formula which gives $u_c = \frac{3}{2} g g L^2 \delta^2 / E$, where $\delta = L/W$. Thus, the dimensionless parameter δ is very important in the problem (as expected: $\delta \gg 1$ is what gives beam theory). Taking E to be of the same order of λ , we realize that $\gamma \sim \delta^{-2}$. Experiments with the code point to $\gamma = 0.25\delta^{-2}$ as an appropriate choice. We implement the code with physical parameters, λ , μ , ϱ , g , L , and W , but set these to achieve the solution of the scaled problem: $\lambda = \varrho = L = 1$, W as W/L , $g = \gamma$, and $\mu = \beta$.

Code. hpl 7: Must explain the code. New concepts here, though not many.

```
from fenics import *
```

```

# Scaled variables
L = 1; W = 0.2
lambda_ = 1
rho = 1
delta = W/L
gamma = 0.25*delta**2
beta = 0.8
mu = beta
g = gamma

# Create mesh and define function space
mesh = BoxMesh(Point(0,0,0), Point(L,W,W), 10, 3, 3)
V = VectorFunctionSpace(mesh, 'P', 1)

# Define boundary conditions
tol = 1E-14

def clamped_boundary(x, on_boundary):
    return on_boundary and (x[0] < tol)

bc = DirichletBC(V, Constant((0,0,0)), clamped_boundary)

def epsilon(u):
    return 0.5*(nabla_grad(u) + nabla_grad(u).T)
#return sym(nabla_grad(u))

def sigma(u):
    return lambda_*nabla_div(u)*Identity(d) + 2*mu*epsilon(u)

# Define variational problem
u = TrialFunction(V)
d = u.geometric_dimension() # no of space dim
v = TestFunction(V)
f = rho*Constant((0,0,g))
T = Constant((0,0,0))
a = inner(sigma(u), epsilon(v))*dx
L = -dot(f, v)*dx + dot(T, v)*ds

# Compute solution
u = Function(V)
solve(a == L, u, bc)

# Plot solution and mesh
plot(u, title='Displacement', mode='displacement')

von_Mises = inner(sigma(u), sigma(u)) - div(u)
V = FunctionSpace(mesh, 'P', 1)
von_Mises = project(von_Mises, V)
plot(von_Mises, title='Stress intensity', mode='displacement')
u_magnitude = sqrt(dot(u,u))
u_magnitude = project(u_magnitude, V)
plot(u_magnitude, 'Displacement magnitude', mode='displacement')
print('min/max u:', u_magnitude.vector().array().min(),
      u_magnitude.vector().array().max())

```

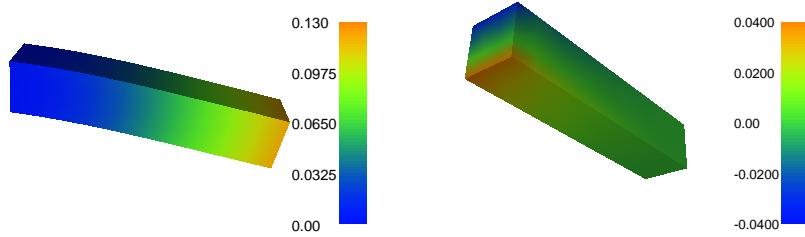


Fig. 3.1 Gravity-induced deformation of a clamped beam: deflection (left) and stress intensity (right).

3.4 The Navier–Stokes equations

Should we here also include coupling to a transport equation? It shows multi-physics capabilities.

3.4.1 Variational formulation

3.4.2 A simple implementation

Chapter 4

Mesh generation, subdomains and boundary conditions

In this chapter, we focus on a fundamental step in the solution of many PDE problems: the generation of a mesh, and the specification of subdomains and boundary conditions. Our starting point is the convection-diffusion equation, which extends the Poisson equation (the diffusion equation) from the previous chapter to take into account the effects of convection.

4.1 Physical problem formulation

We will simulate the conduction of heat in an insulated pipe via both diffusion and convection (transport). The inner diameter of the pipe is 4cm, its thickness is 4mm, the thickness of the surrounding insulation is 10mm, and its length is 50cm. We assume that the temperature of the water at the inlet is 42 degrees centigrade and the temperature of the surrounding air is 22 degrees centigrade. We also assume that the pipe transmits 0.1 liters of water per second. A sketch of the pipe is given in Figure X.

AL 8: Add nice 3D graphics here...

To compute the temperature distribution in the pipe, we need to set boundary conditions, both at the inflow and outflow, as well as on the boundary of the insulating layer which is exposed to the surrounding air. We do this by assuming that the temperature at the inlet is 42 degrees, for the water as well as for the pipe and the insulating layer. We similarly assume the temperature to be 22 degrees in all three layers at the outflow. The boundary of the insulating layer is also assumed to have the temperature 22 degrees.

To compute the temperature distribution, we also need to know the value of the thermal conductivity λ [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$] for water, pipe, and insulation. From a book of physical tables or from the internet, we find the following values that we will use for our simulation: $\lambda_{\text{water}} = 0.6 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $\lambda_{\text{pipe}} = 18 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ (stainless steel), and $\lambda_{\text{insul}} = 0.035 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ (styrofoam). We will also need to know the density and specific heat of wa-

ter, which we set to $\rho = 1 \text{ kg/dm}^3$ and $c = 4.184 \text{ kJ/(kg}\cdot\text{K)}$ (one kcal per $\text{kg}\cdot\text{K}$), respectively.

Finally, we need to know the velocity field for the water flowing through the pipe. We know the total flow rate of water (0.1 liters per second). If the flow is laminar (Poiseuille flow), we know that the velocity profile is a quadratic function in the radius with its maximum at the center and zero velocity on the boundary. We may thus compute the velocity profile from the dimensions of the pipe. In particular, we know that the velocity profile takes the form

$$\beta(x) = (0, 0, C(a - r)^2),$$

where $r = \sqrt{x^2 + y^2}$. The flow rate is then

$$Q = \int_0^a C(a - r)^2 2\pi r dr = 2\pi Ca^4 \int_0^1 s(1 - s)^2 ds = \pi Ca^4 / 6$$

Knowing that $Q = 0.1 \text{ dm}^3/\text{s}$, we can solve for C and find $C = 0.6 \text{ dm}^3/(\pi a^4)$.

4.2 Mathematical problem formulation

We will model the conduction of heat in the pipe using the standard convection-diffusion equation:

$$-\nabla \cdot (\lambda \nabla u) + \nabla \cdot (c\rho\beta u) = f. \quad (4.1)$$

Here, u denotes the temperature, λ is the thermal conductivity, c is the specific heat, ρ is the density, β is the velocity field, and f is the source term. Since our problem does not have a source term, we will set $f = 0$.

The convection-diffusion equation is often stated in the following slightly modified form:

$$-\nabla \cdot (\lambda \nabla u) + c\rho\beta \cdot \nabla u = f.$$

This formulation is equivalent to (4.1) if the velocity field β is divergence free; that is, if $\nabla \cdot \beta = 0$: $\nabla \cdot (\beta u) = (\nabla \cdot \beta)u + \beta \cdot \nabla u = \beta \cdot \nabla u$.

4.3 Scaling the equation

Before we can solve the PDE, we must first introduce dimensionless quantities since, strictly speaking, our program can not work with units, only with numbers. We let L be a reference length, let T be a reference time length, let U be a reference temperature, and let P be a reference power (energy per unit time). We then introduce the following dimensionless quantities:

$$\bar{x} = \frac{x}{L}, \bar{y} = \frac{y}{L}, \bar{z} = \frac{z}{L}, \bar{u} = \frac{u}{U}, \bar{\beta} = \frac{\beta}{LT^{-1}}, \bar{f} = \frac{f}{PL^{-3}}.$$

The dimensionless coordinates \bar{x} , \bar{y} and \bar{z} also lead to dimensionless derivatives: $\bar{\nabla} = (\partial/\partial\bar{x}, \partial/\partial\bar{y}, \partial/\partial\bar{z}) = L\nabla$. Inserting $u = U\bar{u}$, $\beta = L^{-1}T\bar{\beta}$, and $f = L^{-3}P\bar{f}$ into the convection-diffusion equation (4.1) and using $\nabla = L^{-1}\bar{\nabla}$, we obtain

$$-L^{-1}\bar{\nabla} \cdot (\lambda L^{-1}\bar{\nabla}(U\bar{u})) + L^{-1}\bar{\nabla} \cdot (c\rho LT^{-1}\bar{\beta}U\bar{u}) = L^{-3}P\bar{f}.$$

Rearranging the factors L, U, T, P , we obtain

$$-\bar{\nabla} \cdot (LUP^{-1}\lambda\bar{\nabla}\bar{u}) + \bar{\nabla} \cdot (L^3UT^{-1}P^{-1}c\rho\bar{\beta}\bar{u}) = \bar{f}.$$

Finally, we identify the two dimensionless parameters $\bar{\lambda}$ and \bar{c} given by

$$\bar{\lambda} = LUP^{-1}\lambda, \quad \bar{c} = L^3UT^{-1}P^{-1}c\rho.$$

Let's double-check that these are indeed dimensionless quantities. We have

$$\begin{aligned} [\bar{\lambda}] &= [LUP^{-1}\lambda] = [LUP^{-1}] \cdot [\lambda] = [LUP^{-1}] \cdot [W \cdot m^{-1} \cdot K^{-1}] \\ &= [LUP^{-1}] \cdot [L^{-1}U^{-1}P] = [LUP^{-1} \cdot L^{-1}U^{-1}P] = [1]. \end{aligned}$$

Similarly, we have

$$\begin{aligned} [L^3UT^{-1}P^{-1}c\rho] &= [L^3UT^{-1}P^{-1}] \cdot [c] \cdot [\rho] \\ &= [L^3UT^{-1}P^{-1}] \cdot [kJ/(kg \cdot K)] \cdot [kg/dm^3] \\ &= [L^3UT^{-1}P^{-1}] \cdot [PTU^{-1} \cdot L^{-3}] = [1]. \end{aligned}$$

We thus obtain the dimensionless and fully scaled convection-diffusion equation

$$-\bar{\nabla} \cdot (\bar{\lambda}\bar{\nabla}\bar{u}) + \bar{\nabla} \cdot (c\bar{\beta}\bar{u}) = \bar{f}.$$

The reference quantities L , T , U and P may be chosen arbitrarily. If working with very large or very small quantities, one may want to choose for example L to obtain a domain of unit size. However, for our problem this is not necessary. We will therefore make the most straightforward choice which is to use standard SI units. We thus take $L = 1\text{ m}$, $T = 1\text{ s}$, $U = 1\text{ m/s}$, and $P = 1\text{ W}$. The scaled variables and parameters \bar{u} , $\bar{\beta}$, $\bar{\lambda}$ and so on may then be easily computed by expressing everything in standard SI units and then simply dropping the units.

In the following we will simply write u in place of \bar{u} but remember that the u we compute is actually \bar{u} and the actual temperature will be $u\text{K}$:

$$-\nabla \cdot (\lambda\nabla u) + \nabla \cdot (c\beta u) = f. \quad (4.2)$$

Furthermore, since only derivatives of u appear in the equation, adding a constant offset to u does not change the equation. We may therefore work in Kelvin (K) as well as in degrees centigrade without needing to rescale the equation.

4.4 Finite element variational formulation

The finite element variational formulation of the convection diffusion equation is obtained in the same way as for the Poisson equation in the previous chapter, by multiplying the equation with a test function v , integrating over the domain Ω , and integrating terms with second derivatives by parts. For the (scaled) convection-diffusion equation (4.2), we have one such term, namely $-\nabla \cdot (\lambda u)$. For this term, integration by parts gives

$$-\int_{\Omega} (\nabla \cdot (\lambda \nabla u)) v \, dx = \int_{\Omega} \lambda \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} \lambda \nabla u \cdot n v \, ds.$$

Since we assume Dirichlet boundary conditions on the entire boundary, we take the test function v to be zero on $\partial\Omega$ and thus obtain the following variational problem: find $u \in V$ such that

$$\int_{\Omega} \lambda \nabla u \cdot \nabla v \, dx + \int_{\Omega} \nabla \cdot (c\beta u) v \, dx = \int_{\Omega} f v \, dx,$$

for all test functions $v \in V$.

The variational problem can be stated in FEniCS as follows:

```
a = lmbda*dot(grad(u), grad(v))*dx + div(c*beta*u)*v*dx
L = f*v*dx
```

Note the intentional misspelling of `lmbda` to avoid a name clash with the built-in Python keyword `lambda`.

4.5 Mesh generation

4.6 Subdomain markers

4.7 The complete program

```
from fenics import *
from mshr import *
```

```
# Parameters for geometry
a = 0.04
b = a + 0.004
c = a + 0.01
L = 0.5

# Define cylinders
cylinder_a = Cylinder(Point(0, 0, 0), Point(0, 0, L), a, a)
cylinder_b = Cylinder(Point(0, 0, 0), Point(0, 0, L), b, b)
cylinder_c = Cylinder(Point(0, 0, 0), Point(0, 0, L), c, c)

# Define domain and set subdomains
domain = cylinder_c
domain.set_subdomain(1, cylinder_b)
domain.set_subdomain(2, cylinder_a)

# Generate mesh
mesh = generate_mesh(domain, 16)

xmlfile = File('pipe.xml')
xmlfile << mesh

vtkfile = File('pipe.pvd')
vtkfile << mesh
```


Chapter 5

Python programming and PDE solver design

hpl 9: I don't like this title, but have no other good alternative... **AL 10:** Experimenting with new title

5.1 Refactored implementation

Our first programs in this book are all “flat”. That is, they are not organized into logical, reusable units in terms of Python functions. Such flat programs are popular for quickly testing out some software, but not well suited for serious problem solving. We shall therefore at once *refactor* the program, meaning that we divide it into functions, but this is just a reordering of the existing statements. During refactoring, we try make functions as reusable as possible in other contexts, but statements specific to a certain problem or task are also encapsulated in (non-reusable) functions. Being able to distinguish reusable code from specialized code is a key issue when refactoring code, and this ability depends on a good mathematical understanding of the problem at hand (“what is general, what is special?”). In a flat program, general and specialized code (and mathematics) is often mixed together.

5.1.1 A general solver function

We consider the flat program developed in Section 2.1.4. Some of the code in this program is needed to solve any Poisson problem $-\nabla^2 u = f$ on $[0, 1] \times [0, 1]$ with $u = u_0$ on the boundary, while other statements arise from our simple test problem. Let us collect the general, reusable code in a function `solver`. Our special test problem will then just be an application of `solver` with some additional statements. We limit the `solver` function to just *compute the nu-*

numerical solution. Plotting and comparing the solution with the exact solution are considered to be problem-specific activities to be performed elsewhere.

We parameterize `solver` by f , u_0 , and the resolution of the mesh. Since it is so trivial to use higher-order finite element functions by changing the third argument to `FunctionSpace`, we let also the degree of the polynomials in the finite element basis functions be an argument to `solver`.

```
from fenics import *

def solver(f, u0, Nx, Ny, degree=1):
    """
    Solve -Laplace(u)=f on [0,1]x[0,1] with 2*Nx*Ny Lagrange
    elements of specified degree and u=u0 (Expression) on
    the boundary.
    """
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    def u0_boundary(x, on_boundary):
        return on_boundary

    bc = DirichletBC(V, u0, u0_boundary)

    # Define variational problem
    u = TrialFunction(V)
    v = TestFunction(V)
    a = dot(grad(u), grad(v))*dx
    L = f*v*dx

    # Compute solution
    u = Function(V)
    solve(a == L, u, bc)

    return u
```

Plotting for the test problem. The additional tasks we did in our initial program can be placed in other functions. For example, plotting the solution in our particular test problem is placed in an `application_test` function:

```
def application_test():
    """Plot the solution in the test problem."""
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    f = Constant(-6.0)
    u = solver(f, u0, 6, 4, 1)
    # Dump solution to file in VTK format
    u.rename('u', 'u') # name 'u' is used in plot
    vtkfile = File("poisson.pvd")
    vtkfile << u
    # Plot solution and mesh
    plot(u)
```

Make a module! The refactored code is put in a file `ft04_poisson_func.py`. We should make sure that such a file can be imported (and hence reused) in other programs. Then all statements in the main program should appear with a test `if __name__ == '__main__':`. This test is true if the file is executed as a program, but false if the file is imported. If we want to run this file in the same way as we can run `ft04_poisson_func.py`, the main program is simply a call to `application_test()` followed by a call `interactive()` to hold the plot:

```
if __name__ == '__main__':
    application_test()
    # Hold plot
    interactive()
```

5.1.2 Verification and unit tests

The remaining part of our first program is to compare the numerical and the exact solution. Every time we edit the code we must rerun the test and examine that `max_error` is sufficiently small so we know that the code still works. To this end, we shall adopt *unit testing*, meaning that we create a mathematical test and corresponding software that can run all our tests automatically and check that all tests pass. Python has several tools for unit testing. Two very popular ones are `pytest` and `nose`. These are almost identical and very easy to use. More classical unit testing with test classes is offered by the built-in tool `unittest`, but here we are going to use `pytest` (or `nose`) since it demands shorter and clearer code.

Mathematically, our unit test is that the finite element solution of our problem when $f = -6$ equals the exact solution $u = u_0 = 1 + x^2 + 2y^2$. We have already created code that finds the maximum error in the numerical solution. Because of rounding errors, we cannot demand this maximum error to be zero, but we have to use a tolerance, which depends to the number of elements and the degrees of the polynomials in the finite element basis functions. In Section 2.1.6 we reported some experiments with the size of the maximum error. If we want to test that `solver` works for meshes up to $2(20 \times 20)$ elements and cubic Lagrange elements, 10^{-11} is an appropriate tolerance for testing that the maximum error vanishes.

Only three statements are necessary to carry out the unit test. However, we shall embed these statements in software that the testing frameworks `pytest` and `nose` can recognize. This means that each unit test must be placed in a function that

- has a name starting with `test_`
- has no arguments
- implements the test as `assert success, msg`

Regarding the last point, `success` is a boolean expression that is `False` if the test fails, and in that case the string `msg` is written to the screen. When the test fails, `assert` raises an `AssertionError` exception in Python, otherwise the statement runs silently. The `msg` string is optional, so `assert success` is the minimal test. In our case, we will do `assert max_error < tol`, where `tol` is the tolerance (10^{-11}) mentioned above.

A proper *test function* for implementing this unit test in the pytest or nose testing frameworks has the following form. Note that we perform the test for different mesh resolutions and degrees of finite elements.

```
def test_solver():
    """Reproduce u=1+x^2+2y^2 to "machine precision". """
    tol = 1E-11 # This problem's precision
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]**2')
    f = Constant(-6.0)
    for Nx, Ny in [(3,3), (3,5), (5,3), (20,20)]:
        for degree in 1, 2, 3:
            print('solving on 2(%dx%d) mesh with P%d elements'
                  % (Nx, Ny, degree))
            u = solver(f, u0, Nx, Ny, degree)
            # Make a finite element function of the exact u0
            V = u.function_space()
            u0_Function = interpolate(u0, V) # exact solution
            # Check that dof arrays are equal
            u0_array = u0_Function.vector().array() # dof values
            max_error = (u0_array - u.vector().array()).max()
            msg = 'max error: %g for 2(%dx%d) mesh and degree=%d' \
                  % (max_error, Nx, Ny, degree)
            assert max_error < tol, msg
```

We can at any time run

Terminal

```
Terminal> py.test -s -v ft04_poisson_func.py
```

and the pytest tool will run all functions `test_*` in the file and report how the tests go.

We shall make it a habit in this book to encapsulate numerical test problems in unit tests as done above, and we strongly encourage the reader to create similar unit tests whenever a FEniCS solver is implemented. We dare to assert that this is the only serious way do reliable computational science with FEniCS.

Tip: Print messages in test functions

The `assert` statement runs silently when the test passes so users may become uncertain if all the statements in a test function are really executed. A psychological help is to print out something before `assert`

(as we do in the example above) such that it is clear that the test really takes place. (Note that `py.test` needs the `-s` option to show printout from the test functions.)

The next three sections deal with some technicalities about specifying the solution method for linear systems (so that you can solve large problems) and examining array data from the computed solution (so that you can check that the program is correct). These technicalities are scattered around in forthcoming programs. However, the impatient reader who is more interested in seeing the previous program being adapted to a real physical problem, and play around with some interesting visualizations, can safely jump to Section 2.2. Information in the intermediate sections can be studied on demand.

5.2 Useful extensions

hpl 11: Need a little intro.

5.2.1 Controlling the solution process

Sparse LU decomposition (Gaussian elimination) is used by default to solve linear systems of equations in FEniCS programs. This is a very robust and recommended method for a few thousand unknowns in the equation system, and may hence be the method of choice in many 2D and smaller 3D problems. However, sparse LU decomposition becomes slow and memory demanding in large problems. This fact forces the use of iterative methods, which are faster and require much less memory. The forthcoming text tells you how to advantage of state-of-the-art iterative solution methods in FEniCS.

Setting linear solver parameters. Preconditioned Krylov solvers is a type of popular iterative methods that are easily accessible in FEniCS programs. The Poisson equation results in a symmetric, positive definite coefficient matrix, for which the optimal Krylov solver is the Conjugate Gradient (CG) method. However, the CG method requires boundary conditions to be implemented in a symmetric way. This is not the case by default, so then a Krylov solver for non-symmetric system, such as GMRES, is a better choice. Incomplete LU factorization (ILU) is a popular and robust all-round preconditioner, so let us try the GMRES-ILU pair:

```
solve(a == L, u, bc)
    solver_parameters={'linear_solver': 'gmres',
                      'preconditioner': 'ilu'})
# Alternative syntax
```

```
solve(a == L, u, bc,
      solver_parameters=dict(linear_solver='gmres',
                             preconditioner='ilu'))
```

Section 5.2.2 lists the most popular choices of Krylov solvers and preconditioners available in FEniCS.

Linear algebra backend. The actual GMRES and ILU implementations that are brought into action depends on the choice of linear algebra package. FEniCS interfaces several linear algebra packages, called *linear algebra backends* in FEniCS terminology. PETSc is the default choice if FEniCS is compiled with PETSc, otherwise uBLAS. Epetra (Trilinos), Eigen, MTL4 are other supported backends. Which backend to apply can be controlled by setting

```
parameters['linear_algebra_backend'] = backendname
```

where `backendname` is a string, either '`Eigen`', '`PETSc`', '`uBLAS`', '`Epetra`', or '`MTL4`'. All these backends offer high-quality implementations of both iterative and direct solvers for linear systems of equations.

A common platform for FEniCS users is Ubuntu Linux. The FEniCS distribution for Ubuntu contains PETSc, making this package the default linear algebra backend. The default solver is sparse LU decomposition ('`lu`'), and the actual software that is called is then the sparse LU solver from UMFPACK (which PETSc has an interface to). The available linear algebra backends in a FEniCS installation is listed by

```
list_linear_algebra_backends()
```

The `parameters` database. We will normally like to control the tolerance in the stopping criterion and the maximum number of iterations when running an iterative method. Such parameters can be set by accessing the *global parameter database*, which is called `parameters` and which behaves as a nested dictionary. Write

```
info(parameters, verbose=True)
```

to list all parameters and their default values in the database. The nesting of parameter sets is indicated through indentation in the output from `info`. According to this output, the relevant parameter set is named '`krylov_solver`', and the parameters are set like this:

```
prm = parameters['krylov_solver'] # short form
prm['absolute_tolerance'] = 1E-10
prm['relative_tolerance'] = 1E-6
prm['maximum_iterations'] = 1000
```

Stopping criteria for Krylov solvers usually involve the norm of the residual, which must be smaller than the absolute tolerance parameter *or* smaller than the relative tolerance parameter times the initial residual.

To get a printout of the number of actual iterations to reach the stopping criterion, we can insert

```
set_log_level(PROGRESS)
# or
set_log_level(DEBUG)
```

A message with the equation system size, solver type, and number of iterations arises from specifying the argument PROGRESS, while DEBUG results in more information, including CPU time spent in the various parts of the matrix assembly and solve process.

We remark that default values for the global parameter database can be defined in an XML file. To generate such a file from the current set of parameters in a program, run

```
File('fenics_parameters.xml') << parameters
```

If a `fenics_parameters.xml` file is found in the directory where a FEniCS program is run, this file is read and used to initialize the `parameters` object. Otherwise, the file `.config/fenics/fenics_parameters.xml` in the user's home directory is read, if it exists. Another alternative is to load the XML (with any name) manually in the program:

```
File('fenics_parameters.xml') >> parameters
```

The XML file can also be in gzip'ed form with the extension `.xml.gz`.

An extended solver function. Let us extend the previous solver function from `ft04_poisson_func.py` such that it also offers the GMRES+ILU preconditioned Krylov solver.

```
from fenics import *

def solver(
    f, u0, Nx, Ny, degree=1,
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,           # Relative tolerance in Krylov solver
    max_iter=1000,          # Max no of iterations in Krylov solver
    log_level=PROGRESS,     # Amount of solver output
    dump_parameters=False,   # Write out parameter database?
):
    """
    Solve -Laplace(u)=f on [0,1]x[0,1] with 2*Nx*Ny Lagrange
    elements of specified degree and u=u0 (Expression) on
    the boundary.
    """
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    def u0_boundary(x, on_boundary):
        return on_boundary
```

```

bc = DirichletBC(V, u0, u0_boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
a = dot(grad(u), grad(v))*dx
L = f*v*dx

# Compute solution
u = Function(V)

if linear_solver == 'Krylov':
    prm = parameters['krylov_solver'] # short form
    prm['absolute_tolerance'] = abs_tol
    prm['relative_tolerance'] = rel_tol
    prm['maximum_iterations'] = max_iter
    print(parameters['linear_algebra_backend'])
    set_log_level(log_level)
    if dump_parameters:
        info(parameters, True)
    solver_parameters = {'linear_solver': 'gmres',
                         'preconditioner': 'ilu'}
else:
    solver_parameters = {'linear_solver': 'lu'}

solve(a == L, u, bc, solver_parameters=solver_parameters)
return u

def solver_objects(
    f, u0, Nx, Ny, degree=1,
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,           # Relative tolerance in Krylov solver
    max_iter=1000,          # Max no of iterations in Krylov solver
    log_level=PROGRESS,     # Amount of solver output
    dump_parameters=False,  # Write out parameter database?
):
    """As solver, but use objects for linear variational problem
    and solver."""
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    def u0_boundary(x, on_boundary):
        return on_boundary

    bc = DirichletBC(V, u0, u0_boundary)

    # Define variational problem
    u = TrialFunction(V)
    v = TestFunction(V)
    a = dot(grad(u), grad(v))*dx
    L = f*v*dx

```

```

# Compute solution
u = Function(V)
problem = LinearVariationalProblem(a, L, u, bc)
solver = LinearVariationalSolver(problem)

if linear_solver == 'Krylov':
    solver.parameters['linear_solver'] = 'gmres'
    solver.parameters['preconditioner'] = 'ilu'
    prm = solver.parameters['krylov_solver'] # short form
    prm['absolute_tolerance'] = abs_tol
    prm['relative_tolerance'] = rel_tol
    prm['maximum_iterations'] = max_iter
    print(parameters['linear_algebra_backend'])
    set_log_level(log_level)
    if dump_parameters:
        info(parameters, True)
    solver_parameters = {'linear_solver': 'gmres',
                         'preconditioner': 'ilu'}
else:
    solver_parameters = {'linear_solver': 'lu'}

solver.solve()
return u

```

This new `solver` function, found in the file `ft05_poisson_iter.py`, replaces the one in `ft04_poisson_func.py`: it has all the functionality of the previous `solver` function, but can also solve the linear system with iterative methods and report the progress of such solvers.

Remark regarding unit tests. Regarding verification of the new `solver` function in terms of unit tests, it turns out that unit testing in a problem where the approximation error vanishes is gets more complicated when we use iterative methods. The problem is to keep the error due to iterative solution smaller than the tolerance used in the verification tests. First of all this means that the tolerances used in the Krylov solvers must be smaller than the tolerance used in the `assert` test, but this is no guarantee to keep the linear solver error this small. For linear elements and small meshes, a tolerance of 10^{-11} works well in the case of Krylov solvers too (using a tolerance 10^{-12} in those solvers. However, as soon as we switch to P2 elements, it is hard to force the linear solver error below 10^{-6} . Consequently, tolerances in tests depend on the numerical methods. The interested reader is referred to the `test_solver` function in `ft05_poisson_iter.py` for details: this test function tests the numerical solution for direct and iterative linear solvers, for different meshes, and different degrees of the polynomials in the finite element basis functions.

5.2.2 Linear solvers and preconditioners

The following solution methods for linear systems can be accessed in FEniCS programs:

Name	Method
'lu'	sparse LU factorization (Gaussian elim.)
'cholesky'	sparse Cholesky factorization
'cg'	Conjugate gradient method
'gmres'	Generalized minimal residual method
'bicgstab'	Biconjugate gradient stabilized method
'minres'	Minimal residual method
'tfqmr'	Transpose-free quasi-minimal residual method
'richardson'	Richardson method

Possible choices of preconditioners include

Name	Method
'none'	No preconditioner
'ilu'	Incomplete LU factorization
'icc'	Incomplete Cholesky factorization
'jacobi'	Jacobi iteration
'bjacobi'	Block Jacobi iteration
'sor'	Successive over-relaxation
'amg'	Algebraic multigrid (BoomerAMG or ML)
'additive_schwarz'	Additive Schwarz
'hypre_amg'	Hypre algebraic multigrid (BoomerAMG)
'hypre_euclid'	Hypre parallel incomplete LU factorization
'hypre_parasails'	Hypre parallel sparse approximate inverse
'ml_amg'	ML algebraic multigrid

Many of the choices listed above are only offered by a specific backend, so setting the backend appropriately is necessary for being able to choose a desired linear solver or preconditioner. You can also use constructions like

```
prec = 'amg' if has_krylov_solver_preconditioner('amg') \
else 'default'
```

An up-to-date list of the available solvers and preconditioners in FEniCS can be produced by

```
list_linear_solver_methods()
list_krylov_solver_preconditioners()
```

5.2.3 Linear variational problem and solver objects

The `solve(a == L, u, bc)` call is just a compact syntax alternative to a slightly more comprehensive specification of the variational equation and the solution of the associated linear system. This alternative syntax is used in a lot of FEniCS applications and will also be used later in this tutorial, so we show it already now:

```
u = Function(V)
problem = LinearVariationalProblem(a, L, u, bc)
solver = LinearVariationalSolver(problem)
solver.solve()
```

Many objects have an attribute `parameters` corresponding to a parameter set in the global `parameters` database, but local to the object. Here, `solver.parameters` play that role. Setting the CG method with ILU preconditioning as solution method and specifying solver-specific parameters can be done like this:

```
solver.parameters['linear_solver'] = 'gmres'
solver.parameters['preconditioner'] = 'ilu'
prm = solver.parameters['krylov_solver'] # short form
prm['absolute_tolerance'] = 1E-7
prm['relative_tolerance'] = 1E-4
prm['maximum_iterations'] = 1000
```

Settings in the global `parameters` database are propagated to parameter sets in individual objects, with the possibility of being overwritten as done above.

The linear variational problem and solver objects as outlined above are incorporated in an alternative solver function, named `solver_objects`, in `ft05_poisson_iter.py`. Otherwise, this function is parallel to the previously shown `solver` function.

5.2.4 Writing out the discrete solution

We have seen how to grab the degrees of freedom array from a finite element function `u`:

```
u_array = u.vector().array()
```

The elements in `u_array` correspond to function values of `u` at nodes in the mesh. Now, a fundamental question is: What are the coordinates of node `i` whose value is `u_array[i]`? To answer this question, we need to understand how to get our hands on the coordinates, and in particular, the numbering of degrees of freedom and the numbering of vertices in the mesh. We start with P1 (1st order Lagrange) elements where all the nodes are vertices in the mesh.

The function `mesh.coordinates()` returns the coordinates of the vertices as a `numpy` array with shape (M,d) , M being the number of vertices in the mesh and d being the number of space dimensions:

```
>>> from fenics import *
>>>
>>> mesh = UnitSquareMesh(2, 2)
>>> coor = mesh.coordinates()
>>> coor
array([[ 0. ,  0. ],
       [ 0.5,  0. ],
       [ 1. ,  0. ],
       [ 0. ,  0.5],
       [ 0.5,  0.5],
       [ 1. ,  0.5],
       [ 0. ,  1. ],
       [ 0.5,  1. ],
       [ 1. ,  1. ]])
```

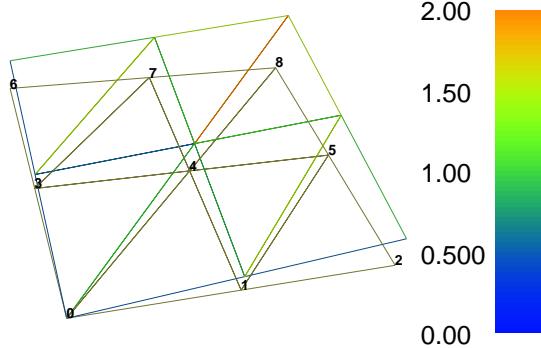
We see from this output that vertices are first numbered along $y = 0$ with increasing x coordinate, then along $y = 0.5$, and so on.

Next we compute a function `u` on this mesh, e.g., the $u = x + y$:

```
>>> V = FunctionSpace(mesh, 'P', 1)
>>> u = interpolate(Expression('x[0]+x[1]'), V)
>>> plot(u, interactive=True)
>>> u_array = u.vector().array()
>>> u_array
array([ 1. ,  0.5,  1.5,  0. ,  1. ,  2. ,  0.5,  1.5,  1. ])
```

We observe that `u_array[0]` is *not* the value of $x + y$ at vertex number 0, since this vertex has coordinates $x = y = 0$. The numbering of the degrees of freedom U_1, \dots, U_N is obviously not the same as the numbering of the vertices.

In the plot of `u`, type `w` to turn on wireframe instead of fully colored surface, `m` to show the mesh, and then `v` to show the numbering of the vertices.



Already in Section 2.1.6 we explained that the vertex values of a `Function` object can be extracted `u.compute_vertex_values()`, which returns an array where element `i` is the value of `u` at vertex `i`:

```
>>> u_at_vertices = u.compute_vertex_values()
>>> for i, x in enumerate(coor):
...     print('vertex %d: u_at_vertices[%d]=%g\tu(%s)=%g' %
...           (i, i, u_at_vertices[i], x, u(x)))
vertex 0: u_at_vertices[0]=0    u([ 0.  0.])=8.46545e-16
vertex 1: u_at_vertices[1]=0.5  u([ 0.5  0. ])=0.5
vertex 2: u_at_vertices[2]=1    u([ 1.  0. ])=1
vertex 3: u_at_vertices[3]=0.5  u([ 0.  0.5])=0.5
vertex 4: u_at_vertices[4]=1    u([ 0.5  0.5])=1
vertex 5: u_at_vertices[5]=1.5  u([ 1.  0.5])=1.5
vertex 6: u_at_vertices[6]=1    u([ 0.  1. ])=1
vertex 7: u_at_vertices[7]=1.5  u([ 0.5  1. ])=1.5
vertex 8: u_at_vertices[8]=2    u([ 1.  1. ])=2
```

Alternatively, we can ask for the mapping from vertex numbering to degrees of freedom numbering in the space V :

```
v2d = vertex_to_dof_map(V)
```

Now, `u_array[v2d[i]]` will give us the value of the degree of freedom in `u` corresponding to vertex `i` (`v2d[i]`). In particular, `u_array[v2d]` is an array with all the elements in the same (vertex numbered) order as `coor`. The inverse map, from degrees of freedom number to vertex number is given by `dof_to_vertex_map(V)`, so `coor[dof_to_vertex_map(V)]` results in an array of all the coordinates in the same order as the degrees of freedom.

For Lagrange elements of degree larger than 1, there are degrees of freedom (nodes) that do not correspond to vertices. **hpl 12:** Anders, is the following true? There is no simple way of getting the coordinates associated with the non-vertex degrees of freedom, so if we want to write out the values of a finite

element solution, the following code snippet does the task at the vertices, and this will work for all kinds of Lagrange elements.

```
def compare_exact_and_numerical_solution(Nx, Ny, degree=1):
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    f = Constant(-6.0)
    u = solver(f, u0, Nx, Ny, degree, linear_solver='direct')
    # Grab exact and numerical solution at the vertices and compare
    V = u.function_space()
    u0_Function = interpolate(u0, V)
    u0_at_vertices = u0_Function.compute_vertex_values()
    u_at_vertices = u.compute_vertex_values()
    coor = V.mesh().coordinates()
    for i, x in enumerate(coor):
        print('vertex %2d (%9g,%9g): error=%g',
              % (i, x[0], x[1],
                 u0_at_vertices[i] - u_at_vertices[i]))
    # Could compute u0(x) - u_at_vertices[i] but this
    # is much more expensive and gives more rounding errors
    center = (0.5, 0.5)
    error = u0(center) - u(center)
    print('numerical error at %s: %g' % (center, error))
```

As expected, the error is either identically zero or about 10^{-15} or 10^{-16} .

Cheap vs expensive function evaluation

Given a `Function` object `u`, we can evaluate its values in various ways:

1. `u(x)` for an arbitrary point `x`
2. `u.vector().array()[i]` for degree of freedom number `i`
3. `u.compute_vertex_values()[i]` at vertex number `i`

The first method, though very flexible, is in general very expensive while the other two are very efficient (but limited to certain points).

To demonstrate the use of point evaluations of `Function` objects, we write out the computed `u` at the center point of the domain and compare it with the exact solution:

```
center = (0.5, 0.5)
error = u0(center) - u(center)
print('numerical error at %s: %g' % (center, error))
```

Trying a $2(3 \times 3)$ mesh, the output from the previous snippet becomes

```
numerical error at (0.5, 0.5): -0.0833333
```

The discrepancy is due to the fact that the center point is not a node in this particular mesh, but a point in the interior of a cell, and `u` varies linearly over the cell while `u0` is a quadratic function. When the center point is a node, as in a $2(t \times 2)$ or $2(4 \times 4)$ mesh, the error is of the order 10^{-15} .

We have seen how to extract the nodal values in a `numpy` array. If desired, we can adjust the nodal values too. Say we want to normalize the solution such that $\max_j U_j = 1$. Then we must divide all U_j values by $\max_j U_j$. The following function performs the task:

```
def normalize_solution(u):
    """Normalize u: return u divided by max(u)."""
    u_array = u.vector().array()
    u_max = u_array.max()
    u_array /= u_max
    u.vector()[:] = u_array
    u.vector().set_local(u_array) # alternative
    return u
```

That is, we manipulate `u_array` as desired, and then we insert this array into `u`'s `Vector` object. The `/=` operator implies an in-place modification of the object on the left-hand side: all elements of the `u_array` are divided by the value `max_u`. Alternatively, one could write `u_array = u_array/max_u`, which implies creating a new array on the right-hand side and assigning this array to the name `u_array`.

Be careful when manipulating degrees of freedom

A call like `u.vector().array()` returns a *copy* of the data in `u.vector()`. One must therefore never perform assignments like `u.vector.array()[:] = ...`, but instead extract the `numpy` array (i.e., a copy), manipulate it, and insert it back with `u.vector()[:] =` or `u.set_local(...)`.

All the code in this subsection can be found in the file `ft05_poisson_iter.py`.

5.2.5 Parameterizing the number of space dimensions

FEniCS makes it is easy to write a unified simulation code that can operate in 1D, 2D, and 3D. We will conveniently make use of this feature in forthcoming examples. As an appetizer, go back to the introductory programs `ft01_poisson_flat.py` or `ft04_poisson_func.py` and change the mesh construction from `UnitSquareMesh(6, 4)` to `UnitCubeMesh(6, 4, 5)`. Now the domain is the unit cube partitioned into $6 \times 4 \times 5$ boxes, and each box is divided into six tetrahedra-shaped finite elements for computations. Run the program and observe that we can solve a 3D problem without any other modifications (!). The visualization allows you to rotate the cube and observe the function values as colors on the boundary.

Generating a hypercube. The syntax for generating a unit interval, square, or box is different, so we need to encapsulate this part of the code.

Given a list or tuple with the divisions into cells in the various spatial direction, the following function returns the mesh in a d -dimensional problem:

```
def unit_hypercube(divisions, degree):
    mesh_classes = [UnitIntervalMesh, UnitSquareMesh, UnitCubeMesh]
    d = len(divisions)
    mesh = mesh_classes[d-1](*divisions)
    V = FunctionSpace(mesh, 'P', degree)
    return V, mesh
```

The construction `mesh_class[d-1]` will pick the right name of the object used to define the domain and generate the mesh. Moreover, the argument `*divisions` sends all the component of the list `divisions` as separate arguments. For example, in a 2D problem where `divisions` has two elements, the statement

```
mesh = mesh_classes[d-1](*divisions)
```

is equivalent to

```
mesh = UnitSquareMesh(divisions[0], divisions[1])
```

Replacing the `Nx` and `parameters by divisions and calling unit_hypercube to create the mesh are the two modifications that we need in any of the previously shown solver functions to turn them into solvers for d -dimensional problems!`

5.2.6 Computing derivatives

In Poisson and many other problems, the gradient of the solution is of interest. The computation is in principle simple: since $u = \sum_{j=1}^N U_j \phi_j$, we have that

$$\nabla u = \sum_{j=1}^N U_j \nabla \phi_j.$$

Given the solution variable `u` in the program, its gradient is obtained by `grad(u)` or `grad(u)`. However, the gradient of a piecewise continuous finite element scalar field is a discontinuous vector field since the ϕ_j has discontinuous derivatives at the boundaries of the cells. For example, using Lagrange elements of degree 1, u is linear over each cell, and the numerical ∇u becomes a piecewise constant vector field. On the contrary, the exact gradient is continuous. For visualization and data analysis purposes we often want the computed gradient to be a continuous vector field. Typically, we want each component of ∇u to be represented in the same way as u itself. To this end, we can project the components of ∇u onto the same function space as we used for u . This means that we solve $w = \nabla u$ approximately by a finite

element method, using the same elements for the components of w as we used for u . This process is known as *projection*.

Not surprisingly, projection is a so common operation in finite element programs that FEniCS has a function for doing the task: `project(q, W)`, which returns the projection of some `Function` or `Expression` object named `q` onto the `FunctionSpace` (if `q` is scalar) or `VectorFunctionSpace` (if `q` is vector-valued) named `W`. Specifically, in our case where `u` is computed and we want to project the vector-valued `grad(u)` onto the `VectorFunctionSpace` where each component has the same `Function` space as `u`:

```
V = u.function_space()
degree = u.ufl_element().degree()
W = VectorFunctionSpace(V.mesh(), 'P', degree)

grad_u = project(grad(u), W)
```

Figure 5.1 shows example of how such a smoothed `gradu(u)` vector field is visualized.

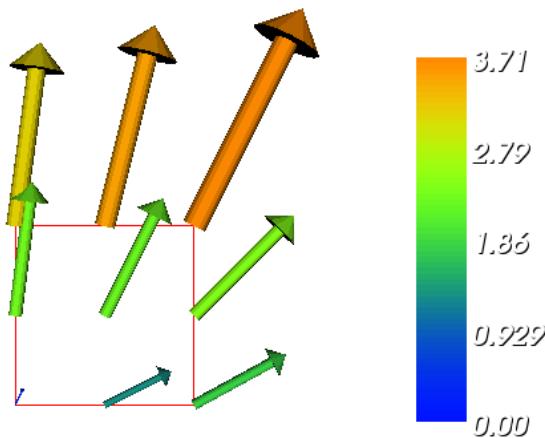


Fig. 5.1 Example of visualizing the vector field ∇u by arrows at the nodes.

The applications of projection are many, including turning discontinuous gradient fields into continuous ones, comparing higher- and lower-order function approximations, and transforming a higher-order finite element solution down to a piecewise linear field, which is required by many visualization packages.

The scalar component fields of the gradient can be extracted as separate fields and, e.g., visualized:

```
grad_u_x, grad_u_y = grad_u.split(deepcopy=True)
plot(grad_u_x, title='x-component of grad(u)')
plot(grad_u_y, title='y-component of grad(u)')
```

The `deepcopy=True` argument signifies a *deep copy*, which is a general term in computer science implying that a copy of the data is returned. (The opposite, `deepcopy=False`, means a *shallow copy*, where the returned objects are just pointers to the original data.)

The `grad_u_x` and `grad_u_y` variables behave as `Function` objects. In particular, we can extract the underlying arrays of nodal values by

```
grad_u_x_array = grad_u_x.vector().array()
grad_u_y_array = grad_u_y.vector().array()
```

The degrees of freedom of the `grad_u` vector field can also be reached by

```
grad_u_array = grad_u.vector().array()
```

but this is a flat `numpy` array where the degrees of freedom for the x component of the gradient is stored in the first part, then the degrees of freedom of the y component, and so on. This is less convenient to work with.

The function `gradient(u)` in `ft05_poisson_iter.py` returns a projected (smoothed) ∇u vector field, given some finite element function `u`:

```
def gradient(u):
    """Return grad(u) projected onto same space as u."""
    V = u.function_space()
    mesh = V.mesh()
    V_g = VectorFunctionSpace(mesh, 'P', 1)
    grad_u = project(grad(u), V_g)
    grad_u.rename('grad(u)', 'continuous gradient field')
    return grad_u
```

Examining the arrays with vertex values of `grad_u_x` and `grad_u_y` quickly reveals that the computed `grad_u` field does not equal the exact gradient $(2x, 4y)$ in this particular test problem where $u = 1 + x^2 + 2y^2$. There are inaccuracies at the boundaries, arising from the approximation problem for w . Increasing the mesh resolution shows, however, that the components of the gradient vary linearly as $2x$ and $4y$ in the interior of the mesh (i.e., as soon as we are one element away from the boundary). The `application_test_gradient` function in `ft05_poisson_iter.py` performs some experiments.

Detour: Manual projection.

Although you will always use `project` to project a finite element function, it can be constructive this point in the tutorial to formulate the projection mathematically and implement its steps manually in FEniCS.

Looking at the component $\partial u / \partial x$ of the gradient, we project the (discrete) derivative $\sum_j U_j \partial \phi_j / \partial x$ onto a function space with basis ϕ_1, ϕ_2, \dots such that the derivative in this space is expressed by the standard sum $\sum_j \bar{U}_j \phi_j$, for suitable (new) coefficients \bar{U}_j .

The variational problem for w reads: find $w \in V^{(g)}$ such that

$$a(w, v) = L(v) \quad \forall v \in \hat{V}^{(g)}, \quad (5.1)$$

where

$$a(w, v) = \int_{\Omega} w \cdot v \, dx, \quad (5.2)$$

$$L(v) = \int_{\Omega} \nabla u \cdot v \, dx. \quad (5.3)$$

The function spaces $V^{(g)}$ and $\hat{V}^{(g)}$ (with the superscript g denoting “gradient”) are vector versions of the function space for u , with boundary conditions removed (if V is the space we used for u , with no restrictions on boundary values, $V^{(g)} = \hat{V}^{(g)} = [V]^d$, where d is the number of space dimensions). For example, if we used piecewise linear functions on the mesh to approximate u , the variational problem for w corresponds to approximating each component field of w by piecewise linear functions.

The variational problem for the vector field w , called `grad_u` in the code, is easy to solve in FEniCS:

```
V_g = VectorFunctionSpace(mesh, 'P', 1)
w = TrialFunction(V_g)
v = TestFunction(V_g)

a = dot(w, v)*dx
L = dot(grad(u), v)*dx
grad_u = Function(V_g)
solve(a == L, grad_u)

plot(grad_u, title='grad(u)')
```

The boundary condition argument to `solve` is dropped since there are no essential boundary conditions in this problem. The new thing is basically that we work with a `VectorFunctionSpace`, since the unknown is now a vector field, instead of the `FunctionSpace` object for scalar fields.

5.2.7 A variable-coefficient Poisson problem

Suppose we have a variable coefficient $p(x, y)$ in the Laplace operator, as in the boundary-value problem

$$\begin{aligned} -\nabla \cdot [p(x, y) \nabla u(x, y)] &= f(x, y) \quad \text{in } \Omega, \\ u(x, y) &= u_0(x, y) \quad \text{on } \partial\Omega. \end{aligned} \tag{5.4}$$

We shall quickly demonstrate that this simple extension of our model problem only requires an equally simple extension of the FEniCS program.

Test problem. Let us continue to use our favorite solution $u(x, y) = 1 + x^2 + 2y^2$ and then prescribe $p(x, y) = x + y$. It follows that $u_0(x, y) = 1 + x^2 + 2y^2$ and $f(x, y) = -8x - 10y$.

Modifications of the PDE solver. What are the modifications we need to do in the previously shown codes to incorporate the variable coefficient p ? from Section 5.2.4?

- `solver` must take `p` as argument,
- `f` in our test problem must be an `Expression` since it is no longer a constant,
- a new `Expression` `p` must be defined for the variable coefficient,
- the formula for $a(u, v)$ in the variational problem is slightly changed.

First we address the modified variational problem. Multiplying the PDE by a test function v and integrating by parts now results in

$$\int_{\Omega} p \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} p \frac{\partial u}{\partial n} v \, ds = \int_{\Omega} f v \, dx.$$

The function spaces for u and v are the same as in Section 2.1.1, implying that the boundary integral vanishes since $v = 0$ on $\partial\Omega$ where we have Dirichlet conditions. The weak form $a(u, v) = L(v)$ then has

$$a(u, v) = \int_{\Omega} p \nabla u \cdot \nabla v \, dx, \tag{5.5}$$

$$L(v) = \int_{\Omega} f v \, dx. \tag{5.6}$$

In the code for solving $-\nabla^2 u = f$ we must replace

```
a = dot(grad(u), grad(v))*dx
```

by

```
a = p*dot(grad(u), grad(v))*dx
```

to solve $-\nabla \cdot (p \nabla u) = f$. Moreover, the definitions of p and f in the test problem read

```
p = Expression('x[0] + x[1]')
f = Expression('-8*x[0] - 10*x[1]')
```

No additional modifications are necessary. The file `ft06_poisson_vc.py` (variable-coefficient Poisson problem in 2D) is a copy of `ft05_poisson_iter.py` with the mentioned changes incorporated. Observe that $p = 1$ recovers the original problem in `ft05_poisson_iter.py`.

You can run it and confirm that it recovers the exact u at the nodes.

Modifications of the flux computations. The flux $-p \nabla u$ may be of particular interest in variable-coefficient Poisson problems as it often has an interesting physical significance. As explained in Section 5.2.6, we normally want the piecewise discontinuous flux or gradient to be approximated by a continuous vector field, using the same elements as used for the numerical solution u . The approximation now consists of solving $w = -p \nabla u$ by a finite element method: find $w \in V^{(g)}$ such that

$$a(w, v) = L(v) \quad \forall v \in V^{(g)}, \quad (5.7)$$

where

$$a(w, v) = \int_{\Omega} w \cdot v \, dx, \quad (5.8)$$

$$L(v) = \int_{\Omega} (-p \nabla u) \cdot v \, dx. \quad (5.9)$$

This problem is identical to the one in Section 5.2.6, except that p enters the integral in L .

The relevant Python statement for computing the flux field take the form

```
flux = project(-p*grad(u),
                VectorFunctionSpace(mesh, 'P', degree))
```

An appropriate function for computing the flux based on u and p is

```
def flux(u, p):
    """Return p*grad(u) projected onto same space as u."""
    V = u.function_space()
    mesh = V.mesh()
    degree = u.ufl_element().degree()
    V_g = VectorFunctionSpace(mesh, 'P', degree)
    flux_u = project(-p*grad(u), V_g)
    flux_u.rename('flux(u)', 'continuous flux field')
    return flux_u

def application_test_flux(Nx=6, Ny=4):
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
```

```

p = Expression('x[0] + x[1]')
f = Expression('-8*x[0] - 10*x[1]')
u = solver(p, f, u0, Nx, Ny, 1, linear_solver='direct')
u.rename('u', 'solution')
flux_u = flux(u, p)
# Grab each component as a scalar field
flux_u_x, flux_u_y = flux_u.split(deepcopy=True)
flux_u_x.rename('flux(u)_x', 'x-component of flux(u)')
flux_u_y.rename('flux(u)_y', 'y-component of flux(u)')
plot(u, title=u.label())
plot(flux_u, title=flux_u.label())
plot(flux_u_x, title=flux_u_x.label())
plot(flux_u_y, title=flux_u_y.label())

u_exact = lambda x, y: 1 + x**2 + 2*y**2
flux_x_exact = lambda x, y: -(x+y)*2*x
flux_y_exact = lambda x, y: -(x+y)*4*y

coor = u.function_space().mesh().coordinates()
if len(coor) < 50:
    # Quite large errors for coarse meshes, but the error
    # decreases with increasing resolution
    for i, value in enumerate(flux_u_x.compute_vertex_values()):
        print('vertex %d, %s, -p*u_x=%g, error=%g' %
              (i, tuple(coor[i]), value,
               flux_x_exact(*coor[i]) - value))
    for i, value in enumerate(flux_u_y.compute_vertex_values()):
        print('vertex %d, %s, -p*u_y=%g, error=%g' %
              (i, tuple(coor[i]), value,
               flux_y_exact(*coor[i]) - value))
else:
    # Compute integrated L2 error of the flux components
    # (Will this work for unstructured mesh? Need to think about that)
    xv = coor.T[0]
    yv = coor.T[1]

def compute_errors(u, u_exact):
    """Compute various measures of the error u - u_exact, where
    u is a finite element Function and u_exact is an Expression."""

    # Compute error norm (for very small errors, the value can be
    # negative so we run abs(assemble(error)) to avoid failure in sqrt

    V = u.function_space()

    # Function - Expression
    error = (u - u_exact)**2*dx
    E1 = sqrt(abs(assemble(error)))

    # Explicit interpolation of u_e onto the same space as u:
    u_e = interpolate(u_exact, V)
    error = (u - u_e)**2*dx
    E2 = sqrt(abs(assemble(error)))

```

```

# Explicit interpolation of u_exact to higher-order elements,
# u will also be interpolated to the space Ve before integration
Ve = FunctionSpace(V.mesh(), 'P', 5)
u_e = interpolate(u_exact, Ve)
error = (u - u_e)**2*dx
E3 = sqrt(abs(assemble(error)))

# fenics.errornorm interpolates u and u_e to a space with
# given degreee, and creates the error field by subtracting
# the degrees of freedom, then the error field is integrated
# TEMPORARY BUG - doesn't accept Expression for u_e
#E4 = errornorm(u_e, u, normtype='l2', degree=3)
# Manual implementation errornorm to get around the bug:
def errornorm(u_exact, u, Ve):
    u_Ve = interpolate(u, Ve)
    u_e_Ve = interpolate(u_exact, Ve)
    e_Ve = Function(Ve)
    # Subtract degrees of freedom for the error field
    e_Ve.vector()[:] = u_e_Ve.vector().array() - u_Ve.vector().array()
    # More efficient computation (avoids the rhs array result above)
    #e_Ve.assign(u_e_Ve)                                # e_Ve = u_e_Ve
    #e_Ve.vector().axpy(-1.0, u_Ve.vector())           # e_Ve += -1.0*u_Ve
    error = e_Ve**2*dx(Ve.mesh())
    return sqrt(abs(assemble(error))), e_Ve
E4, e_Ve = errornorm(u_exact, u, Ve)

# Infinity norm based on nodal values
u_e = interpolate(u_exact, V)
E5 = abs(u_e.vector().array() - u.vector().array()).max()

# H1 seminorm
error = dot(grad(e_Ve), grad(e_Ve))*dx
E6 = sqrt(abs(assemble(error)))

# Collect error measures in a dictionary with self-explanatory keys
errors = {'u - u_exact': E1,
          'u - interpolate(u_exact,V)': E2,
          'interpolate(u,Ve) - interpolate(u_exact,Ve)': E3,
          'errornorm': E4,
          'infinity norm (of dofs)': E5,
          'grad(error) H1 seminorm': E6}

return errors

def convergence_rate(u_exact, f, u0, p, degrees,
                     n=[2***(k+3) for k in range(5)]):
    """
    Compute convergence rates for various error norms for a
    sequence of meshes with Nx=Ny=b and P1, P2, ...,
    Pdegrees elements. Return rates for two consecutive meshes:
    rates[degree][error_type] = r0, r1, r2, ...
    """
    h = {} # Discretization parameter, h[degree][experiment]

```

```

E = {} # Error measure(s), E[degree][experiment][error_type]
P_degrees = 1,2,3,4
num_meshes = 5

# Perform experiments with meshes and element types
for degree in P_degrees:
    n = 4 # Coarsest mesh division
    h[degree] = []
    E[degree] = []
    for i in range(num_meshes):
        n *= 2
        h[degree].append(1.0/n)
        u = solver(p, f, u0, n, n, degree,
                    linear_solver='direct')
        errors = compute_errors(u, u_exact)
        E[degree].append(errors)
        print('2*%dx%d P%d mesh, %d unknowns, E1=%g' %
              (n, n, degree, u.function_space().dim(),
               errors['u - u_exact']))

# Convergence rates
from math import log as ln # log is a fenics name too
error_types = list(E[1][0].keys())
rates = {}
for degree in P_degrees:
    rates[degree] = {}
    for error_type in sorted(error_types):
        rates[degree][error_type] = []
        for i in range(num_meshes):
            Ei = E[degree][i][error_type]
            Eim1 = E[degree][i-1][error_type]
            r = ln(Ei/Eim1)/ln(h[degree][i]/h[degree][i-1])
            rates[degree][error_type].append(round(r,2))
return rates

def convergence_rate_sin():
    """Compute convergence rates for u=sin(x)*sin(y) solution."""
    omega = 1.0
    u_exact = Expression('sin(omega*pi*x[0])*sin(omega*pi*x[1])',
                         omega=omega)
    f = 2*omega**2*pi**2*u_exact
    u0 = Constant(0)
    p = Constant(1)
    # Note: P4 for n>=128 seems to break down
    rates = convergence_rates(u_exact, f, u0, p, degrees=4,
                               n=[2***(k+3) for k in range(5)])
    # Print rates
    print('\n\n')
    for error_type in error_types:
        print(error_type)
        for degree in P_degrees:
            print('P%d: %s' %
                  (degree, str(rates[degree][error_type])[1:-1]))

def structured_mesh(u, divisions):

```

```

"""Represent u on a structured mesh."""
# u must have P1 elements, otherwise interpolate to P1 elements
u2 = u if u.ufl_element().degree() == 1 else \
    interpolate(u, FunctionSpace(mesh, 'P', 1))
mesh = u.function_space().mesh()
from BoxField import fenics_function2BoxField
u_box = fenics_function2BoxField(
    u2, mesh, divisions, uniform_mesh=True)
return u_box

def application_structured_mesh(model_problem=1):
    if model_problem == 1:
        # Numerical solution is exact
        u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
        p = Expression('x[0] + x[1]')
        f = Expression('-8*x[0] - 10*x[1]')
        flux_u_x_exact = lambda x, y: -(x + y)*2*x
        nx = 6; ny = 4
    elif model_problem == 2:
        # Mexican hat solution
        from sympy import exp, sin, pi  # for use in math formulas
        import sympy as sym
        H = lambda x: exp(-16*(x-0.5)**2)*sin(3*pi*x)
        x, y = sym.symbols('x[0], x[1]')
        u = H(x)*H(y)
        u_c = sym.printing.ccode(u)
        # '-exp(-16*pow(x - 0.5, 2) - 16*pow(y - 0.5, 2))*'
        # 'sin(3*M_PI*x)*sin(3*M_PI*y)'
        u_c = u_c.replace('M_PI', 'DOLFIN_PI')
        print('u in C:', u_c)
        u0 = Expression(u_c)

        p = 1  # Don't use Constant(1) here (!)
        f = sym.diff(-p*sym.diff(u, x), x) + \
            sym.diff(-p*sym.diff(u, y), y)
        f = sym.simplify(f)
        f_c = sym.printing.ccode(f)
        f_c = f_c.replace('M_PI', 'DOLFIN_PI')
        f = Expression(f_c)
        flux_u_x_exact = sym.lambdify([x, y], -p*sym.diff(u, x),
                                       modules='numpy')
        print('f in C:', f_c)
        p = Constant(1)
        nx = 22; ny = 22

        u = solver(p, f, u0, nx, ny, 1, linear_solver='direct')
        u_box = structured_mesh(u, (nx, ny))
        u_ = u_box.values  # numpy array
        X = 0; Y = 1       # for indexing in x and y direction

        # Iterate over 2D mesh points (i,j)
        print('u_ is defined on a structured mesh with %s points' %
              str(u_.shape))
        if u.function_space().dim() < 100:

```

```

for j in range(u_.shape[1]):
    for i in range(u_.shape[0]):
        print('u[%d,%d]=u(%g,%g)=%g' %
              (i, j,
               u_box.grid.coor[X][i], u_box.grid.coor[X][j],
               u_[i,j]))

# Make surface plot
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
fig = plt.figure()
ax = fig.gca(projection='3d')
cv = u_box.grid.coorv # vectorized mesh coordinates
ax.plot_surface(cv[X], cv[Y], u_, cmap=cm.coolwarm,
                rstride=1, cstride=1)
plt.title('Surface plot of solution')
plt.savefig('tmp0.png'); plt.savefig('tmp0.pdf')

# Make contour plot
fig = plt.figure()
ax = fig.gca()
cs = ax.contour(cv[X], cv[Y], u_, 7) # 7 levels
plt.clabel(cs) # add labels to contour lines
plt.axis('equal')
plt.title('Contour plot of solution')
plt.savefig('tmp1.png'); plt.savefig('tmp1.pdf')

# Plot u along a line y=const and compare with exact solution
start = (0, 0.4)
x, u_val, y_fixed, snapped = u_box.gridline(start, direction=X)
u_e_val = [u0((x_, y_fixed)) for x_ in x]

plt.figure()
plt.plot(x, u_val, 'r-')
plt.plot(x, u_e_val, 'bo')
plt.legend(['P1 elements', 'exact'], loc='best')
plt.title('Solution along line y=%g, % y_fixed')
plt.xlabel('x'); plt.ylabel('u')
plt.savefig('tmp2.png'); plt.savefig('tmp2.pdf')

flux_u = flux(u, p)
flux_u_x, flux_u_y = flux_u.split(deepcopy=True)

# Plot the numerical and exact flux along the same line
flux2_x = flux_u_x if flux_u_x.ufl_element().degree() == 1 \
           else interpolate(flux_x,
                            FunctionSpace(u.function_space().mesh(),
                                          'P', 1))
flux_u_x_box = structured_mesh(flux2_x, (nx,ny))
x, flux_u_val, y_fixed, snapped = \
    flux_u_x_box.gridline(start, direction=X)
y = y_fixed

```

```

plt.figure()
plt.plot(x, flux_u_val, 'r-')
plt.plot(x, flux_u_x_exact(x, y_fixed), 'bo')
plt.legend(['P1 elements', 'exact'], loc='best')
plt.title('Flux along line y=%g' % y_fixed)
plt.xlabel('x'); plt.ylabel('u')
plt.savefig('tmp3.png'); plt.savefig('tmp3.pdf')

plt.show()

def solver_linalg(
    p, f, u0, Nx, Ny, degree=1,
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,           # Relative tolerance in Krylov solver
    max_iter=1000,          # Max no of iterations in Krylov solver
    log_level=PROGRESS,     # Amount of solver output
    dump_parameters=False,   # Write out parameter database?
    assembly='variational', # or 'matvec' or 'system'
    start_vector='zero',    # or 'random'
):
    """
    Solve -div(p*grad(u))=f on [0,1]x[0,1] with 2*Nx*Ny Lagrange
    elements of specified degree and u=u0 (Expression) on
    the boundary.
    """
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    def u0_boundary(x, on_boundary):
        return on_boundary

    bc = DirichletBC(V, u0, u0_boundary)

    # Define variational problem
    u = TrialFunction(V)
    v = TestFunction(V)
    a = dot(p*grad(u), grad(v))*dx
    L = f*v*dx

    # Compute solution
    u = Function(V)
    U = u.vector()
    if initial_guess == 'random':
        import numpy as np
        np.random.seed(10) # for testing
        U[:] = numpy.random.uniform(-100, 100, n)

    if assembly == 'variational':
        if linear_solver == 'Krylov':
            prm = parameters['krylov_solver'] # short form
            prm['absolute_tolerance'] = abs_tol
            prm['relative_tolerance'] = rel_tol

```

```

prm['maximum_iterations'] = max_iter
prm['nonzero_initial_guess'] = True
print(parameters['linear_algebra_backend'])
set_log_level(log_level)
if dump_parameters:
    info(parameters, True)
solver_parameters = {'linear_solver': 'gmres',
                     'preconditioner': 'ilu'}
else:
    solver_parameters = {'linear_solver': 'lu'}

solve(a == L, u, bc, solver_parameters=solver_parameters)
A = None # Cannot return coefficient matrix
else:
    if assembly == 'matvec':
        A = assemble(a)
        b = assemble(L)
        bc.apply(A, b)
        if linear_solver == 'direct':
            solve(A, U, b)
        else:
            solver = KrylovSolver('gmres', 'ilu')
            prm = solver.parameters
            prm['absolute_tolerance'] = abs_tol
            prm['relative_tolerance'] = rel_tol
            prm['maximum_iterations'] = max_iter
            prm['nonzero_initial_guess'] = True
            solver.solve(A, U, b)
    elif assembly == 'system':
        A, b = assemble_system(a, L, [bc])
        if linear_solver == 'direct':
            solve(A, U, b)
        else:
            solver = KrylovSolver('cg', 'ilu')
            prm = solver.parameters
            prm['absolute_tolerance'] = abs_tol
            prm['relative_tolerance'] = rel_tol
            prm['maximum_iterations'] = max_iter
            prm['nonzero_initial_guess'] = True
            solver.solve(A, U, b)
return u, A

def application_linalg():
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    p = Expression('x[0] + x[1]')
    f = Expression('-8*x[0] - 10*x[1]')
    meshes = [2, 8, 32, 128]
    for n in meshes:
        for assembly in 'variational', 'matvec', 'system':
            print('--- %dx%d mesh, %s assembly ---' % (n, n, assembly))
            u, A = solver_linalg(
                p, f, u0, n, n, linear_solver='Krylov',
                assembly=assembly)
            if A is not None and u.function_space().dim() < 10:

```

```

import numpy as np
np.set_printoptions(precision=2)
print('A: %s assembly\n' % assembly, A.array())

def solver_bc(
    p, f,                      # Coefficients in the PDE
    boundary_conditions,        # Dict of boundary conditions
    Nx, Ny,                     # Cell division of the domain
    degree=1,                   # Polynomial degree
    subdomains=[],               # List of SubDomain objects in domain
    linear_solver='Krylov',     # Alt: 'direct'
    abs_tol=1E-5,                # Absolute tolerance in Krylov solver
    rel_tol=1E-3,                # Relative tolerance in Krylov solver
    max_iter=1000,               # Max no of iterations in Krylov solver
    log_level=PROGRESS,          # Amount of solver output
    dump_parameters=False,        # Write out parameter database?
    debug=False,
):
    """
    Solve -div(p*grad(u))=f on [0,1]x[0,1] with 2*Nx*Ny Lagrange
    elements of specified degree and Dirichlet, Neumann, or Robin
    conditions on the boundary. Piecewise constant p over subdomains
    are also allowed.
    """
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    tol = 1E-14

    # Subdomains in the domain?
    import numpy as np
    if subdomains:
        # subdomains is list of SubDomain objects,
        # p is array of corresponding constant values of p
        # in each subdomain
        if not isinstance(p, (list, tuple, np.ndarray)):
            raise TypeError(
                'p must be array if we have subdomains, not %s'
                % type(p))
        materials = CellFunction('size_t', mesh)
        materials.set_all(0) # "the rest"
        for m, subdomain in enumerate(subdomains[1:], 1):
            subdomain.mark(materials, m)

        p_values = p
        V0 = FunctionSpace(mesh, 'DG', 0)
        p = Function(V0)
        help = np.asarray(materials.array(), dtype=np.int32)
        p.vector()[:] = np.choose(help, p_values)
    else:
        if not isinstance(p, (Expression, Constant)):
            raise TypeError(
                'p is type %s, must be Expression or Constant'

```

```
% type(p))

# Boundary subdomains
class BoundaryX0(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[0]) < tol

class BoundaryX1(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[0] - 1) < tol

class BoundaryY0(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[1]) < tol

class BoundaryY1(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[1] - 1) < tol

# Mark boundaries
boundary_parts = FacetFunction('size_t', mesh)
boundary_parts.set_all(9999)
bx0 = BoundaryX0()
bx1 = BoundaryX1()
by0 = BoundaryY0()
by1 = BoundaryY1()
bx0.mark(boundary_parts, 0)
bx1.mark(boundary_parts, 1)
by0.mark(boundary_parts, 2)
by1.mark(boundary_parts, 3)
# boundary_parts.array() is a numpy array

ds = Measure('ds', domain=mesh, subdomain_data=boundary_parts)

# boundary_conditions is a dict of dicts:
# {0: {'Dirichlet': u0},
#  1: {'Robin': (r, s)},
#  2: {'Neumann': g}},
#  3: {'Neumann', 0} }

bcs = [] # List of Dirichlet conditions
for n in boundary_conditions:
    if 'Dirichlet' in boundary_conditions[n]:
        bcs.append(
            DirichletBC(V, boundary_conditions[n]['Dirichlet'],
                        boundary_parts, n))

if debug:
    # Print the vertices that are on the boundaries
    coor = mesh.coordinates()
    for x in coor:
        if bx0.inside(x, True): print('%s is on x=0' % x)
        if bx1.inside(x, True): print('%s is on x=1' % x)
        if by0.inside(x, True): print('%s is on y=0' % x)
```

```

if by1.inside(x, True): print('%s is on y=1' % x)

# Print the Dirichlet conditions
print('No of Dirichlet conditions:', len(bcs))
d2v = dof_to_vertex_map(V)
for bc in bcs:
    bc_dict = bc.get_boundary_values()
    for dof in bc_dict:
        print('dof %2d: u=%g' % (dof, bc_dict[dof]))
        if V.ufl_element().degree() == 1:
            print(' at point %s' %
                  (str(tuple(coor[d2v[dof]].tolist()))))

# Collect Neumann integrals
u = TrialFunction(V)
v = TestFunction(V)

Neumann_integrals = []
for n in boundary_conditions:
    if 'Neumann' in boundary_conditions[n]:
        if boundary_conditions[n]['Neumann'] != 0:
            g = boundary_conditions[n]['Neumann']
            Neumann_integrals.append(g*v*ds(n))

# Collect Robin integrals
Robin_a_integrals = []
Robin_L_integrals = []
for n in boundary_conditions:
    if 'Robin' in boundary_conditions[n]:
        r, s = boundary_conditions[n]['Robin']
        Robin_a_integrals.append(r*u*v*ds(n))
        Robin_L_integrals.append(r*s*v*ds(n))

# Simpler Robin integrals
Robin_integrals = []
for n in boundary_conditions:
    if 'Robin' in boundary_conditions[n]:
        r, s = boundary_conditions[n]['Robin']
        Robin_integrals.append(r*(u-s)*v*ds(n))

# Define variational problem, solver_bc
a = dot(p*grad(u), grad(v))*dx + \
      sum(Robin_a_integrals)
L = f*v*dx - sum(Neumann_integrals) + sum(Robin_L_integrals)

# Simpler variational formulation
F = dot(p*grad(u), grad(v))*dx + \
      sum(Robin_integrals) - f*v*dx + sum(Neumann_integrals)
a, L = lhs(F), rhs(F)

# Compute solution
u = Function(V)

```

```

if linear_solver == 'Krylov':
    prm = parameters['krylov_solver'] # short form
    prm['absolute_tolerance'] = abs_tol
    prm['relative_tolerance'] = rel_tol
    prm['maximum_iterations'] = max_iter
    print(parameters['linear_algebra_backend'])
    set_log_level(log_level)
    if dump_parameters:
        info(parameters, True)
    solver_parameters = {'linear_solver': 'gmres',
                         'preconditioner': 'ilu'}
else:
    solver_parameters = {'linear_solver': 'lu'}

solve(a == L, u, bcs, solver_parameters=solver_parameters)
return u, p # Note: p may be modified (Function on V0)

def application_bc_test():
    # Define manufactured solution in sympy and derive f, g, etc.
    import sympy as sym
    x, y = sym.symbols('x[0] x[1]') # UFL needs x[0] for x etc.
    u = 1 + x**2 + 2*y**2
    f = -sym.diff(u, x, 2) - sym.diff(u, y, 2) # -Laplace(u)
    f = sym.simplify(f)
    u_00 = u.subs(x, 0) # x=0 boundary
    u_01 = u.subs(x, 1) # x=1 boundary
    g = -sym.diff(u, y).subs(y, 1) # x=1 boundary, du/dn=-du/dy
    r = 1000 # any function can go here
    s = u

    # Turn to C/C++ code for UFL expressions
    f = sym.printing.ccode(f)
    u_00 = sym.printing.ccode(u_00)
    u_01 = sym.printing.ccode(u_01)
    g = sym.printing.ccode(g)
    r = sym.printing.ccode(r)
    s = sym.printing.ccode(s)
    print('Test problem (C/C++):\nu = %s\nf = %s' % (u, f))
    print('u_00: %s\nu_01: %s\ng = %s\nr = %s\ns = %s' %
          (u_00, u_01, g, r, s))

    # Turn into FEniCS objects
    u_00 = Expression(u_00)
    u_01 = Expression(u_01)
    f = Expression(f)
    g = Expression(g)
    r = Expression(r)
    s = Expression(s)
    u_exact = Expression(sym.printing.ccode(u))

    boundary_conditions = {
        0: {'Dirichlet': u_00}, # x=0
        1: {'Dirichlet': u_01}, # x=1
        2: {'Robin': (r, s)}, # y=0
    }

```

```

3: {'Neumann': g})}           # y=1

p = Constant(1)
Nx = Ny = 2
u, p = solver_bc(
    p, f, boundary_conditions, Nx, Ny, degree=1,
    linear_solver='direct',
    debug=2*Nx*Ny < 50, # for small problems only
)

# Compute max error in infinity norm
u_e = interpolate(u_exact, u.function_space())
import numpy as np
max_error = np.abs(u_e.vector().array() -
                    u.vector().array()).max()
print('Max error:', max_error)

# Print numerical and exact solution at the vertices
if u.function_space().dim() < 50: # (small problems only)
    u_e_at_vertices = u_e.compute_vertex_values()
    u_at_vertices = u.compute_vertex_values()
    coor = u.function_space().mesh().coordinates()
    for i, x in enumerate(coor):
        print('vertex %2d (%9g,%9g): error=%g %g vs %g'
              % (i, x[0], x[1],
                 u_e_at_vertices[i] - u_at_vertices[i],
                 u_e_at_vertices[i], u_at_vertices[i]))

def test_solvers_bc():
    """Reproduce u=1+x^2+2y^2 to with different solvers."""
    tol = 3E-12 # Appropriate tolerance for these tests (P2, 20x20 mesh)
    import sympy as sym
    x, y = sym.symbols('x[0] x[1]')
    u = 1 + x**2 + 2*y**2
    f = -sym.diff(u, x, 2) - sym.diff(u, y, 2)
    f = sym.simplify(f)
    u_00 = u.subs(x, 0) # x=0 boundary
    u_01 = u.subs(x, 1) # x=1 boundary
    g = -sym.diff(u, y).subs(y, 1) # x=1 boundary
    r = 1000 # arbitrary function can go here
    s = u

    # Turn to C/C++ code for UFL expressions
    f = sym.printing.ccode(f)
    u_00 = sym.printing.ccode(u_00)
    u_01 = sym.printing.ccode(u_01)
    g = sym.printing.ccode(g)
    r = sym.printing.ccode(r)
    s = sym.printing.ccode(s)
    print('Test problem (C/C++):\nu = %s\nf = %s' % (u, f))
    print('u_00: %s\nu_01: %s\ng = %s\nr = %s\ns = %s' %
          (u_00, u_01, g, r, s))

    # Turn into FEniCS objects

```

```

u_00 = Expression(u_00)
u_01 = Expression(u_01)
f = Expression(f)
g = Expression(g)
r = Expression(r)
s = Expression(s)
u_exact = Expression(sym.printing.ccode(u))

boundary_conditions = {
    0: {'Dirichlet': u_00},
    1: {'Dirichlet': u_01},
    2: {'Robin': (r, s)},
    3: {'Neumann': g}}

p = Constant(1)

for Nx, Ny in [(3,3), (3,5), (5,3), (20,20)]:
    for degree in 1, 2, 3:
        for linear_solver in ['direct']:
            print('solving on 2(%dx%dx) mesh with P%d elements'
                  % (Nx, Ny, degree)),
            print(' %s solver, %s function' %
                  (linear_solver, solver_func.__name__))
            u, p = solver_bc(
                p, f, boundary_conditions, Nx, Ny, degree,
                linear_solver=linear_solver,
                abs_tol=0.1*tol,
                rel_tol=0.1*tol)
            # Make a finite element function of the exact u0
            V = u.function_space()
            u_e_Function = interpolate(u_exact, V) # exact solution
            # Check that dof arrays are equal
            u_e_array = u_e_Function.vector().array() # dof values
            max_error = (u_e_array - u.vector().array()).max()
            msg = 'max error: %g for 2(%dx%d) mesh, degree=%d,\n\
                  %s solver, %s' % \
                  (max_error, Nx, Ny, degree, linear_solver,
                   solver_func.__name__)
            print(msg)
            assert max_error < tol, msg

def application_bc_test_2mat():
    tol = 1E-14 # Tolerance for coordinate comparisons

    class Omega0(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] <= 0.5+tol

    class Omega1(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] >= 0.5-tol

    subdomains = [Omega0(), Omega1()]
    p_values = [2.0, 13.0]

```

```

u_exact = Expression(
    'x[1] <= 0.5? 2*x[1]*p_1/(p_0+p_1) : '
    '((2*x[1]-1)*p_0 + p_1)/(p_0+p_1)',
    p_0=p_values[0], p_1=p_values[1])

boundary_conditions = {
    0: {'Neumann': 0},
    1: {'Neumann': 0},
    2: {'Dirichlet': Constant(0)}, # y=0
    3: {'Dirichlet': Constant(1)}, # y=1
}

f = Constant(0)
Nx = Ny = 2
u, p = solver_bc(
    p_values, f, boundary_conditions, Nx, Ny, degree=1,
    linear_solver='direct', subdomains=subdomains,
    debug=2*Nx*Ny < 50, # for small problems only
)

# Compute max error in infinity norm
u_e = interpolate(u_exact, u.function_space())
import numpy as np
max_error = np.abs(u_e.vector().array() -
                    u.vector().array()).max()
print('Max error:', max_error)

# Print numerical and exact solution at the vertices
if u.function_space().dim() < 50: # (small problems only)
    u_e_at_vertices = u_e.compute_vertex_values()
    u_at_vertices = u.compute_vertex_values()
    coor = u.function_space().mesh().coordinates()
    for i, x in enumerate(coor):
        print('vertex %2d (%9g,%9g): error=%g %g vs %g'
              % (i, x[0], x[1],
                  u_e_at_vertices[i] - u_at_vertices[i],
                  u_e_at_vertices[i], u_at_vertices[i]))


def test_solvers_bc_2mat():
    tol = 2E-13 # Tolerance for comparisons

    class Omega0(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] <= 0.5+tol

    class Omega1(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] >= 0.5-tol

    subdomains = [Omega0(), Omega1()]
    p_values = [2.0, 13.0]
    boundary_conditions = {

```

```

0: {'Neumann': 0},
1: {'Neumann': 0},
2: {'Dirichlet': Constant(0)}, # y=0
3: {'Dirichlet': Constant(1)}, # y=1
}

f = Constant(0)
u_exact = Expression(
    'x[1] <= 0.5? 2*x[1]*p_1/(p_0+p_1) : '
    '((2*x[1]-1)*p_0 + p_1)/(p_0+p_1)',
    p_0=p_values[0], p_1=p_values[1])

for Nx, Ny in [(2,2), (2,4), (8,4)]:
    for degree in 1, 2, 3:
        u, p = solver_bc(
            p_values, f, boundary_conditions, Nx, Ny, degree,
            linear_solver='direct', subdomains=subdomains,
            debug=False)

        # Compute max error in infinity norm
        u_e = interpolate(u_exact, u.function_space())
        import numpy as np
        max_error = np.abs(u_e.vector().array() -
                           u.vector().array()).max()
        assert max_error < tol, 'max error: %g' % max_error

def application_flow_around_circle(obstacle='rectangle'):
    tol = 1E-14 # Tolerance for coordinate comparisons

    class Circle(SubDomain):
        def inside(self, x, on_boundary):
            return ((x[0]-0.5)**2 + (x[1]-0.5)**2) <= 0.2**2

    class Rectangle(SubDomain):
        def inside(self, x, on_boundary):
            return 0.3 <= x[0] <= 0.7 and 0.3 <= x[1] <= 0.7

    obstacle = Circle() if obstacle == 'circle' else Rectangle()
    subdomains = [None, obstacle]
    p_values = [1.0, 1E-4]

    boundary_conditions = {
        0: {'Neumann': 0},
        1: {'Neumann': 0},
        2: {'Dirichlet': Constant(1)}, # y=0
        3: {'Dirichlet': Constant(0)}, # y=1
    }

    f = Constant(0)
    Nx = Ny = 50
    u, p = solver_bc(
        p_values, f, boundary_conditions, Nx, Ny, degree=1,
        linear_solver='direct', subdomains=subdomains)

```

```

v = flux(u, p)
file = File('porous_media_flow.pvd')
file << u
file << v
plot(u)
plot(v)

if __name__ == '__main__':
    #application_test()
    #application_test_flux(Nx=20, Ny=20)
    #convergence_rate()
    #application_structured_mesh(2)
    #application_linalg()
    #application_bc_test_2mat()
    application_flow_around_circle()
    #test_solvers_bc()
    # Hold plot
    interactive()

```

Plotting the flux vector field is naturally as easy as plotting the gradient (see Section 5.2.6):

```

plot(flux, title='flux field')

flux_x, flux_y = flux.split(deepcopy=True) # extract components
plot(flux_x, title='x-component of flux (-p*grad(u))')
plot(flux_y, title='y-component of flux (-p*grad(u))')

```

For data analysis of the nodal values of the flux field we can grab the underlying `numpy` arrays (demands a `deepcopy=True` in the split of `flux`):

```

flux_x_array = flux_x.vector().array()
flux_y_array = flux_y.vector().array()

```

The function `application_test_flux` in the program `ft06_poisson_vc.py` demonstrates the computations described above.

5.2.8 Creating the linear system explicitly

Given $a(u, v) = L(v)$, the discrete solution u is computed by inserting $u = \sum_{j=1}^N U_j \phi_j$ into $a(u, v)$ and demanding $a(u, v) = L(v)$ to be fulfilled for N test functions $\hat{\phi}_1, \dots, \hat{\phi}_N$. This implies

$$\sum_{j=1}^N a(\phi_j, \hat{\phi}_i) U_j = L(\hat{\phi}_i), \quad i = 1, \dots, N,$$

which is nothing but a linear system,

$$AU = b,$$

where the entries in A and b are given by

$$A_{ij} = a(\phi_j, \hat{\phi}_i), \\ b_i = L(\hat{\phi}_i).$$

The examples so far have specified the left- and right-hand side of the variational formulation and then asked FEniCS to assemble the linear system and solve it. An alternative is to explicitly call functions for assembling the coefficient matrix A and the right-side vector b , and then solve the linear system $AU = b$ with respect to the U vector. Instead of `solve(a == L, u, b)` we now write

```
A = assemble(a)
b = assemble(L)
bc.apply(A, b)
u = Function(V)
U = u.vector()
solve(A, U, b)
```

The variables `a` and `L` are as before. That is, `a` refers to the bilinear form involving a `TrialFunction` object (e.g., `u`) and a `TestFunction` object (`v`), and `L` involves a `TestFunction` object (`v`). From `a` and `L`, the `assemble` function can compute A and b .

The matrix A and vector b are first assembled without incorporating essential (Dirichlet) boundary conditions. Thereafter, the call `bc.apply(A, b)` performs the necessary modifications of the linear system such that `u` is guaranteed to equal the prescribed boundary values. When we have multiple Dirichlet conditions stored in a list `bcs`, as explained in Section 5.4.2, we must apply each condition in `bcs` to the system:

```
# bcs is a list of DirichletBC objects
for bc in bcs:
    bc.apply(A, b)
```

There is an alternative function `assemble_system`, which can assemble the system and take boundary conditions into account in one call:

```
A, b = assemble_system(a, L, bcs)
```

The `assemble_system` function incorporates the boundary conditions in the element matrices and vectors, prior to assembly. The conditions are also incorporated in a symmetric way to preserve eventual symmetry of the coefficient matrix. With `bc.apply(A, b)` the matrix `A` is modified in an nonsymmetric way.

Note that the solution `u` is, as before, a `Function` object. The degrees of freedom, $U = A^{-1}b$, are filled into `u`'s `Vector` object (`u.vector()`) by the `solve` function.

The object `A` is of type `Matrix`, while `b` and `u.vector()` are of type `Vector`. We may convert the matrix and vector data to `numpy` arrays by calling the `array()` method as shown before. If you wonder how essential boundary conditions are incorporated in the linear system, you can print out `A` and `b` before and after the `bc.apply(A, b)` call:

```
A = assemble(a)
b = assemble(L)
if mesh.num_cells() < 16: # print for small meshes only
    print(A.array())
    print(b.array())
bc.apply(A, b)
if mesh.num_cells() < 16:
    print(A.array())
    print(b.array())
```

With access to the elements in `A` through a `numpy` array we can easily perform computations on this matrix, such as computing the eigenvalues (using the `eig` function in `numpy.linalg`). We can alternatively dump `A.array()` and `b.array()` to file in MATLAB format and invoke MATLAB or Octave to analyze the linear system. Dumping the arrays to MATLAB format is done by

```
import scipy.io
scipy.io.savemat('Ab.mat', {'A': A.array(), 'b': b.array()})
```

Writing `load Ab.mat` in MATLAB or Octave will then make the array variables `A` and `b` available for computations.

Matrix processing in Python or MATLAB/Octave is only feasible for small PDE problems since the `numpy` arrays or matrices in MATLAB file format are dense matrices. FEniCS also has an interface to the eigensolver package SLEPc, which is a preferred tool for computing the eigenvalues of large, sparse matrices of the type encountered in PDE problems (see `demo/la/eigenvalue` in the FEniCS source code tree for a demo).

By default, `solve(A, U, b)` applies sparse LU decomposition as solver. Specification of an iterative solver and preconditioner is done through two optional arguments:

```
solve(A, U, b, 'cg', 'ilu')
```

Appropriate names of solvers and preconditioners are found in Section 5.2.2.

To control tolerances in the stopping criterion and the maximum number of iterations, one can explicitly form a `KrylovSolver` object and set items in its `parameters` attribute (see also Section 5.2.3):

```
solver = KrylovSolver('cg', 'ilu')
prm = solver.parameters
prm['absolute_tolerance'] = 1E-7
prm['relative_tolerance'] = 1E-4
prm['maximum_iterations'] = 1000
u = Function(V)
```

```
U = u.vector()
set_log_level(DEBUG)
solver.solve(A, U, b)
```

The function `solver_linalg` in the program file `ft06_poisson_vc.py` implements a solver function where the user can choose between different types of assembly: the variational (`solve(a == L, u, bc)`), assembling the matrix and right-hand side separately, and assembling the system such that the coefficient matrix preserves symmetry. The function `application_linalg` runs a test problem on sequence of meshes and solves the problem with symmetric and non-symmetric modification of the coefficient matrix. One can monitor the number of Krylov method iteration and realize that with a symmetric coefficient matrix, the Conjugate Gradient method requires slightly fewer iterations than GMRES in the non-symmetric case. Taking into account that the Conjugate Gradient method has less work per iteration, there is some efficiency to be gained by using `assemble_system`.

hpl 13: Running `application_linalg`, the results are strange: Why does the `solve(a==L, ...)` method need many more iterations than `solve(A, U, b, ...)` when we use the same Krylov parameter settings? Something wrong with the settings?

The choice of start vector for the iterations in a linear solver is often important. With the `solver.solve(A, U, b)` call the default start vector is the zero vector. A start vector with random numbers in the interval $[-100, 100]$ can be computed as

```
n = u.vector().array().size
U = u.vector()
U[:] = numpy.random.uniform(-100, 100, n)
solver.parameters['nonzero_initial_guess'] = True
solver.solve(A, U, b)
```

Note that we must turn off the default behavior of setting the start vector (“initial guess”) to zero, and then the provided value of `U` is used as start vector.

Creating the linear system explicitly in a program can have some advantages in more advanced problem settings. For example, A may be constant throughout a time-dependent simulation, so we can avoid recalculating A at every time level and save a significant amount of simulation time.

5.2.9 Taking advantage of structured mesh data

When finite element computations are done on a structured rectangular mesh, maybe with uniform partitioning, VTK-based tools for completely unstructured 2D/3D meshes are not required. Instead we can use visualization and data analysis tools for *structured data*. Such data typically appear in finite

difference simulations and image analysis. Analysis and visualization of structured data are faster and easier than doing the same with data on unstructured meshes, and the collection of tools to choose among is much larger. We shall demonstrate the potential of such tools and how they allow for tailored and flexible visualization and data analysis.

A necessary first step is to transform our `mesh` object to an object representing a rectangle with equally-shaped *rectangular* cells. The second step is to transform the one-dimensional array of nodal values to a two-dimensional array holding the values at the corners of the cells in the structured mesh. We want to access a value by its i and j indices, i counting cells in the x direction, and j counting cells in the y direction. This transformation is in principle straightforward, yet it frequently leads to obscure indexing errors, so using software tools to ease the work is advantageous.

In the directory `src/modules`, associated with this booklet, we have included a Python module `BoxField` that can take a finite element function u computed by a FEniCS software and represent it on a structured box-shaped mesh and assign or extract values by multi-dimensional indexing: `[i]` in 1D, `[i,j]` in 2D, and `[i,j,k]` in 3D. Given a finite element function u , the following function returns a `BoxField` object that represents u on a structured mesh:

```
def structured_mesh(u, divisions):
    """Represent u on a structured mesh."""
    # u must have P1 elements, otherwise interpolate to P1 elements
    u2 = u if u.ufl_element().degree() == 1 else \
        interpolate(u, FunctionSpace(mesh, 'P', 1))
    mesh = u.function_space().mesh()
    from BoxField import fenics_function2BoxField
    u_box = fenics_function2BoxField(
        u2, mesh, divisions, uniform_mesh=True)
    return u_box
```

Note that we can only turn functions on meshes with P1 elements into `BoxField` objects, so if u is based on another element type, we first interpolate the scalar field onto a mesh with P1 elements. Also note that to use the function, we need to know the divisions into cells in the various spatial directions (`divisions`).

The `u_box` object contains several useful data structures:

- `u_box.grid`: object for the structured mesh
- `u_box.grid.coor[X]`: grid coordinates in $X=0$ direction
- `u_box.grid.coor[Y]`: grid coordinates in $Y=1$ direction
- `u_box.grid.coor[Z]`: grid coordinates in $Z=2$ direction
- `u_box.grid.coorv[X]`: vectorized version of `u_box.grid.coor[X]` (for vectorized computations or surface plotting)
- `u_box.grid.coorv[Y]`: vectorized version of `u_box.grid.coor[Y]`
- `u_box.grid.coorv[Z]`: vectorized version of `u_box.grid.coor[Z]`

- `u_box.values`: numpy array holding the `u` values; `u_box.values[i,j]` holds `u` at the mesh point with coordinates `(u_box.grid.coor[X], u_box.grid.coor[Y])`

Iterating over points and values. Let us go back to the `solver` function in the `ft06_poisson_vc.py` code from Section 5.2.7, compute `u`, map it onto a `BoxField` object for a structured mesh representation, and write out the coordinates and function values at all mesh points:

```
u = solver(p, f, u0, nx, ny, 1, linear_solver='direct')
u_box = structured_mesh(u, (nx, ny))
u_ = u_box.values      # numpy array
X = 0; Y = 1           # for indexing in x and y direction

# Iterate over 2D mesh points (i,j)
print('u_ is defined on a structured mesh with %s points' %
      str(u_.shape))
for j in range(u_.shape[1]):
    for i in range(u_.shape[0]):
        print('u[%d,%d]=u(%g,%g)=%g' %
              (i, j,
               u_box.grid.coor[X][i], u_box.grid.coor[Y][j],
               u_[i,j]))
```

Finite difference approximations. Note that with `u_`, we can easily express finite difference approximation of derivatives:

```
x = u_box.grid.coor[X]
dx = x[1] - x[0]
u_xx = (u_[i-1,j] - 2*u_[i,j] + u_[i+1,j])/dx**2
```

Surface plot. The ability to access a finite element field in the way one can access a finite difference-type of field is handy in many occasions, including visualization and data analysis. With Matplotlib we can create a surface plot, see Figure 5.2 (upper left):

```
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
fig = plt.figure()
ax = fig.gca(projection='3d')
cv = u_box.grid.coorv # vectorized mesh coordinates
ax.plot_surface(cv[X], cv[Y], u_, cmap=cm.coolwarm,
                rstride=1, cstride=1)
plt.title('Surface plot of solution')
```

The key issue is to know that the coordinates needed for the surface plot is in `u_box.grid.coorv` and that the values are in `u_`.

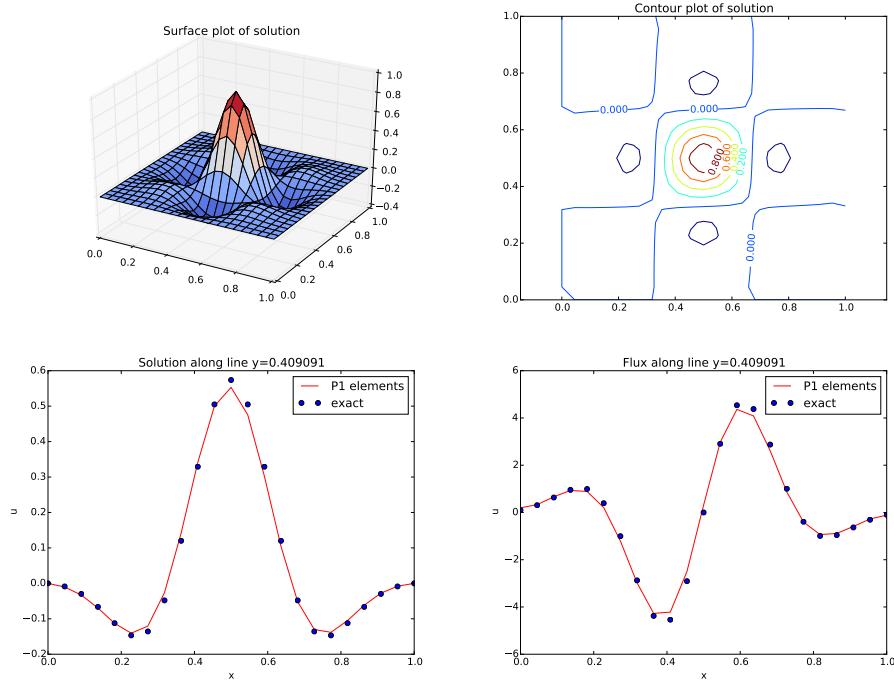


Fig. 5.2 Various plots of the solution on a structured mesh.

Contour plot. A contour plot can also be made by Matplotlib:

```
fig = plt.figure()
ax = fig.gca()
levels = [1.5, 2.0, 2.5, 3.5]
cs = ax.contour(cv[X], cv[Y], u_, levels=levels)
plt.clabel(cs) # add labels to contour lines
plt.axis('equal')
plt.title('Contour plot of solution')
```

The result appears in Figure 5.2 (upper right).

Curve plot through the mesh. A handy feature of BoxField objects is the ability to give a start point in the grid and a direction, and then extract the field and corresponding coordinates along the nearest line of mesh points. In 3D fields one can also extract data in a plane. Say we want to plot u along the line $y = 0.4$. The mesh points, x , and the u values along this line, u_val , are extracted by

```
start = (0, 0.4)
X = 0
x, u_val, y_fixed, snapped = u_box.gridline(start, direction=X)
```

The variable `snapped` is true if the line had to be snapped onto a gridline and in that case `y_fixed` holds the snapped (altered) y value. To avoid interpolation in the structured mesh, `snapped` is in fact *always* true.

A comparison of the numerical and exact solution along the line $y = 0.5$ (snapped from $y = 0.4$) is made by the following code:

```
start = (0, 0.4)
x, u_val, y_fixed, snapped = u_box.gridline(start, direction=X)
u_e_val = [u0((x_, y_fixed)) for x_ in x]

plt.figure()
plt.plot(x, u_val, 'r-')
plt.plot(x, u_e_val, 'bo')
plt.legend(['P1 elements', 'exact'], loc='upper left')
plt.title('Solution along line y=%g' % y_fixed)
plt.xlabel('x'); plt.ylabel('u')
```

See Figure 5.2 (lower left) for the resulting curve plot.

Curve plot of the flux. Let us also compare the numerical and exact flux $-p\partial u/\partial x$ along the same line as above:

```
flux_u = flux(u, p)
flux_u_x, flux_u_y = flux_u.split(deepcopy=True)

# Plot the numerical and exact flux along the same line
flux2_x = flux_u_x if flux_u_x.ufl_element().degree() == 1 \
    else interpolate(flux_x,
                     FunctionSpace(u.function_space().mesh(),
                                   'P', 1))
flux_u_x_box = structured_mesh(flux_u_x, (nx,ny))
x, flux_u_val, y_fixed, snapped = \
    flux_u_x_box.gridline(start, direction=X)
y = y_fixed

plt.figure()
plt.plot(x, flux_u_val, 'r-')
plt.plot(x, flux_u_x_exact(x, y_fixed), 'bo')
plt.legend(['P1 elements', 'exact'], loc='upper right')
plt.title('Flux along line y=%g' % y_fixed)
plt.xlabel('x'); plt.ylabel('u')
```

The second `plt.plot` command requires a Python function `flux_u_x_exact(x,y)` to be available for the exact flux expression.

Note that Matplotlib is one choice of plotting package. With the unified interface in the SciTools package¹ one can access Matplotlib, Gnuplot, MATLAB, OpenDX, VisIt, and other plotting engines through the same API.

Test problem. The graphics referred to in Figure 5.2 correspond to a test problem with prescribed solution $u_e = H(x)H(y)$, where

¹<https://github.com/hplgit/scitools>

$$H(x) = e^{-16(x-\frac{1}{2})^2} \sin(3\pi x).$$

We just fit a function $f(x, y)$ in the PDE (can choose $p = 1$), and notice that $u = 0$ along the boundary of the unit square. Although it is easy to carry out the differentiation of f by hand and hardcode the resulting expressions in an `Expression` object, a more reliable habit is to use Python's symbolic computing engine, SymPy, to perform mathematics and automatically turn formulas into C++ syntax for `Expression` objects. A short introduction was given in Section 3.2.2.

We start out with defining the exact solution in `sympy`:

```
from sympy import exp, sin, pi # for use in math formulas
import sympy as sym
H = lambda x: exp(-16*(x-0.5)**2)*sin(3*pi*x)
x, y = sym.symbols('x[0], x[1]')
u = H(x)*H(y)
```

Define symbolic coordinates as required in Expression objects

Note that we would normally write `x, y = sym.symbols('x y')`, but if we want the resulting expressions to be have valid syntax for `Expression` objects, and then x reads `x[0]` and y must be `x[1]`. This is easily accomplished with `sympy` by defining the names of x and y as `x[0]` and `x[1]: x, y = sym.symbols('x[0] x[1]')`.

Turning the expression for `u` into C or C++ syntax for `Expression` objects needs two steps. First we ask for the C code of the expression,

```
u_c = sym.printing.ccode(u)
```

Printing out `u_c` gives (the output is here manually broken into two lines):

```
-exp(-16*pow(x[0] - 0.5, 2) - 16*pow(x[1] - 0.5, 2))*  
sin(3*M_PI*x[0])*sin(3*M_PI*x[1])
```

The necessary syntax adjustment is replacing the symbol `M_PI` for π in C/C++ by `pi` (or `DOLFIN_PI`):

```
u_c = u_c.replace('M_PI', 'pi')
u0 = Expression(u_c)
```

Thereafter, we can progress with the computation of $f = -\nabla \cdot (p\nabla u)$:

```
p = 1
f = sym.diff(-p*sym.diff(u, x), x) + sym.diff(-p*sym.diff(u, y), y)
f = sym.simplify(f)
f_c = sym.printing.ccode(f)
f_c = f_c.replace('M_PI', 'pi')
f = Expression(f_c)
```

We also need a Python function for the exact flux $-p\partial u/\partial x$:

```
flux_u_x_exact = sym.lambdify([x, y], -p*sym.diff(u, x),
                               modules='numpy')
```

It remains to define `p = Constant(1)` and set `nx` and `ny` before calling `solver` to compute the finite element solution of this problem.

5.3 Postprocessing computations

hpl 11: Need a little intro.

5.3.1 Computing functionals

After the solution u of a PDE is computed, we occasionally want to compute functionals of u , for example,

$$\frac{1}{2} \|\nabla u\|^2 \equiv \frac{1}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx, \quad (5.10)$$

which often reflects some energy quantity. Another frequently occurring functional is the error

$$\|u_e - u\| = \left(\int_{\Omega} (u_e - u)^2 \, dx \right)^{1/2}, \quad (5.11)$$

where u_e is the exact solution. The error is of particular interest when studying convergence properties. Sometimes the interest concerns the flux out of a part Γ of the boundary $\partial\Omega$,

$$F = - \int_{\Gamma} p \nabla u \cdot \mathbf{n} \, ds, \quad (5.12)$$

where \mathbf{n} is an outward unit normal at Γ and p is a coefficient (see the problem in Section 5.2.7 for a specific example). All these functionals are easy to compute with FEniCS, and this section describes how it can be done.

Energy functional. The integrand of the energy functional (5.10) is described in the UFL language in the same manner as we describe weak forms:

```
energy = 0.5*dot(grad(u), grad(u))*dx
E = assemble(energy)
```

The `assemble` call performs the integration. It is possible to restrict the integration to subdomains, or parts of the boundary, by using a mesh function to mark the subdomains as explained in Section 5.4.4.

Error functional. Computation of (5.11) is typically done by

```
error = (u - u_exact)**2*dx
E = sqrt(abs(assemble(error)))
```

The exact solution u_e is here in a `Function` or `Expression` object `u_exact`, while `u` is the finite element approximation. (Sometimes, for very small error values, the result of `assemble(error)` can be a (very small) negative number, so we have used `abs` in the expression for `E` above to ensure a positive value for the `sqrt` function.)

As will be explained and demonstrate in Section 5.3.2, the integration of $(u - u_{\text{exact}})^{**2}dx$ can result in too optimistic convergence rates unless one is careful how `u_exact` is transferred onto a mesh. The general recommendation for reliable error computation is to use the `errornorm` function (see `pydoc fenics.errornorm` and Section 5.3.2 for more information):

```
E = errornorm(u_exact, u)
```

Flux Functionals. To compute flux integrals like $F = - \int_{\Gamma} p \nabla u \cdot \mathbf{n} ds$ we need to define the \mathbf{n} vector, referred to as *facet normal* in FEniCS. If the surface domain Γ in the flux integral is the complete boundary we can perform the flux computation by

```
n = FacetNormal(mesh)
flux = -p*dot(grad(u), n)*ds
total_flux = assemble(flux)
```

Although `grad(u)` and `grad(u)` are interchangeable in the above expression when `u` is a scalar function, we have chosen to write `grad(u)` because this is the right expression if we generalize the underlying equation to a vector Laplace/Poisson PDE. With `grad(u)` we must in that case write `dot(n, grad(u))`.

It is possible to restrict the integration to a part of the boundary using a mesh function to mark the relevant part, as explained in Section 5.4.4. Assuming that the part corresponds to subdomain number `i`, the relevant syntax for the variational formulation of the flux is `-p*dot(grad(u), n)*ds(i)`.

5.3.2 Computing convergence rates

hpl 15: Newer FEniCS examples have `dx(degree)`. Should explain that syntax. Also `Expression(string, degree)`.

To illustrate error computations and convergence of finite element solutions, we have included a function `convergence_rate` in the `ft06_poisson_vc.py` program. This is a tool that is very handy when verifying finite element codes and will therefore be explained in detail here.

The L^2 norm of the error in a finite element approximation u , u_e being the exact solution, is given by

Various ways of computing the error.

$$E = \left(\int_{\Omega} (u_e - u)^2 dx \right)^{1/2},$$

and implemented in FEniCS by

```
error = (u - u_e)**2*dx
E = sqrt(abs(assemble(error)))
```

Sometimes, for very small error values, the result of `assemble(error)` can be a (very small) negative number, so we have used `abs` in the expression for `E` above to ensure a positive value for the `sqrt` function.

We remark that `u_e` will, in the expression above, be interpolated onto the function space `V` before `assemble` can perform the integration over the domain. This implies that the exact solution used in the integral will vary linearly over the cells, and not as a sine function, if `V` corresponds to linear Lagrange elements. This situation may yield a smaller error `u - u_e` than what is actually true. More accurate representation of the exact solution is easily achieved by interpolating the formula onto a space defined by higher-order elements, say of third degree:

```
Ve = FunctionSpace(mesh, 'P', degree=3)
u_e_Ve = interpolate(u_e, Ve)
error = (u - u_e_Ve)**2*dx
E = sqrt(assemble(error))
```

To achieve complete mathematical control of which function space the computations are carried out in, we can explicitly interpolate `u` to the same space:

```
u_Ve = interpolate(u, Ve)
error = (u_Ve - u_e_Ve)**2*dx
```

The square in the expression for `error` will be expanded and lead to a lot of terms that almost cancel when the error is small, with the potential of introducing significant rounding errors. The function `errornorm` is available for avoiding this effect by first interpolating `u` and `u_exact` to a space with higher-order elements, then subtracting the degrees of freedom, and then performing the integration of the error field. The usage is simple:

```
E = errornorm(u_exact, u, normtype='L2', degree=3)
```

It is illustrative to look at the short implementation of `errornorm`:

```
def errornorm(u_exact, u, Ve):
    u_Ve = interpolate(u, Ve)
    u_e_Ve = interpolate(u_exact, Ve)
    e_Ve = Function(Ve)
    # Subtract degrees of freedom for the error field
    e_Ve.vector()[:] = u_e_Ve.vector().array() - \
        u_Ve.vector().array()
    error = e_Ve**2*dx
```

```
    return sqrt(assemble(error))
```

The `errornorm` procedure turns out to be identical to computing the expression $(u_e - u)^{**2} * dx$ directly in the present test case.

Sometimes it is of interest to compute the error of the gradient field: $\|\nabla(u - u_e)\|$ (often referred to as the H^1 seminorm of the error). Given the error field `e_Ve` above, we simply write

```
H1seminorm = sqrt(assemble(dot(grad(e_Ve), grad(e_Ve))*dx))
```

All the various types of error computations here are placed in a function `compute_errors` in `ft06_poisson_vc.py`: **hpl 16**: Necessary to repeat code? New info is essentiall the return dict. **hpl 17**: Anders, I (in 2010...) ran into problems with `fenics.errornorm`, see comments in the code below, and made the version below. We should check out these problems again and adjust `fenics.errornorm` if necessary.

```
def compute_errors(u, u_exact):
    """Compute various measures of the error u - u_exact, where
    u is a finite element Function and u_exact is an Expression."""

    # Compute error norm (for very small errors, the value can be
    # negative so we run abs(assemble(error)) to avoid failure in sqrt

    V = u.function_space()

    # Function - Expression
    error = (u - u_exact)**2*dx
    E1 = sqrt(abs(assemble(error)))

    # Explicit interpolation of u_e onto the same space as u:
    u_e = interpolate(u_exact, V)
    error = (u - u_e)**2*dx
    E2 = sqrt(abs(assemble(error)))

    # Explicit interpolation of u_exact to higher-order elements,
    # u will also be interpolated to the space Ve before integration
    Ve = FunctionSpace(V.mesh(), 'P', 5)
    u_e = interpolate(u_exact, Ve)
    error = (u - u_e)**2*dx
    E3 = sqrt(abs(assemble(error)))

    # fenics.errornorm interpolates u and u_e to a space with
    # given degreee, and creates the error field by subtracting
    # the degrees of freedom, then the error field is integrated
    # TEMPORARY BUG - doesn't accept Expression for u_e
    #E4 = errornorm(u_e, u, normtype='l2', degree=3)
    # Manual implementation errornorm to get around the bug:
    def errornorm(u_exact, u, Ve):
        u_Ve = interpolate(u, Ve)
        u_e_Ve = interpolate(u_exact, Ve)
        e_Ve = Function(Ve)
        # Subtract degrees of freedom for the error field
```

```

e_Ve.vector()[:] = u_e_Ve.vector().array() - u_Ve.vector().array()
# More efficient computation (avoids the rhs array result above)
#e_Ve.assign(u_e_Ve) # e_Ve = u_e_Ve
#e_Ve.vector().axpy(-1.0, u_Ve.vector()) # e_Ve += -1.0*u_Ve
error = e_Ve**2*dx(Ve.mesh())
return sqrt(abs(assemble(error))), e_Ve
E4, e_Ve = errornorm(u_exact, u, Ve)

# Infinity norm based on nodal values
u_e = interpolate(u_exact, V)
E5 = abs(u_e.vector().array() - u.vector().array()).max()

# H1 seminorm
error = dot(grad(e_Ve), grad(e_Ve))*dx
E6 = sqrt(abs(assemble(error)))

# Collect error measures in a dictionary with self-explanatory keys
errors = {'u - u_exact': E1,
          'u - interpolate(u_exact,V)': E2,
          'interpolate(u,Ve) - interpolate(u_exact,Ve)': E3,
          'errornorm': E4,
          'infinity norm (of dofs)': E5,
          'grad(error) H1 seminorm': E6}

return errors

```

Computing convergence rates empirically. Calling the `solver` function for finer and finer meshes enables us to study the convergence rate. Define the element size $h = 1/n$, where n is the number of cell divisions in x and y direction (`n=Nx=Ny` in the code). We perform experiments with $h_0 > h_1 > h_2 \dots$ and compute the corresponding errors E_0, E_1, E_3 and so forth. Assuming $E_i = Ch_i^r$ for unknown constants C and r , we can compare two consecutive experiments, $E_i = Ch_i^r$ and $E_{i-1} = Ch_{i-1}^r$, and solve for r :

$$r = \frac{\ln(E_i/E_{i-1})}{\ln(h_i/h_{i-1})}.$$

The r values should approach the expected convergence rate `degree+1` as i increases.

The procedure above can easily be turned into Python code. Here we run through a different types of elements (P1, P2, P3, and P4), perform experiments over a series of refined meshes, and for each experiment report the six error types as returned by `compute_errors`:

```

def convergence_rate(u_exact, f, u0, p, degrees,
                     n=[2**k+3 for k in range(5)]):
    """
    Compute convergence rates for various error norms for a
    sequence of meshes with Nx=Ny=b and P1, P2, ...,
    Pdegrees elements. Return rates for two consecutive meshes:
    rates[degree][error_type] = r0, r1, r2, ...
    """

```

```

h = {} # Discretization parameter, h[degree][experiment]
E = {} # Error measure(s), E[degree][experiment][error_type]
P_degrees = 1,2,3,4
num_meshes = 5

# Perform experiments with meshes and element types
for degree in P_degrees:
    n = 4 # Coarsest mesh division
    h[degree] = []
    E[degree] = []
    for i in range(num_meshes):
        n *= 2
        h[degree].append(1.0/n)
        u = solver(p, f, u0, n, n, degree,
                    linear_solver='direct')
        errors = compute_errors(u, u_exact)
        E[degree].append(errors)
        print('2*(%dx%d) P%d mesh, %d unknowns, E1=%g' %
              (n, n, degree, u.function_space().dim(),
               errors['u - u_exact']))
    # Convergence rates
    from math import log as ln # log is a fenics name too
    error_types = list(E[1][0].keys())
    rates = {}
    for degree in P_degrees:
        rates[degree] = {}
        for error_type in sorted(error_types):
            rates[degree][error_type] = []
        for i in range(num_meshes):
            Ei = E[degree][i][error_type]
            Eim1 = E[degree][i-1][error_type]
            r = ln(Ei/Eim1)/ln(h[degree][i]/h[degree][i-1])
            rates[degree][error_type].append(round(r,2))
    return rates

def convergence_rate_sin():
    """Compute convergence rates for u=sin(x)*sin(y) solution."""
    omega = 1.0
    u_exact = Expression('sin(omega*pi*x[0])*sin(omega*pi*x[1])',
                         omega=omega)
    f = 2*omega**2*pi**2*u_exact
    u0 = Constant(0)
    p = Constant(1)
    # Note: P4 for n>=128 seems to break down
    rates = convergence_rates(u_exact, f, u0, p, degrees=4,
                               n=[2***(k+3) for k in range(5)])
    # Print rates
    print('\n\n')
    for error_type in error_types:
        print(error_type)
        for degree in P_degrees:
            print('P%d: %s' %
                  (degree, str(rates[degree][error_type])[1:-1]))

```

Note how we make a complete general function `convergence_rate`, aimed at any 2D Poisson problem in the class we now can solve, and then call this general function in `convergence_rate_sin` for a special test case.

Test problem. Section 5.2.6 specifies a more complicated solution,

$$u(x, y) = \sin(\omega\pi x)\sin(\omega\pi y)$$

on the unit square. This choice implies $f(x, y) = 2\omega^2\pi^2 u(x, y)$. With ω restricted to an integer it follows that $u_0 = 0$.

We need to define the appropriate boundary conditions, the exact solution, and the f function in the code:

```
def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, Constant(0.0), boundary)

omega = 1.0
u_e = Expression('sin(omega*pi*x[0])*sin(omega*pi*x[1])',
                 omega=omega)

f = 2*pi**2*omega**2*u_e
```

Experiments. Calling `convergence_rate_sin()` gives some interesting results. Using the error measure E5 based on the infinity norm of the difference of the degrees of freedom, we have

	element	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
P1		1.99	1.97	1.99	2.0	2.0
P2		3.99	3.96	3.99	4.0	3.99
P3		3.96	3.89	3.96	3.99	4.0
P4		3.75	4.99	5.0	5.0	

The computations with P4 elements on a 128×128 with a direct solver (UMFPACK) on a small laptop broke down. Otherwise we achieve expected results: the error goes like h^{d+1} for elements of degree d . Also L^2 norms based on the `errorenorm` gives the expected h^{d+1} rate for u and h^d for ∇u .

However, using `(u - u_exact)**2` for the error computation, which implies interpolating `u_exact` onto the same space as `u`, results in h^4 convergence for P2 elements.

	element	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
P1		1.98	1.94	1.98	2.0	2.0
P2		3.98	3.95	3.99	3.99	3.99
P3		3.69	4.03	4.01	3.95	2.77

This is an example where it is important to interpolate `u_exact` to a higher-order space (polynomials of degree 3 are sufficient here) to avoid computing a too optimistic convergence rate.

Checking convergence rates is the next best method for verifying PDE codes (the best being a numerical solution without approximation errors as in Section 5.2.4 and many other places in this tutorial).

5.4 Multiple domains and boundaries

hpl 11: Need a little intro.

5.4.1 Combining Dirichlet and Neumann conditions

Let us make a slight extension of our two-dimensional Poisson problem from Chapter 2 and add a Neumann boundary condition. The domain is still the unit square, but now we set the Dirichlet condition $u = u_0$ at the left and right sides, $x = 0$ and $x = 1$, while the Neumann condition

$$-\frac{\partial u}{\partial n} = g$$

is applied to the remaining sides $y = 0$ and $y = 1$. The Neumann condition is also known as a *natural boundary condition* (in contrast to an essential boundary condition).

PDE problem. Let Γ_D and Γ_N denote the parts of $\partial\Omega$ where the Dirichlet and Neumann conditions apply, respectively. The complete boundary-value problem can be written as

$$-\nabla^2 u = f \text{ in } \Omega, \quad (5.13)$$

$$u = u_0 \text{ on } \Gamma_D, \quad (5.14)$$

$$-\frac{\partial u}{\partial n} = g \text{ on } \Gamma_N. \quad (5.15)$$

Again we choose $u = 1 + x^2 + 2y^2$ as the exact solution and adjust f , g , and u_0 accordingly:

$$\begin{aligned} f &= -6, \\ g &= \begin{cases} -4, & y = 1 \\ 0, & y = 0 \end{cases} \\ u_0 &= 1 + x^2 + 2y^2. \end{aligned}$$

For ease of programming we may introduce a g function defined over the whole of Ω such that g takes on the right values at $y = 0$ and $y = 1$. One possible extension is

$$g(x, y) = -4y.$$

Variational formulation. The first task is to derive the variational problem. This time we cannot omit the boundary term arising from the integration by parts, because v is only zero on Γ_D . We have

$$-\int_{\Omega} (\nabla^2 u)v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} \frac{\partial u}{\partial n} v \, ds,$$

and since $v = 0$ on Γ_D ,

$$-\int_{\partial\Omega} \frac{\partial u}{\partial n} v \, ds = -\int_{\Gamma_N} \frac{\partial u}{\partial n} v \, ds = \int_{\Gamma_N} gv \, ds,$$

by applying the boundary condition on Γ_N . The resulting weak form reads

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx + \int_{\Gamma_N} gv \, ds = \int_{\Omega} fv \, dx. \quad (5.16)$$

Expressing this equation in the standard notation $a(u, v) = L(v)$ is straightforward with

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (5.17)$$

$$L(v) = \int_{\Omega} fv \, dx - \int_{\Gamma_N} gv \, ds. \quad (5.18)$$

Implementation. How does the Neumann condition impact the implementation? Let us go back to the very simplest file, `ft01_poisson_flat.py`, from Section 2.1.4, we realize that the statements remain almost the same. Only two adjustments are necessary:

- The function describing the boundary where Dirichlet conditions apply must be modified.
- The new boundary term must be added to the expression in `L`.

The first adjustment can be coded as

```
def Dirichlet_boundary(x, on_boundary):
```

```

if on_boundary:
    if x[0] == 0 or x[0] == 1:
        return True
    else:
        return False
else:
    return False

```

A more compact implementation reads

```

def Dirichlet_boundary(x, on_boundary):
    return on_boundary and (x[0] == 0 or x[0] == 1)

```

Never use `==` for comparing real numbers!

A list like `x[0] == 1` should never be used if `x[0]` is a real number, because rounding errors in `x[0]` may make the test fail even when it is mathematically correct. Consider

```

>>> 0.1 + 0.2 == 0.3
False
>>> 0.1 + 0.2
0.3000000000000004

```

Comparison of real numbers need to use tolerances! The values of the tolerances depend on the size of the numbers involved in arithmetic operations:

```

>>> abs(0.1+0.2 - 0.3)
5.551115123125783e-17
>>> abs(1.1+1.2 - 2.3)
0.0
>>> abs(10.1+10.2 - 20.3)
3.552713678800501e-15
>>> abs(100.1+100.2 - 200.3)
0.0
>>> abs(1000.1+1000.2 - 2000.3)
2.2737367544323206e-13
>>> abs(10000.1+10000.2 - 20000.3)
3.637978807091713e-12

```

For numbers around unity, tolerances as low as $3 \cdot 10^{-16}$ can be used (in fact, this tolerance is known as the constant `DOLFIN_EPS` in FEniCS), otherwise an appropriate tolerance must be found.

Testing for `x[0] == 1` should therefore be implemented as

```

tol = 1E-14
if abs(x[0] - 1) < tol:
    ...

```

Here is a new boundary function using tolerances in the test:

```
def Dirichlet_boundary(x, on_boundary):
    tol = 1E-14 # tolerance for coordinate comparisons
    return on_boundary and \
        (abs(x[0]) < tol or abs(x[0] - 1) < tol)
```

The second adjustment of our program concerns the definition of L , where we have to add a boundary integral and a definition of the g function to be integrated:

```
g = Expression('-4*x[1]')
L = f*v*dx - g*v*ds
```

The `ds` variable implies a boundary integral, while `dx` implies an integral over the domain Ω . No more modifications are necessary.

5.4.2 Multiple Dirichlet conditions

The PDE problem from the previous section applies a function $u_0(x,y)$ for setting Dirichlet conditions at two parts of the boundary. Having a single function to set multiple Dirichlet conditions is seldom possible. The more general case is to have m functions for setting Dirichlet conditions on m parts of the boundary. The purpose of this section is to explain how such multiple conditions are treated in FEniCS programs.

Let us return to the case from Section 5.4.1 and define two separate functions for the two Dirichlet conditions:

$$\begin{aligned} -\nabla^2 u &= -6 \text{ in } \Omega, \\ u &= u_L \text{ on } \Gamma_0, \\ u &= u_R \text{ on } \Gamma_1, \\ -\frac{\partial u}{\partial n} &= g \text{ on } \Gamma_N. \end{aligned}$$

Here, Γ_0 is the boundary $x = 0$, while Γ_1 corresponds to the boundary $x = 1$. We have that $u_L = 1 + 2y^2$, $u_R = 2 + 2y^2$, and $g = -4y$.

Functions for marking Dirichlet boundaries. For the left boundary Γ_0 we define the usual triple of a function for the boundary value, a function for defining the boundary of interest, and a `DirichletBC` object:

```
u_L = Expression('1 + 2*x[1]*x[1]')

def left_boundary(x, on_boundary):
    tol = 1E-14 # tolerance for coordinate comparisons
    return on_boundary and abs(x[0]) < tol

Gamma_0 = DirichletBC(V, u_L, left_boundary)
```

For the boundary $x = 1$ we write a similar code snippet:

```
u_R = Expression('2 + 2*x[1]*x[1]')

def right_boundary(x, on_boundary):
    tol = 1E-14 # tolerance for coordinate comparisons
    return on_boundary and abs(x[0] - 1) < tol

Gamma_1 = DirichletBC(V, u_R, right_boundary)
```

The various essential conditions are then collected in a list and used in the solution process:

```
bcs = [Gamma_0, Gamma_1]
...
solve(a == L, u, bcs)
# or
problem = LinearVariationalProblem(a, L, u, bcs)
solver = LinearVariationalSolver(problem)
solver.solve()
```

In other problems, where the u values are constant at a part of the boundary, we may use a simple `Constant` object instead of an `Expression` object.

5.4.3 Working with subdomains

Solving PDEs in domains made up of different materials is a frequently encountered task. In FEniCS, these kind of problems are handled by defining subdomains inside the domain. The subdomains may represent the various materials. We can thereafter define material properties through functions, known in FEniCS as *mesh functions*, that are piecewise constant in each subdomain. A simple example with two materials (subdomains) in 2D will demonstrate the basic steps in the process.

Suppose we want to solve

$$\nabla \cdot [k(x,y)\nabla u(x,y)] = 0, \quad (5.19)$$

in a domain Ω consisting of two subdomains where k takes on a different value in each subdomain. For simplicity, yet without loss of generality, we choose for the current implementation the domain $\Omega = [0,1] \times [0,1]$ and divide it into two equal subdomains, as depicted in Figure 5.3,

$$\Omega_0 = [0,1] \times [0,1/2], \quad \Omega_1 = [0,1] \times (1/2,1].$$

We define $k(x,y) = k_0$ in Ω_0 and $k(x,y) = k_1$ in Ω_1 , where $k_0 > 0$ and $k_1 > 0$ are given constants.

Physically, the present problem may correspond to heat conduction, where the heat conduction in Ω_1 is more efficient than in Ω_0 . An alternative inter-

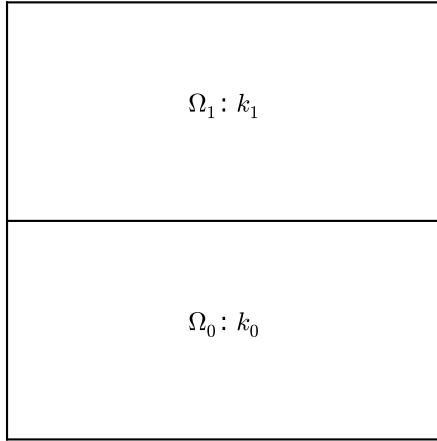


Fig. 5.3 Medium with discontinuous material properties.

pretation is flow in porous media with two geological layers, where the layers' ability to transport the fluid differ.

Expression objects with if test. The simplest way of implementing a variable k is to define an `Expression` object where we return the appropriate k value depending on the position in space. Since we need some testing on the coordinates, the most straightforward approach is to define a subclass of `Expression`, where we can use a full Python method instead of just a C++ string formula for specifying a function. The method that defines the function is called `eval`:

```
class K(Expression):
    def set_k_values(self, k0, k1):
        self.k0, self.k1 = k0, k1

    def eval(self, value, x):
        """x: spatial point, value[0]: function value."""
        # Fill in-place value[0] for scalar function,
        # value[:] for vector function (no return)

        tol = 1E-14 # Tolerance for coordinate comparisons
        if x[1] <= 0.5+tol:
            value[0] = self.k0
        else:
            value[0] = self.k1

    # Initialize
    k = K()
    k.set_k_values(1, 0.01)
```

The `eval` method gives great flexibility in defining functions, but a downside is that C++ calls up `eval` in Python for each point x , which is a slow process,

and the number of calls is proportional to the number of numerical integration points in the mesh (about the number of degrees of freedom). Function expressions in terms of strings are compiled to efficient C++ functions, being called from C++, so we should try to express functions as string expressions if possible. (The `eval` method can also be defined through C++ code, but this is much more complicated and not covered here.) The idea is to use inline if tests in C++:

```
tol = 1E-14
k0 = 1.0
k1 = 0.01
k = Expression('x[1] <= 0.5+tol? k0 : k1',
               tol=tol, k0=k0, k1=k1)
```

The method with if tests on the location is feasible when the subdomains have very simple shapes. A completely general method, utilizing *mesh functions*, is described next.

Mesh functions. We now address how to specify the subdomains Ω_0 and Ω_1 so that the method also works for subdomains of any shape. For this purpose we need to use subclasses of class `SubDomain`, not only plain functions as we have used so far for specifying boundaries. Consider the boundary function

```
def boundary(x, on_boundary):
    tol = 1E-14
    return on_boundary and abs(x[0]) < tol
```

for defining the boundary $x = 0$. Instead of using such a stand-alone function, we can create an instance (or object) of a subclass of `SubDomain`, which implements the `inside` method as an alternative to the `boundary` function:

```
class Boundary(SubDomain):
    def inside(self, x, on_boundary):
        tol = 1E-14
        return on_boundary and abs(x[0]) < tol

boundary = Boundary()
bc = DirichletBC(V, Constant(0), boundary)
```

A word about computer science terminology may be used here: The term *instance* means a Python object of a particular type (such as `SubDomain`, `Function`, `FunctionSpace`, etc.). Many use *instance* and *object* as interchangeable terms. In other computer programming languages one may also use the term *variable* for the same thing. We mostly use the well-known term *object* in this text.

A subclass of `SubDomain` with an `inside` method offers functionality for marking parts of the domain or the boundary. Now we need to define one class for the subdomain Ω_0 where $y \leq 1/2$ and another for the subdomain Ω_1 where $y \geq 1/2$:

```
tol = 1E-14 # Tolerance for coordinate comparisons
```

```

class Omega0(SubDomain):
    def inside(self, x, on_boundary):
        return x[1] <= 0.5+tol

class Omega1(SubDomain):
    def inside(self, x, on_boundary):
        return x[1] >= 0.5-tol

```

Notice the use of `<=` and `>=` in both tests. For a cell to belong to, e.g., Ω_1 , the `inside` method must return `True` for all the vertices `x` of the cell. So to make the cells at the internal boundary $y = 1/2$ belong to Ω_1 , we need the test `x[1] >= 0.5`. However, because of potential rounding errors in the coordinates `x[1]`, we use a tolerance in the comparisons: `x[1] >= 0.5-tol`.

The next task is to use a *mesh function* to mark all cells in Ω_0 with the subdomain number 0 and all cells in Ω_1 with the subdomain number 1. Our convention is to number subdomains as 0,1,2,....

A `MeshFunction` object is a discrete function that can be evaluated at a set of so-called *mesh entities*. Examples of mesh entities are cells, facets, and vertices. A `MeshFunction` over cells is suitable to represent subdomains (materials), while a `MeshFunction` over facets is used to represent pieces of external or internal boundaries. Mesh functions over vertices can be used to describe continuous fields. The specialized classes `CellFunction` and `FacetFunction` are used to construct mesh functions of cells and facets, respectively.

Since we need to define subdomains of Ω in the present example, we make use of a `CellFunction`. The constructor is fed with two arguments: 1) the type of value: `'int'` for integers, `'uint'` for positive (unsigned) integers, `'double'` for real numbers, and `'bool'` for logical values; 2) a `Mesh` object. Alternatively, the constructor can take just a filename and initialize the `CellFunction` from data in a file.

We start with creating a `CellFunction` whose values are non-negative integers (`'uint'`) for numbering the subdomains. The appropriate code for two subdomains then reads

```

materials = CellFunction('size_t', mesh)
# Mark subdomains with numbers 0 and 1
subdomain0 = Omega0()
subdomain0.mark(materials, 0)
subdomain1 = Omega1()
subdomain1.mark(materials, 1)

# Alternative
materials.set_all(0)
subdomain1.mark(materials, 1)

```

Calling `materials.array()` returns a `numpy` array of the subdomain values. That is, `materials.array()[i]` is the subdomain value of cell number `i`. This array is used to look up the subdomain or material number of a specific element.

We need a function `k` that is constant in each subdomain Ω_0 and Ω_1 . Since we want `k` to be a finite element function, it is natural to choose a space of functions that is constant over each element. The family of discontinuous Galerkin methods, in FEniCS denoted by 'DG', is suitable for this purpose. Since we want functions that are piecewise constant, the value of the degree parameter is zero:

```
V0 = FunctionSpace(mesh, 'DG', 0)
k = Function(V0)
```

To fill `k` with the right values in each element, we loop over all cells (i.e., indices in `materials.array()`), extract the corresponding subdomain number of a cell, and assign the corresponding k value to the `k.vector()` array:

```
k_values = [1.5, 50] # values of k in the two subdomains
for cell_no in range(len(materials.array())):
    material_no = materials.array()[cell_no]
    k.vector()[cell_no] = k_values[material_no]
```

Long loops in Python are known to be slow, so for large meshes it is preferable to avoid such loops and instead use *vectorized code*. Normally this implies that the loop must be replaced by calls to functions from the `numpy` library that operate on complete arrays (in efficient C code). The functionality we want in the present case is to compute an array of the same size as `materials.array()`, but where the value `i` of an entry in `materials.array()` is replaced by `k_values[i]`. Such an operation is carried out by the `numpy` function `choose`:

```
help = numpy.asarray(materials.array(), dtype=numpy.int32)
k.vector()[:] = numpy.choose(help, k_values)
```

The `help` array is required since `choose` cannot work with `materials.array()` because this array has elements of type `uint32`. We must therefore transform this array to an array `help` with standard `int32` integers.

The next section exemplifies a complete solver with a piecewise constant coefficient, like k , defined through `SubDomain` objects, combined with different types of boundary conditions.

C++ strings for subdomain definitions. The `SubDomain` class in Python is convenient, but leads to lots of function calls from C++ to Python, which are slow. In large problems, the subdomains should be defined through C++ code. This is easy to achieve using the `CompiledSubDomain` object. Consider the definition of classes `Omega0` and `Omega1` above in Python. The key strings that define these subdomain can be expressed in C++ syntax and fed to `CompiledSubDomain` as follows:

```
tol = 1E-14 # Tolerance for coordinate comparisons

subdomain0 = CompiledSubDomain(
    'x[1] <= boundary+tol', tol=1E-14, boundary=0.5)
subdomain1 = CompiledSubDomain(
```

```
'x[1] >= boundary-tol', tol=1E-14, boundary=0.5)
```

As seen, one can have parameters in the strings and specify their values by keyword arguments. The resulting objects, `subdomain0` and `subdomain1`, can be used as ordinary `SubDomain` objects.

Compiled subdomain strings can be applied for specifying boundaries as well, e.g.,

```
y_R = CompiledSubDomain('on_boundary && near(x[1], R, eps=tol)',
                        tol=1E-14, R=2) # y=2
```

It is possible to feed the C++ string (without parameters) directly as the third argument to `DirichletBC` without explicitly constructing a `CompiledSubDomain` object:

```
bc1 = DirichletBC(V, value, 'on_boundary && near(x[1], 2, 1E-14)')
```

5.4.4 Multiple Neumann, Robin, and Dirichlet condition

Consider the model problem from Section 5.4.2 where we had both Dirichlet and Neumann conditions. The term `v*g*ds` in the expression for `L` implies a boundary integral over the complete boundary, or in FEniCS terms, an integral over all exterior facets. However, the contributions from the parts of the boundary where we have Dirichlet conditions are erased when the linear system is modified by the Dirichlet conditions. We would like, from an efficiency point of view, to integrate `v*g*ds` only over the parts of the boundary where we actually have Neumann conditions. And more importantly, in other problems one may have different Neumann conditions or other conditions like the Robin type condition. With the mesh function concept we can mark different parts of the boundary and integrate over specific parts. The same concept can also be used to treat multiple Dirichlet conditions. The forthcoming text illustrates how this is done.

Three types of boundary conditions. We extend our repertoire of boundary conditions to three types: Dirichlet, Neumann, and Robin. Dirichlet conditions apply to some parts $\Gamma_{D,0}, \Gamma_{D,1}, \dots$, of the boundary:

$$u_{0,0} \text{ on } \Gamma_{D,0}, \quad u_{0,1} \text{ on } \Gamma_{D,1}, \dots$$

where $u_{0,i}$ are prescribed functions, $i = 0, 1, \dots$. On other parts, $\Gamma_{N,0}, \Gamma_{N,1}, \dots$, and so on, we have Neumann conditions

$$-p \frac{\partial u}{\partial n} = g_0 \text{ on } \Gamma_{N,0}, \quad -p \frac{\partial u}{\partial n} = g_1 \text{ on } \Gamma_{N,1}, \quad \dots$$

Finally, we have *Robin conditions*

$$-p \frac{\partial u}{\partial n} = r(u - s),$$

where r and s are specified functions. The Robin condition is most often used to model heat transfer to the surroundings and arise naturally from Newton's cooling law. In that case, r is a heat transfer coefficient, and s is the temperature of the surroundings. Both can be space and time-dependent. The Robin conditions apply at some parts $\Gamma_{R,0}$, $\Gamma_{R,1}$, and so forth:

$$-p \frac{\partial u}{\partial n} = r_0(u - s_0) \text{ on } \Gamma_{R,0}, \quad -p \frac{\partial u}{\partial n} = r_1(u - s_1) \text{ on } \Gamma_{R,1}, \quad \dots$$

A general model problem. With the notation above, the model problem to be solved with multiple Dirichlet, Neumann, and Robin conditions can formally be defined as

$$-\nabla \cdot (p \nabla u) = -f, \text{ in } \Omega, \tag{5.20}$$

$$u = u_{0,i} \text{ on } \Gamma_{D,i}, \quad i = 0, 1, \dots \tag{5.21}$$

$$-p \frac{\partial u}{\partial n} = g_i \text{ on } \Gamma_{N,i}, \quad i = 0, 1, \dots \tag{5.22}$$

$$-p \frac{\partial u}{\partial n} = r_i(u - s_i) \text{ on } \Gamma_{R,i}, \quad i = 0, 1, \dots \tag{5.23}$$

Variational formulation. Integration by parts of $-\int_{\Omega} v \nabla \cdot (p \nabla u) dx$ becomes as usual

$$-\int_{\Omega} v \nabla \cdot (p \nabla u) dx = \int_{\Omega} p \nabla u \cdot \nabla v dx - \int_{\partial \Omega} p \frac{\partial u}{\partial n} v ds.$$

The boundary integral does not apply to the parts of the boundary where we have Dirichlet conditions ($\Gamma_{D,i}$). Moreover, on the remaining parts, we must split the boundary integral into the parts where we have Neumann and Robin conditions such that we insert the right conditions as integrands. Specifically, we have

$$\begin{aligned} -\int_{\partial \Omega} p \frac{\partial u}{\partial n} v ds &= -\sum_i \int_{\Gamma_{N,i}} p \frac{\partial u}{\partial n} ds - \sum_i \int_{\Gamma_{R,i}} p \frac{\partial u}{\partial n} ds \\ &= \sum_i \int_{\Gamma_{N,i}} g_i ds + \sum_i \int_{\Gamma_{R,i}} r_i(u - s_i) ds. \end{aligned}$$

The variational formulation then becomes

$$F = \int_{\Omega} p \nabla u \cdot \nabla v \, dx + \sum_i \int_{\Gamma_{N,i}} g_i v \, ds + \sum_i \int_{\Gamma_{R,i}} r_i(u - s_i)v \, ds - \int_{\Omega} f v \, dx = 0. \quad (5.24)$$

We have been used to writing this variational formulation in the standard notation $a(u, v) = L(v)$, which requires that we identify all integrals with *both* u and v , and collect these in $a(u, v)$, while the remaining integrals with v and not u go into $L(v)$. The integral from the Robin condition must of this reason be split in two parts:

$$\int_{\Gamma_{R,i}} r_i(u - s_i)v \, ds = \int_{\Gamma_{R,i}} r_i u v \, ds - \int_{\Gamma_{R,i}} r_i s_i v \, ds.$$

We then have

$$a(u, v) = \int_{\Omega} p \nabla u \cdot \nabla v \, dx + \sum_i \int_{\Gamma_{R,i}} r_i u v \, ds, \quad (5.25)$$

$$L(v) = \int_{\Omega} f v \, dx - \sum_i \int_{\Gamma_{N,i}} g_i v \, ds + \sum_i \int_{\Gamma_{R,i}} r_i s_i v \, ds. \quad (5.26)$$

Implementation of boundary conditions. Looking at our previous `solver` functions for solving the 2D Poisson equation, the following new aspects must be taken care of:

1. definition of a mesh function over the boundary,
2. marking each side as a subdomain, using the mesh function,
3. splitting a boundary integral into parts.

A general approach to the first task is to mark each of the desired boundaries with markers 0, 1, 2, and so forth. Here we aim at the four sides of the unit square, marked with 0 ($x = 0$), 1 ($x = 1$), 2 ($y = 0$), and 3 ($y = 1$). The marking of boundaries makes use of a mesh function object, but contrary to Section 5.4.3, this is not a function over cells, but a function over cell facets. We apply the `FacetFunction` for this purpose:

```
boundary_parts = FacetFunction('size_t', mesh)
```

As in Section 5.4.3 we use a subclass of `SubDomain` to identify the various parts of the mesh function. Problems with domains of more complicated geometries may set the mesh function for marking boundaries as part of the mesh generation. In our case, the $x = 0$ boundary can be marked by

```
class BoundaryX0(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[0]) < tol

bx0 = BoundaryX0()
bx0.mark(boundary_parts, 0)
```

Similarly, we make the classes `BoundaryX1` for the $x = 1$ boundary, `BoundaryY0` for the $y = 0$ boundary, and `BoundaryY1` for the $y = 1$ boundary, and mark these as subdomains 1, 2, and 3, respectively.

For generality of the implementation, we let the user specify what kind of boundary condition that applies to each of the four boundaries. We set up a Python dictionary for this purpose, with the key as subdomain number and the value as a dictionary specifying the kind of condition as key and a function as its value. For example,

```
boundary_conditions = {
    0: {'Dirichlet': u0},
    1: {'Robin': (r, s)},
    2: {'Neumann': g},
    3: {'Neumann', 0}}
```

specifies

- a Dirichlet condition, with values implemented by an `Expression` or `Constant` object `u0`, on subdomain 0, i.e., the $x = 1$ boundary;
- a Robin condition (5.4.4) on subdomain 1, $x = 1$, with `Expression` or `Constant` objects `r` and `s` specifying r and s ;
- a Neumann condition $\partial u / \partial n = g$ on subdomain 2, $y = 0$, where an `Expression` or `Constant` object `g` implements the value `g`;
- a homogeneous Neumann condition $\partial u / \partial n = 0$ on subdomain 3, $y = 1$.

As explained in Section 5.4.2, multiple Dirichlet conditions must be collected in a list of `DirichletBC` objects. Based on the `boundary_conditions` data structure above, we can construct this list by the following snippet:

```
bcs = [] # List of Dirichlet conditions
for n in boundary_conditions:
    if 'Dirichlet' in boundary_conditions[n]:
        bcs.append(
            DirichletBC(V, boundary_conditions[n]['Dirichlet'],
                        boundary_parts, n))
```

The new aspect of the variational problem is the two distinct boundary integrals over $\Gamma_{N,i}$ and $\Gamma_{R,i}$. Having a mesh function over exterior cell facets (our `boundary_parts` object), where subdomains (boundary parts) are numbered as 0, 1, 2, ..., the special symbol `ds(0)` implies integration over subdomain (part) 0, `ds(1)` denotes integration over subdomain (part) 1, and so on. The idea of multiple `ds`-type objects generalizes to volume integrals too: `dx(0)`, `dx(1)`, etc., are used to integrate over subdomain 0, 1, etc., inside Ω .

Before we have `ds(n)` for integers `n` defined, we must do

```
ds = Measure('ds', domain=mesh, subdomain_data=boundaries_parts)
```

Similarly, if we want integration of different parts of the domain, we redefine `dx` as

```
dx = Measure('dx', domain=mesh, subdomain_data=domains)
```

where `domains` is a `CellFunction` defining subdomains in Ω .

Suppose we have a Robin condition with values r and s on subdomain R , a Neumann condition with value g on subdomain N , the variational form can be written

```
a = dot(grad(u), grad(v))*dx + r*u*v*ds(R)
L = f*v*dx - g*v*ds(N) + r*s*v*ds(R)
```

In our case things get a bit more complicated since the information about integrals in Neumann and Robin conditions are in the `boundary_conditions` data structure. We can collect all Neumann conditions by the code

```
u = TrialFunction(V)
v = TestFunction(V)
Neumann_integrals = []
for n in boundary_conditions:
    if 'Neumann' in boundary_conditions[n]:
        if boundary_conditions[n]['Neumann'] != 0:
            g = boundary_conditions[n]['Neumann']
            Neumann_integrals.append(g*v*ds(n))
```

Applying `sum(Neumann_integrals)` will apply the `+` operator to the variational forms in the `Neumann_integrals` list and result in the integrals we need for the right-hand side `L` of the variational form.

The integrals in the Robin condition can similarly be collected in lists:

```
Robin_a_integrals = []
Robin_L_integrals = []
for n in boundary_conditions:
    if 'Robin' in boundary_conditions[n]:
        r, s = boundary_conditions[n]['Robin']
        Robin_a_integrals.append(r*u*v*ds(n))
        Robin_L_integrals.append(r*s*v*ds(n))
```

We are now in a position to define the `a` and `L` expressions in the variational formulation:

```
a = dot(p*grad(u), grad(v))*dx +
     sum(Robin_a_integrals)
L = f*v*dx - sum(Neumann_integrals) + sum(Robin_L_integrals)
```

Simplified handling of the variational formulation. We carefully ordered the terms in the variational formulation above into the a and L parts. This requires a splitting of the Robin condition and makes the `a` and `L` expressions less readable (still we think understanding this splitting is key for any finite element programmer!). Fortunately, UFL allow us to specify the complete variational form (5.24) as *one expression* and offer tools to extract what goes into the bilinear form $a(u, v)$ and the linear form $L(v)$:

```
F = dot(p*grad(u), grad(v))*dx +
     sum(Robin_integrals) - f*v*dx + sum(Neumann_integrals)
a, L = lhs(F), rhs(F)
```

This time we can more naturally define the integrals from the Robin condition as $r*(u-s)*v*ds(n)$:

```
Robin_integrals = []
for n in boundary_conditions:
    if 'Robin' in boundary_conditions[n]:
        r, s = boundary_conditions[n]['Robin']
        Robin_integrals.append(r*(u-s)*v*ds(n))
```

The complete code is in the `solver_bc` function in the `ft06_poisson_vc.py` file.

Test problem. Let us continue to use $u_e = 1 + x^2 + 2y^2$ as the exact solution, and set $p = 1$ and $f = -6$ in the PDE. Our domain is the unit square, and we assign Dirichlet conditions at $x = 0$ and $x = 1$, a Neumann condition at $y = 1$, and a Robin condition at $y = 0$. With the given u_e , we realize that the Neumann condition is $-4y$ (which means -4 at $y = 1$), while the Robin condition can be selected in many ways. Since $\partial u / \partial n = -\partial u / \partial y = 0$ at $y = 0$, we can select $s = u$ and have r arbitrary in the Robin condition.

The boundary parts are $\Gamma_{D,0}$: $x = 0$, $\Gamma_{D,1}$: $x = 1$, $\Gamma_{R,0}$: $y = 0$, and $\Gamma_{N,0}$: $y = 1$.

When implementing this test problem (and especially other test problems with more complicated expressions), it is advantageous to use symbolic computing. Below we define u_e as a `sympy` expression and derive other functions from their mathematical definitions. Then we turn these expressions into C/C++ code, which can be fed into `Expression` objects.

```
def application_bc_test():
    # Define manufactured solution in sympy and derive f, g, etc.
    import sympy as sym
    x, y = sym.symbols('x[0] x[1]') # UFL needs x[0] for x etc.
    u = 1 + x**2 + 2*y**2
    f = -sym.diff(u, x, 2) - sym.diff(u, y, 2) # -Laplace(u)
    f = sym.simplify(f)
    u_00 = u.subs(x, 0) # x=0 boundary
    u_01 = u.subs(x, 1) # x=1 boundary
    g = -sym.diff(u, y).subs(y, 1) # x=1 boundary, du/dn=-du/dy
    r = 1000 # any function can go here
    s = u

    # Turn to C/C++ code for UFL expressions
    f = sym.printing.ccode(f)
    u_00 = sym.printing.ccode(u_00)
    u_01 = sym.printing.ccode(u_01)
    g = sym.printing.ccode(g)
    r = sym.printing.ccode(r)
    s = sym.printing.ccode(s)
    print('Test problem (C/C++):\nu = %s\nf = %s' % (u, f))
    print('u_00: %s\nu_01: %s\ng = %s\nr = %s\ns = %s' %
          (u_00, u_01, g, r, s))

    # Turn into FEniCS objects
```

```

u_00 = Expression(u_00)
u_01 = Expression(u_01)
f = Expression(f)
g = Expression(g)
r = Expression(r)
s = Expression(s)
u_exact = Expression(sym.printing.ccode(u))

boundary_conditions = {
    0: {'Dirichlet': u_00},    # x=0
    1: {'Dirichlet': u_01},    # x=1
    2: {'Robin': (r, s)},    # y=0
    3: {'Neumann': g}}       # y=1

p = Constant(1)
Nx = Ny = 2
u, p = solver_bc(
    p, f, boundary_conditions, Nx, Ny, degree=1,
    linear_solver='direct',
    debug=2*Nx*Ny < 50, # for small problems only
)

# Compute max error in infinity norm
u_e = interpolate(u_exact, u.function_space())
import numpy as np
max_error = np.abs(u_e.vector().array() -
                   u.vector().array()).max()
print('Max error:', max_error)

# Print numerical and exact solution at the vertices
if u.function_space().dim() < 50: # (small problems only)
    u_e_at_vertices = u_e.compute_vertex_values()
    u_at_vertices = u.compute_vertex_values()
    coor = u.function_space().mesh().coordinates()
    for i, x in enumerate(coor):
        print('vertex %2d (%9g,%9g): error=%g %g vs %g'
              % (i, x[0], x[1],
                 u_e_at_vertices[i] - u_at_vertices[i],
                 u_e_at_vertices[i], u_at_vertices[i]))

```

This simple test problem is turned into a real unit test for different function spaces in the function `test_solver_bc`.

Debugging the setting of boundary conditions. It is easy to make mistakes when implementing a problem with many different types of boundary conditions, as in the present case. Some helpful debugging output is to run through all vertex coordinates and check if the `SubDomain.inside` method marks the vertex as on the boundary. Another useful printout is to list which degrees of freedom that are subject to Dirichlet conditions, and for first-order Lagrange elements, add the corresponding vertex coordinate to the output.

```

if debug:
    # Print the vertices that are on the boundaries

```

```

coor = mesh.coordinates()
for x in coor:
    if bx0.inside(x, True): print('%s is on x=0' % x)
    if bx1.inside(x, True): print('%s is on x=1' % x)
    if by0.inside(x, True): print('%s is on y=0' % x)
    if by1.inside(x, True): print('%s is on y=1' % x)
# Print the Dirichlet conditions
print('No of Dirichlet conditions:', len(bcs))
d2v = dof_to_vertex_map(V)
for bc in bcs:
    bc_dict = bc.get_boundary_values()
    for dof in bc_dict:
        print('dof %d: u=%g, % (dof, bc_dict[dof]))'
              if V.ufl_element().degree() == 1:
                  print(', at point %s' %
                        (str(tuple(coor[d2v[dof]].tolist())))))

```

In addition, it is helpful to print the exact and the numerical solution at all the vertices as shown in Section 5.2.4.

Implementation of multiple subdomains. Section 5.4.3 explains how to deal with multiple subdomains of Ω and a piecewise constant coefficient function p that takes on different constant values in the different subdomains. We can easily add this type of p coefficient to the `solver_bc` function. The signature of the function is

```

def solver_bc(
    p, f,                      # Coefficients in the PDE
    boundary_conditions,        # Dict of boundary conditions
    Nx, Ny,                     # Cell division of the domain
    degree=1,                   # Polynomial degree
    subdomains=[],               # List of SubDomain objects in domain
    linear_solver='Krylov',     # Alt: 'direct'
    abs_tol=1E-5,                # Absolute tolerance in Krylov solver
    rel_tol=1E-3,                # Relative tolerance in Krylov solver
    max_iter=1000,               # Max no of iterations in Krylov solver
    log_level=PROGRESS,          # Amount of solver output
    dump_parameters=False,       # Write out parameter database?
    debug=False,
    ):
    ...
    return u, p    # p may be modified

```

If `subdomain` is an empty list, we assume there are no subdomains, and p is an `Expression` or `Constant` object specifying a formula for p . If not, `subdomain` is a list of `SubDomain` objects, defining different parts of the domain. The first element is a dummy object, defining “the rest” of the domain. The next elements define specific geometries in the `inside` methods. We start by marking all elements with subdomain number 0, this will then be “the rest” after marking subdomains 1, 2, and so on. The next step is to define `p` as a piecewise constant function over cells and fill it with values. We assume that the user-argument `p` is an array (or list) holding the values of p in the

different parts corresponding to `subdomains`. The returned `p` is needed for flux computations. If there are no subdomains, the returned `p` is just the original `p` argument.

The appropriate code for computing `p` becomes

```
import numpy as np
if subdomains:
    # subdomains is list of SubDomain objects,
    # p is array of corresponding constant values of p
    # in each subdomain
    materials = CellFunction('size_t', mesh)
    materials.set_all(0) # "the rest"
    for m, subdomain in enumerate(subdomains[1:], 1):
        subdomain.mark(materials, m)

    p_values = p
    V0 = FunctionSpace(mesh, 'DG', 0)
    p = Function(V0)
    help = np.asarray(materials.array(), dtype=np.int32)
    p.vector()[:] = np.choose(help, p_values)
```

We define $p(x, y) = p_0$ in Ω_0 and $k(x, y) = p_1$ in Ω_1 , where $p_0 > 0$ and $p_1 > 0$ are given constants. As boundary conditions, we choose $u = 0$ at $y = 0$, $u = 1$ at $y = 1$, and $\partial u / \partial n = 0$ at $x = 0$ and $x = 1$. One can show that the exact solution is now given by

$$u(x, y) = \begin{cases} \frac{2yp_1}{p_0+p_1}, & y \leq 1/2 \\ \frac{(2y-1)p_0+p_1}{p_0+p_1}, & y \geq 1/2 \end{cases} \quad (5.27)$$

As long as the element boundaries coincide with the internal boundary $y = 1/2$, this piecewise linear solution should be exactly recovered by Lagrange elements of any degree. We can use this property to verify the implementation and make a unit test for a series of function spaces:

```
def test_solvers_bc_2mat():
    tol = 2E-13 # Tolerance for comparisons

    class Omega0(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] <= 0.5+tol

    class Omega1(SubDomain):
        def inside(self, x, on_boundary):
            return x[1] >= 0.5-tol

    subdomains = [Omega0(), Omega1()]
    p_values = [2.0, 13.0]
    boundary_conditions = {
        0: {'Neumann': 0},
        1: {'Neumann': 0},
        2: {'Dirichlet': Constant(0)}, # y=0
        3: {'Dirichlet': Constant(1)}, # y=1
```

```

        }

f = Constant(0)
u_exact = Expression(
    'x[1] <= 0.5? 2*x[1]*p_1/(p_0+p_1) : '
    '((2*x[1]-1)*p_0 + p_1)/(p_0+p_1)',
    p_0=p_values[0], p_1=p_values[1])

for Nx, Ny in [(2,2), (2,4), (8,4)]:
    for degree in 1, 2, 3:
        u, p = solver_bc(
            p_values, f, boundary_conditions, Nx, Ny, degree,
            linear_solver='direct', subdomains=subdomains,
            debug=False)

        # Compute max error in infinity norm
        u_e = interpolate(u_exact, u.function_space())
        import numpy as np
        max_error = np.abs(u_e.vector().array() -
                           u.vector().array()).max()
        assert max_error < tol, 'max error: %g' % max_error

```

5.4.5 Refactoring of a solver function into solver and problem classes

A FEniCS solver for a PDE can be implemented in a general way, but the problem-dependent data, like boundary conditions, must be specified in each case by the user. The implementation in the previous section required the user to supply a `boundary_conditions` dictionary with specifications of the boundary condition on each of the four sides of the unit square. If we, e.g., want two Dirichlet conditions at one side, as our mathematical formulation of the problem in the previous section in fact supports, this is not possible without extending the `solver_bc` function.

A different software design is to introduce a problem class and methods, supplied by the user from case to case, where boundary conditions and other input data are defined. Such a design is used in a lot of more advanced FEniCS application codes, and it is time to exemplify it here. As a counterpart to the solver function, we introduce a solver class, but all the arguments for various input data are instead method calls to an instance of a *problem class*. This puts a somewhat greater burden on the programmer, but it allows for more flexibility, and the code for, e.g., boundary conditions can be more tailored to the problem at hand than the code we introduced in the `solver_bc` function in the previous section.

The solver class will need problem information and for this purpose call up the methods in a problem class. For example, the solver gets the f and p functions in the PDE problem by calling `problem.f_rhs()` and

`problem.p_coeff()`. The mesh object and the polynomial degree of the elements are supposed to be returned from `problem.mesh_degree()`. Furthermore, the problem class defines the boundary conditions in the problem as lists of minimal information from which the solver can build proper data structures.

The solver class is a wrapping of the previous `solver_bc` and `flux` functions as methods in a class, but some of the code for handling boundary conditions in `solver_bc` is now delegated to the user in the problem class.

```
from fenics import *
import numpy as np

class PoissonSolver(object):
    def __init__(self, problem, debug=False):
        self.mesh, degree = problem.mesh_degree()
        self.V = V = FunctionSpace(self.mesh, 'P', degree)
        Dirichlet_cond = problem.Dirichlet_conditions()
        if isinstance(Dirichlet_cond, (Expression)):
            # Just one Expression for Dirichlet conditions on
            # the entire boundary
            self.bcs = [DirichletBC(
                V, Dirichlet_cond,
                lambda x, on_boundary: on_boundary)]
        else:
            # Boundary SubDomain markers
            self.bcs = [
                DirichletBC(V, value, boundaries, index)
                for value, boundaries, index
                in Dirichlet_cond]

        if debug:
            # Print the Dirichlet conditions
            print('No of Dirichlet conditions:', len(self.bcs))
            coor = self.mesh.coordinates()
            d2v = dof_to_vertex_map(V)
            for bc in self.bcs:
                bc_dict = bc.get_boundary_values()
                for dof in bc_dict:
                    print('dof %2d: u=%g' % (dof, bc_dict[dof]))
                    if V.ufl_element().degree() == 1:
                        print(' at point %s' %
                              (str(tuple(coor[d2v[dof]].tolist())))))

    u = TrialFunction(V)
    v = TestFunction(V)
    p = problem.p_coeff()
    self.p = p # store for flux computations
    f = problem.f_rhs()
    F = dot(p*grad(u), grad(v))*dx
    F -= f*v*dx
    F -= sum([g*v*ds_
              for g, ds_ in problem.Neumann_conditions()])
    F += sum([r*(u-s)*ds_
              for r, s, ds_ in problem.Neumann_conditions()])
```

```

        for r, s, ds_ in problem.Robin_conditions())
self.a, self.L = lhs(F), rhs(F)

if debug and V.dim() < 50:
    A = assemble(self.a)
    print('A:\n', A.array())
    b = assemble(self.L)
    print('b:\n', b.array())

def solve(self, linear_solver='direct'):
    # Compute solution
    self.u = Function(self.V)

    if linear_solver == 'Krylov':
        solver_parameters = {'linear_solver': 'gmres',
                             'preconditioner': 'ilu'}
    else:
        solver_parameters = {'linear_solver': 'lu'}

    solve(self.a == self.L, self.u, self.bcs,
          solver_parameters=solver_parameters)
    return self.u

def flux(self):
    """Compute and return flux -p*grad(u)."""
    mesh = self.u.function_space().mesh()
    degree = self.u.ufl_element().degree()
    V_g = VectorFunctionSpace(mesh, 'P', degree)
    self.flux_u = project(-self.p*grad(self.u), V_g)
    self.flux_u.rename('flux(u)', 'continuous flux field')
    return self.flux_u

class PoissonProblem(object):
    """Abstract base class for problems."""
    def solve(self, linear_solver='direct',
              abs_tol=1E-6, rel_tol=1E-5, max_iter=1000):
        self.solver = PoissonSolver(self)
        prm = parameters['krylov_solver'] # short form
        prm['absolute_tolerance'] = abs_tol
        prm['relative_tolerance'] = rel_tol
        prm['maximum_iterations'] = max_iter
        return self.solver.solve(linear_solver)

    def solution(self):
        return self.solver.u

    def mesh_degree(self):
        """Return mesh, degree."""
        raise NotImplementedError('Must implement mesh!')

    def p_coeff(self):
        return Constant(1.0)

    def f_rhs(self):

```

```

    return Constant(0.0)

def Dirichlet_conditions(self):
    """Return list of (value,boundary_parts,index) triplets,
    or an Expression (if Dirichlet values only)."""
    return []

def Neumann_conditions(self):
    """Return list of (g,ds(n)) pairs."""
    return []

def Robin_conditions(self):
    """Return list of (r,u,ds(n)) triplets."""
    return []

```

Note that this is a general Poisson problem solver that works in any number of space dimensions and with any mesh and composition of boundary conditions.

Tip: Be careful with the `mesh` variable!

In classes, one often stores the mesh in `self.mesh`. When you need the mesh, it is easy to write just `mesh`, but this gives rise to peculiar error messages, since `mesh` is a Python module imported by `from fenics import *` and already available as a name in your file. When encountering strange error messages in statements containing a variable `mesh`, make sure you use `self.mesh`.

Below is the specific problem class for solving a scaled 2D Poisson problem. We have a two-material domain where a rectangle $[0.3, 0.7] \times [0.3, 0.7]$ is embedded in the unit square and where p has a constant value inside the rectangle and another value outside. On $x = 0$ and $x = 1$ we have homogeneous Neumann conditions, and on $y = 0$ and $y = 1$ we have the Dirichlet conditions $u = 1$ and $u = 0$, respectively.

```

class Problem1(PoissonProblem):
    """
        -div(p*grad(u))=f on the unit square.
        General Dirichlet, Neumann, or Robin condition along each
        side. Can have multiple subdomains with p constant in
        each subdomain.
    """
    def __init__(self, Nx, Ny):
        """Initialize mesh, boundary parts, and p."""
        self.mesh = UnitSquareMesh(Nx, Ny)
        tol = 1E-14

        class BoundaryX0(SubDomain):
            def inside(self, x, on_boundary):
                return on_boundary and abs(x[0]) < tol

```

```

class BoundaryX1(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[0] - 1) < tol

class BoundaryY0(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[1]) < tol

class BoundaryY1(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary and abs(x[1] - 1) < tol

# Mark boundaries
#self.boundary_parts = FacetFunction('size_t', mesh)
self.boundary_parts = FacetFunction('uint', self.mesh)
self.boundary_parts.set_all(9999)
self.bx0 = BoundaryX0()
self.bx1 = BoundaryX1()
self.by0 = BoundaryY0()
self.by1 = BoundaryY1()
self.bx0.mark(self.boundary_parts, 0)
self.bx1.mark(self.boundary_parts, 1)
self.by0.mark(self.boundary_parts, 2)
self.by1.mark(self.boundary_parts, 3)
self.ds = Measure(
    'ds', domain=self.mesh,
    subdomain_data=self.boundary_parts)

# The domain is the unit square with an embedded rectangle
class Rectangle(SubDomain):
    def inside(self, x, on_boundary):
        return 0.3 <= x[0] <= 0.7 and 0.3 <= x[1] <= 0.7

    self.materials = CellFunction('size_t', self.mesh)
    self.materials.set_all(0) # "the rest"
    subdomain = Rectangle()
    subdomain.mark(self.materials, 1)
    self.V0 = FunctionSpace(self.mesh, 'DG', 0)
    self.p = Function(self.V0)
    help = np.asarray(self.materials.array(), dtype=np.int32)
    p_values = [1, 1E-3]
    self.p.vector()[:] = np.choose(help, p_values)

    def mesh_degree(self):
        return self.mesh, 2

    def p_coeff(self):
        return self.p

    def f_rhs(self):
        return Constant(0)

    def Dirichlet_conditions(self):

```

```

    """Return list of (value,boundary) pairs."""
    return [(1.0, self.boundary_parts, 2),
            (0.0, self.boundary_parts, 3)]

def Neumann_conditions(self):
    """Return list of g*ds(n) values."""
    return [(0, self.ds(0)), (0, self.ds(1))]

```

A specific problem can be solved by

```

def demo():
    problem = PoissonProblem1(Nx=20, Ny=20)
    problem.solve(linear_solver='direct')
    u = problem.solution()
    u.rename('u', 'potential') # name 'u' is used in plot
    plot(u)
    flux_u = problem.solver.flux()
    plot(flux_u)
    vtkfile = File('poisson.pvd')
    vtkfile << u
    interactive()

def test_PoissonSolver():
    """Recover numerical solution to "machine precision". """
    class TestProblemExact(PoissonProblem):
        def __init__(self, Nx, Ny):
            """Initialize mesh, boundary parts, and p."""
            self.mesh = UnitSquareMesh(Nx, Ny)
            self.u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')

        def mesh_degree(self):
            return self.mesh, 1

        def f_rhs(self):
            return Constant(-6.0)

        def Dirichlet_conditions(self):
            return self.u0

    problem = TestProblemExact(Nx=2, Ny=2)
    problem.solve(linear_solver='direct')
    u = problem.solution()
    u_e = interpolate(problem.u0, u.function_space())
    max_error = np.abs(u_e.vector().array() -
                       u.vector().array()).max()
    tol = 1E-14
    assert max_error < tol, 'max error: %g' % max_error

if __name__ == '__main__':
    #demo()
    test_PoissonSolver()

```

The complete code is found in the file `ft08_poisson_class.py`.

Pros and cons of solver/problem classes vs solver function

What are the advantages of class `Solver` and `Problem` over the function implementation in Section 5.4.4? The primary advantage is that the class version works for any mesh and any composition of boundary conditions, while the solver function is tied to a mesh over the unit square, only one type of boundary condition on each side, and a piecewise constant p function. The programmer has to supply more code in the class version, but gets greater flexibility. The disadvantage of the class version is that it applies the class concept so one needs experience with Python class programming.

References

- [1] M. S. Alnæs, A. Logg, K. B. Ølgaard, M. E. Rognes, and G. N. Wells. Unified Form Language: A domain-specific language for weak formulations of partial differential equations. *ACM Transactions on Mathematical Software*, 40(2), 2014. doi:10.1145/2566630, arXiv:1211.4047.
- [2] Douglas N. Arnold and Anders Logg. Periodic table of the finite elements. *SIAM News*, 2014.
- [3] W. B. Bickford. *A First Course in the Finite Element Method*. Irwin, 2nd edition, 1994.
- [4] Dietrich Braess. *Finite Elements*. Cambridge University Press, Cambridge, third edition, 2007.
- [5] Susanne C. Brenner and L. Ridgway Scott. *The Mathematical Theory of Finite Element Methods*, volume 15 of *Texts in Applied Mathematics*. Springer, New York, third edition, 2008.
- [6] Philippe G. Ciarlet. *The Finite Element Method for Elliptic Problems*, volume 40 of *Classics in Applied Mathematics*. SIAM, Philadelphia, PA, 2002. Reprint of the 1978 original [North-Holland, Amsterdam; MR0520174 (58 #25001)].
- [7] J. Donea and A. Huerta. *Finite Element Methods for Flow Problems*. Wiley Press, 2003.
- [8] K. Eriksson, D. Estep, P. Hansbo, and C. Johnson. *Computational Differential Equations*. Cambridge University Press, 1996.
- [9] A. Ern and J.-L. Guermond. *Theory and Practice of Finite Elements*. Springer, 2004.
- [10] Python Software Foundation. The Python tutorial.
<http://docs.python.org/2/tutorial>.
- [11] M. Gockenbach. *Understanding and Implementing the Finite Element Method*. SIAM, 2006.
- [12] T. J. R. Hughes. *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall, 1987.
- [13] J. M. Kinder and P. Nelson. *A Student's Guide to Python for Physical Modeling*. Princeton University Press, 2015.

- [14] J. Kiusalaas. *Numerical Methods in Engineering With Python*. Cambridge University Press, 2005.
- [15] R. H. Landau, M. J. Paez, and C. C. Bordeianu. *Computational Physics: Problem Solving with Python*. Wiley, third edition, 2015.
- [16] H. P. Langtangen. *Python Scripting for Computational Science*. Springer, third edition, 2009.
- [17] H. P. Langtangen. *A Primer on Scientific Programming With Python*. Texts in Computational Science and Engineering. Springer, fifth edition, 2016.
- [18] H. P. Langtangen and L. R. Hellevik. Brief tutorials on scientific Python. <http://hplgit.github.io/bumpy/doc/web/index.html>.
- [19] H. P. Langtangen and A. Logg. *The Advanced FEniCS Tutorial - Writing State-of-the-art Finite Element Solvers in Hours*. Springer, 2016.
- [20] M. G. Larson and F. Bengzon. *The Finite Element Method: Theory, Implementation, and Applications*. Texts in Computational Science and Engineering. Springer, 2013.
- [21] A. Logg, K.-A. Mardal, and G. N. Wells. *Automated Solution of Partial Differential Equations by the Finite Element Method*. Springer, 2012.
- [22] M. Pilgrim. *Dive into Python*. Apress, 2004. <http://www.diveintopython.net>.
- [23] A. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations*. Springer Series in Computational Mathematics. Springer, 1994.
- [24] A. Henderson Squillacote. *The Paraview Guide*. Kitware, 2007.

Index

- abstract variational formulation, 14
- assemble**, 96
- assemble_system**, 96
- assembly of linear systems, 96
- boundary conditions, 120
- boundary specification (class), 117
- boundary specification (function), 20, 22
- BoxField**, 99
- C++ expression syntax, 21
- CG finite element family, 20
- CompiledSubDomain**, 119
- compute vertex values, 71
- contour plot, 100
- degrees of freedom, 23
- degrees of freedom array, 26, 76
- degrees of freedom array (vector field), 76
- dimension-independent code, 73
- Dirichlet boundary conditions, 20, 120
- DirichletBC**, 20
- dof to vertex map, 71
- energy functional, 104
- error functional, 104
- Expresion**, 28
- Expression**, 20
- expression syntax (C++), 21
- Expression with parameters, 28
- finite element specifications, 20
- flux functional, 105
- ft02_diffusion_flat1.py**, 38
- ft05_poisson_iter.py**, 65, 69, 76
- ft06_poisson_vc.py**, 78
- functionals, 104
- FunctionSpace**, 20
- heterogeneous media, 115
- info** function, 64
- interpolation, 29
- KrylovSolver, 97
- Lagrange finite element family, 20
- linear algebra backend, 64
- linear systems (in FEniCS), 96
- LinearVariationalProblem**, 69
- LinearVariationalSolver**, 69
- Mesh**, 19
- MTL4, 64
- multi-material domain, 115
- near**, 120

Neumann boundary conditions, 111, 120
 nodal values array, 26, 76
 numbering
 cell vertices, 26
 degrees of freedom, 26
 P1 element, 20
parameters database, 64
pdftk, 33
 Periodic Table of the Finite Elements,
 20
PETSc, 64
plot, 33
 plotting, 33
 Poisson's equation, 11
 Poisson's equation with variable coefficient, 78
project, 75
 projection, 74, 75
 random start vector (linear systems),
 98
rename, 24
 Robin boundary conditions, 120
 Robin condition, 121
 rotate PDF plots, 33
scitools, 98
SLEPc, 97
 structured mesh, 98
 surface plot (structured mesh), 100
sympy, 102
 test function, 12
TestFunction, 20
 time-dependent PDEs, 35
 trial function, 12
TrialFunction, 20
 Trilinos, 64
uBLAS, 64
UFL, 23
UMFPACK, 64
 unit testing, 61
 variational formulation, 12