Hans Petter Langtangen[*], Anders Logg[†]

Solving PDEs in Minutes - The FEniCS Tutorial Volume I

Sep 23, 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 Mathematical Sciences, Chalmers University of Technology and Center for Biomedical Computing, Simula Research Laboratory.

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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* [24]. This tutorial is a further development of the opening chapter in [24].

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 [24]. 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 Plesser, Marie Rognes, and Hans Joachim Scroll. Ekkehard Ellmann as well as two anonymous reviewers provided a series of suggestions and improvements.

Special thank goes to Benjamin Kehlet for all his work with the `mshr` tool and for quickly implementing our requests in this tutorial.

Oslo and Smögen, August 2016 *Hans Petter Langtangen, Anders Logg*

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, mshr, 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++ code from high-level mathematical abstractions. FIAT is the finite element backend of FEniCS, responsible for generating finite element basis functions, UFL implements the abstract mathematical language by which users may express variational problems, and mshr provides FEniCS with mesh generation capabilities.

1.2 What you will learn

The goal of this tutorial is to 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 short and 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 at how easy it is to solve PDEs with FEniCS!

1.4 Obtaining the software

Reading this tutorial obviously requires access to the FEniCS software. 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 well[1] 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 page. Once you have installed Docker, just copy the following line into a terminal window:

Terminal

[1] Running 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.

```
Terminal> curl -s https://get.fenicsproject.org | bash
```

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-enabled[2] terminal:

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 repository for this book.

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

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 Python language. A natural starting point for beginners is the classical *Python Tutorial* [11], or a tutorial geared towards scientific computing [20]. In the latter, you will also find pointers to other tutorials for scientific computing in Python. Among ordinary books we recommend the general introduction *Dive into Python* [25] as well as texts that focus on scientific computing with Python [15–19].

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.

1.6.2 The finite element method

There exist many good books on the finite element method. The books typically fall in either of two categories: the abstract mathematical version of the method or the engineering "structural analysis" formulation. FEniCS builds heavily on concepts from the abstract mathematical exposition. The first author has in development a book [22] 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 [23] is our recommended introduction to the finite element method, with a mathematical notation that goes well with FEniCS. An easy-to-read book, which also provides a good general background for using FEniCS, is Gockenbach [12]. The book by Donea and Huerta [8] has a similar style, but aims at readers with interest

in fluid flow problems. Hughes [14] 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* [9] 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 [10], Quarteroni and Valli [26], or Ciarlet [7].

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

Most books on a programming language start with a "Hello, World!" program. That is, one is curious about how a very fundamental task is expressed in the language, and writing a text to the screen can be such a task. In the world of *finite element methods for PDEs*, the most fundamental task must be to solve the Poisson equation. Our counterpart to the classical "Hello, World!" program therefore solves

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

$$u(\boldsymbol{x}) = u_{\mathrm{D}}(\boldsymbol{x}), \quad \boldsymbol{x} \text{ on } \partial\Omega\,. \tag{2.2}$$

Here, $u = u(\boldsymbol{x})$ is the unknown function, $f = f(\boldsymbol{x})$ 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 for 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 a similar program in most other software frameworks for PDEs require much more code and more technically difficult programming.

What makes FEniCS attractive?

Although many frameworks have a really elegant "Hello, World!" example on the Poisson equation, FEniCS is to our knowledge the only framework where the code stays compact and nice, very close to the mathematical formulation, also when the complexity increases with, e.g., systems of PDEs and mixed finite elements for computing on massively high-performance parallel platforms.

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 very brief introduction to the topic in this tutorial, but reading a proper book on the

finite element method in addition is encouraged. Section 1.6.2 contains a list of some suitable books. Experience shows that you can work with FEniCS as a tool to solve your PDEs even without thorough knowledge of the finite element method, as long as you get somebody to help you with formulating the PDE as a variational problem.

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:

$$-\int_\Omega (\nabla^2 u)v \,\mathrm{d}x = \int_\Omega fv \,\mathrm{d}x\,. \tag{2.4}$$

A common rule when we derive variational formulations is that we try to keep the order of the derivatives of u and v as low as possible (this will enlarge the collection of finite elements that can be used in the problem). Here, we have a second-order spatial derivative of u, which can be transformed to a first-derivative of u and v by applying the technique of integration by parts. A Laplace term will always be subject to integration by parts[1]. The formula reads

$$-\int_\Omega (\nabla^2 u)v \,\mathrm{d}x = \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x - \int_{\partial\Omega} \frac{\partial u}{\partial n} v \,\mathrm{d}s, \tag{2.5}$$

where $\frac{\partial u}{\partial n} = \nabla u \cdot n$ is the derivative of u in the outward normal direction n on the boundary.

Another feature of variational formulations is that the test function v is required to vanish on the parts of the boundary where the solution u is known (the book [22] explains in detail why this requirement is necessary). In the present problem, this means 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

$$\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x = \int_\Omega fv \,\mathrm{d}x\,. \tag{2.6}$$

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 (possi-

[1] Integration by parts in more than one space dimension is based on Gauss' divergence theorem. Simply take (2.5) as the formula to be used.

bly 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

$$\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x \quad \forall v \in \hat{V}\,. \tag{2.7}$$

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

$$V = \{v \in H^1(\Omega) : v = u_{\mathrm{D}} \text{ on } \partial\Omega\},$$
$$\hat{V} = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}\,.$$

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

$$\int_\Omega \nabla u_h \cdot \nabla v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x \quad \forall v \in \hat{V}_h \subset \hat{V}\,. \tag{2.8}$$

This variational problem, together with a suitable definition of the function spaces V_h and $\hat{V}_h$, uniquely define our approximate numerical solution of Poisson's equation (2.1). The mathematical framework may seem complicated at first glance, but the good news is that 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:

$$a(u,v) = L(v)\,. \tag{2.9}$$

For the Poisson equation, we have:

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x, \tag{2.10}$$

$$L(v) = \int_\Omega f v \,\mathrm{d}x\,. \tag{2.11}$$

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:

- 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).
- Express the PDE as a (discrete) variational problem: find $u \in V$ such that $a(u,v) = L(v)$ for all $v \in \hat{V}$.

2.1.3 Choosing a test problem

The Poisson problem (2.1)–(2.2) has so far featured a general domain Ω and general functions u_{D} for the boundary conditions and f for the right-hand side. For our first implementation we will need to make specific choices for Ω, u_{D}, and f. It will be wise to construct a 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

$$u_{\mathrm{e}}(x,y) = 1 + x^2 + 2y^2\,. \tag{2.12}$$

By inserting (2.12) into the Poisson equation (2.1), we find that $u_{\mathrm{e}}(x,y)$ is a solution if

$$f(x,y) = -6, \quad u_{\mathrm{D}}(x,y) = u_{\mathrm{e}}(x,y) = 1 + x^2 + 2y^2,$$

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 5.3.4. 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.

2.2 FEniCS implementation

2.2.1 The complete program

A FEniCS program for solving our test problem for the Poisson equation in 2D with the given choices of u_{D}, 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 condition
u_D = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]', degree=2)

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u_D, 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 and mesh
u.rename('u', 'solution')
plot(u)
plot(mesh)

# Save solution to file in VTK format
vtkfile = File('poisson/solution.pvd')
```

```
vtkfile << u


# Compute error in L2 norm
error_L2 = errornorm(u_D, u, 'L2')

# Compute maximum error at vertices
vertex_values_u_D = u_D.compute_vertex_values(mesh)
vertex_values_u = u.compute_vertex_values(mesh)
import numpy as np
error_max = np.max(np.abs(vertex_values_u_D - vertex_values_u))

# Print errors
print('error_L2  =', error_L2)
print('error_max =', error_max)

# Hold plot
interactive()
```

The complete code can be found in the file `ft01_poisson.py`.

2.2.2 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.py`:

- Use a terminal window.
- Use an integrated 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.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` or `fenicsproject start`.

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 L^2 and maximum norms 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}.

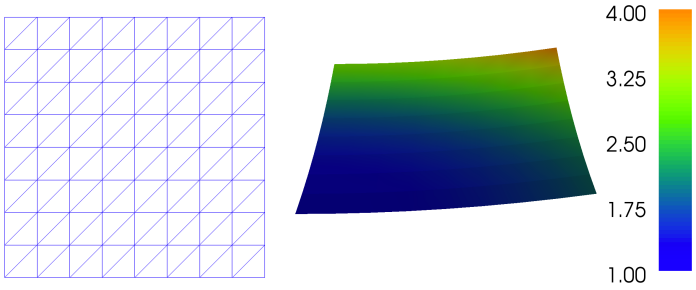


Fig. 2.1 Plot of the solution in the first FEniCS example.

Spyder. Many prefer to work in an integrated development environment that provides 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.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.py` in the blank cell of this notebook, then press Shift+Enter to execute the cell. The file `ft01_poisson.py` will then 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**.

2.3 Dissection of the program

We shall now dissect our FEniCS program in detail. 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_{D}), 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.

2.3.1 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.

2.3.2 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.

2.3.3 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 Elements [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.

2.3.4 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)
```

2.3.5 Defining the boundary and the boundary conditions

The next step is to specify the boundary condition: $u = u_{\mathrm{D}}$ on $\partial\Omega$. This is done by

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

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

Boundary conditions of the type $u = u_{\mathrm{D}}$ 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`.

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

```
u_D = 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

$u_{\mathrm{D}}(x,y) = 1 + x^2 + 2y^2$, the formula string can be written as `1 + x[0]*x[0] + 2*x[1]*x[1]`:

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

We set the degree to 2 so that `u_D` may represent the exact quadratic solution to our test problem.

String expressions must have valid C++ syntax!

The string argument to an `Expression` object must obey C++ syntax. Most Python syntax for mathematical expressions is 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 $f(x) = e^{-\kappa\pi^2 t}\sin(\pi k x)$ 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 `boundary` specifies which points that belong to the part of the boundary where the boundary condition should be applied:

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

A function like `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 `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 `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 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 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 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)
```

Never use == for comparing real numbers!

A comparison 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
0.30000000000000004
```

Comparison of real numbers needs to be made with 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 of unit size, 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 appropriately scaled tolerance must be used.

2.3.6 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)
```

2.3.7 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 $\nabla u \cdot \nabla v \, \mathrm{d}x$ and $f v \, \mathrm{d}x$. 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, 24] and is an integral part of FEniCS.

2.3.8 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 is often used 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.

2.3.9 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.

2.3.10 Exporting and post-processing the solution

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

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

The `solution.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 `solution.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 Paraview web page.

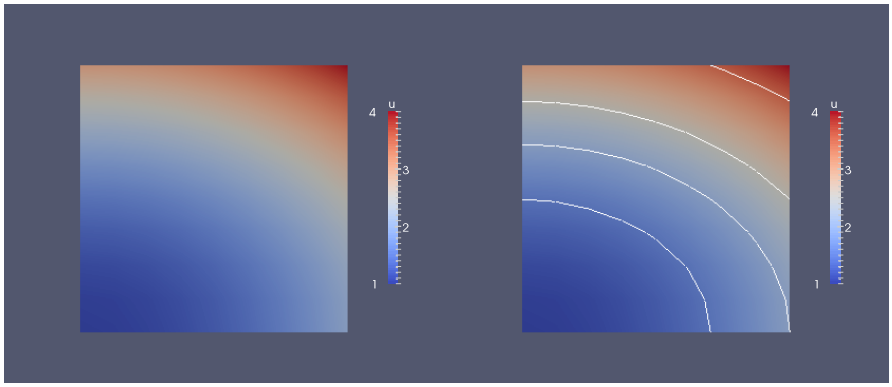


Fig. 2.2 Visualization of the solution of the test problem in ParaView, with contour lines added in the right plot.

2.3.11 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_D`,

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

$$E = \sqrt{\int_\Omega (u_{\mathrm{D}} - u)^2 \,\mathrm{d}x}\,.$$

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_L2 = errornorm(u_D, 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_D` and `u` at all vertices, and then subtract the results:

```
vertex_values_u_D = u_D.compute_vertex_values(mesh)
vertex_values_u = u.compute_vertex_values(mesh)
import numpy as np
error_max = np.max(np.abs(vertex_values_u_D - vertex_values_u))
```

We have here used the maximum and absolute value functions from `numpy`, because these are much more efficient for large arrays (a factor of 30) than Python's built-n `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 $2 \cdot 10^{-15}$.

2.3.12 Examining 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:

$$u = \sum_{j=1}^{N} U_j \phi_j \,. \tag{2.13}$$

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 values $U_1, \ldots, U_N$. The values $U_1, \ldots, U_N$ 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 locations 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 in the vector U directly by

```
nodal_values_u = 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:

```
array_u = nodal_values_u.array()
```

With `numpy` arrays we can write MATLAB-like code to analyze the data. Indexing is done with square brackets: `array_u[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 `array_u` is equal to the number of vertices, and each `array_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 5.2.6 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:

```
vertex_values_u = u.compute_vertex_values()
```

Note that for P_1 elements the arrays `array_u` and `vertex_values_u` have the same lengths and contain the same values, albeit in different order.

2.4 Deflection of a membrane

Our first FEniCS program for the Poisson equation targeted a simple test problem where we could 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

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

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:

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

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.

2.4.1 Scaling the equation

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

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

where

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

With an appropriate scaling, 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 this particular case 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

$$-\nabla^2 w = 4\exp\left(-\beta^2(x^2 + (y - R_0)^2)\right), \tag{2.16}$$

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 $\beta \to 0$, we have a special case with solution $w = 1 - x^2 - y^2$.

Given a computed scaled solution w, the physical deflection can be computed 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.

2.4.2 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)
mesh = generate_mesh(domain, 20)
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.

2.4.3 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
```

2.4.4 Defining the variational problem

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)
```

2.4.5 Plotting the solution

It is of interest to visualize the pressure p along with the deflection w so that we can examine membrane's response to the pressure. 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 save the fields to file in VTK format:

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

vtkfile_w = File('poisson_membrane/deflection.pvd')
vtkfile_w << w
vtkfile_p = File('poisson_membrane/load.pvd')
vtkfile_p << p
```

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

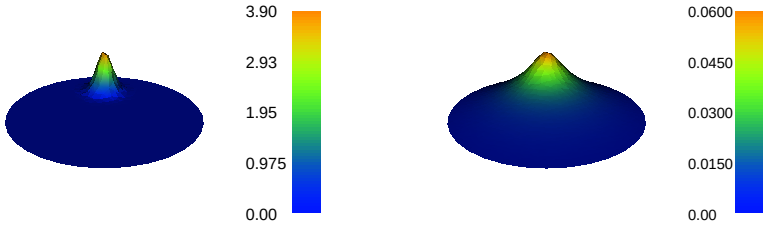


Fig. 2.3 Load (left) and resulting deflection (right) of a circular membrane.

2.4.6 Making 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 $100u$')
plt.savefig('poisson_membrane/plot.pdf')
plt.savefig('poisson_membrane/plot.png')

# Hold plots
interactive()
plt.show()
```

The complete code can be found in the file `ft02_poisson_membrane.py`.

The resulting curve plot appears in Figure 2.4. It is seen how the localized input (p) is heavily damped and smoothened in the output (w). This reflects a typical property of the Poisson equation.

2.4.7 Visualizing the solution in ParaView

ParaView is a powerful tool for visualizing scalar and vector fields, including those computed by FEniCS.

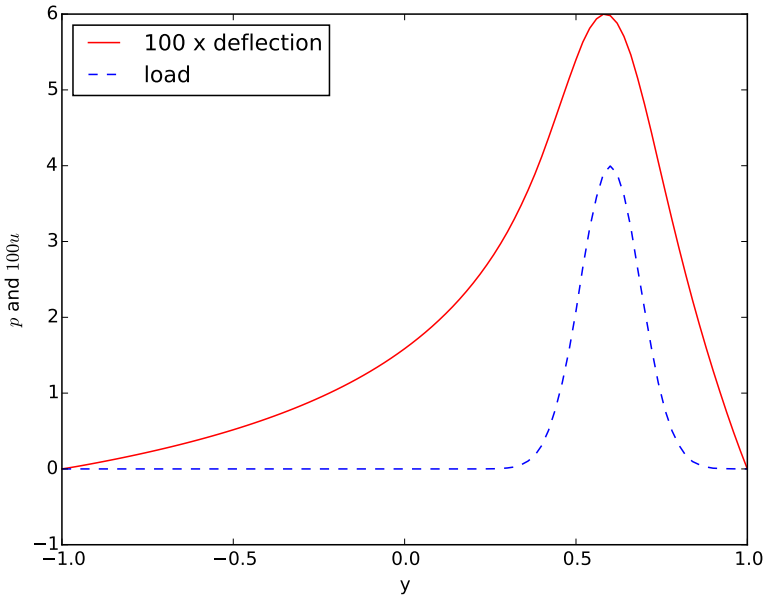


Fig. 2.4 Comparison of membrane load and deflection.

Our program writes the fields w and p to file as finite element functions. We choose the names of these files to be `membrane_deflection.pvd` for w and `membrane_load.pvd` for p. These files are in VTK format and their data can be visualized in ParaView. We now give a detailed account for how to visualize the fields w and p 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 will 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 color spectrum and choose another color, say yellow, then double click at the right and 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.
13. To plot a 2D scalar field as a surface, load the field, click **Apply** to plot it, then select from the **Filters** pulldown menu the filter *Warp By Scalar*, click **Apply**, then toggle the **2D** button to **3D** in the Layout `#1` window (upper row of buttons in that window). Now you can rotate the figure. The height of the surface is very low, so go to the *Properties (Warp By Scalar1)* window to the left in the GUI and give a *Scale Factor* of 20 and re-click **Apply** to lift the surface by a factor of 20. Figure 2.5 (right) shows the result.

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 [27] (free PDF available) and to the ParaView tutorial as well as an instruction video.

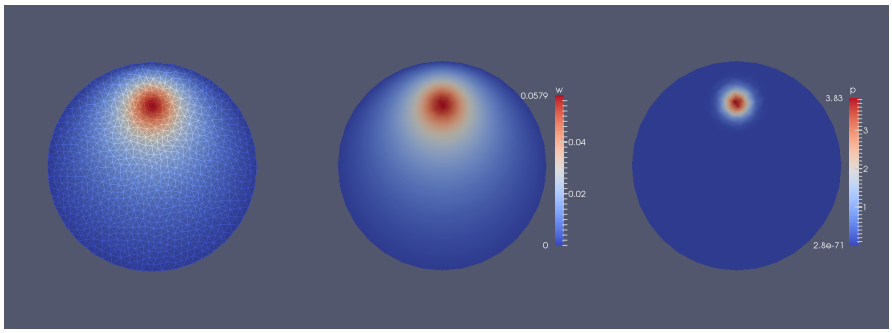


Fig. 2.5 Default visualizations in ParaView: deflection (left, middle) and pressure load (right).

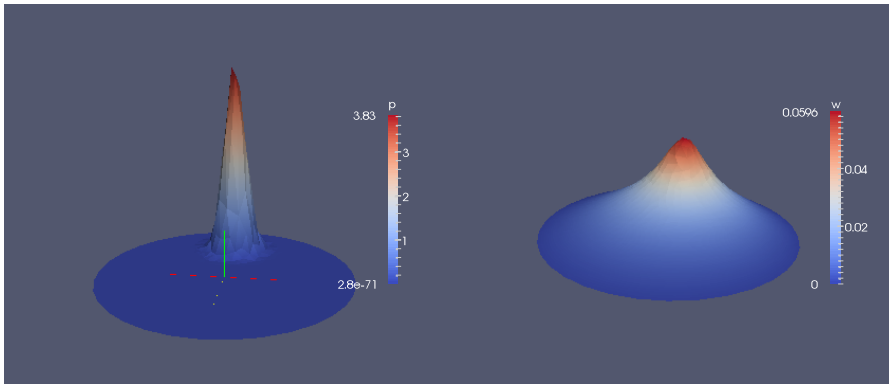


Fig. 2.6 Use of Warp By Scalar filter to create lifted surfaces (with different vertical scales!) in ParaView: load (left) and deflection (right).

2.4.8 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')`.

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.

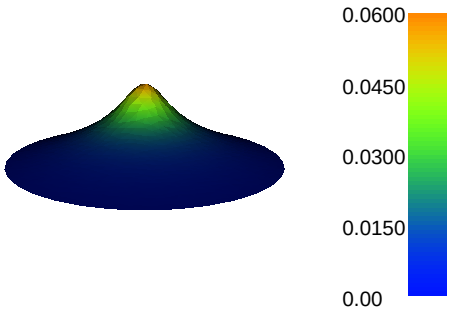


Fig. 2.7 Plot of the deflection of a membrane using the built-in visualization tool.

Built-in plotting on Mac OS X and in Docker

The built-in plotting in FEniCS may not work as expected when either running on Mac OS X or when running inside a FEniCS Docker container. FEniCS supports plotting using the `plot()` command on Mac OS X. However, the keyboard shortcuts `h`, `p`, `P` and so on may fail to work. When running inside a Docker container, plotting is not supported since Docker does not interact with your windowing system. For Docker users who need plotting, it is recommended to either work within

a Jupyter/FEniCS notebook (command `fenicsproject notebook`) or rely on Paraview or other external tools for visualization.

Exercise 2.1: Visualize a solution in a cube

Solve the problem $-\nabla^2 u = f$ on the unit cube $[0,1]\times[0,1]\times[0,1]$ with $u_0 = 1+x^2+2y^2-4z^2$ on the boundary. Visualize the solution. Explore both the built-in visualization tool and ParaView.

Solution. As hinted by the filename in this exercise, a good starting point is the `solver` function in the program `ft03_poisson_solver.py`, which solves the corresponding 2D problem. Only two lines in the body of `solver` needs to be changed (!): `mesh = ....` Replace this line with

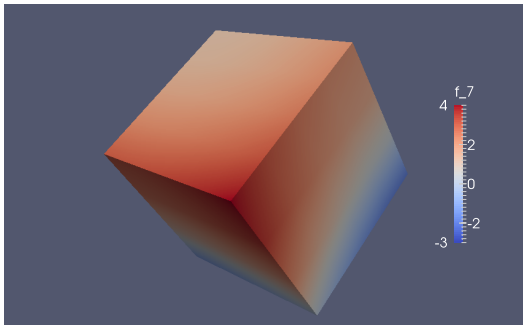
```
mesh = UnitCubeMesh(Nx, Ny, Nz)
```

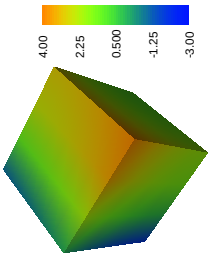
and add `Nz` as argument to `solver`. We implement the new u_0 function in `application_test` and realize that the proper $f(x,y,z)$ function in this new case is 2.

```
u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1] - 4*x[2]*x[2]')
f = Constant(2.0)
u = solver(f, u0, 6, 4, 3, 1)
```

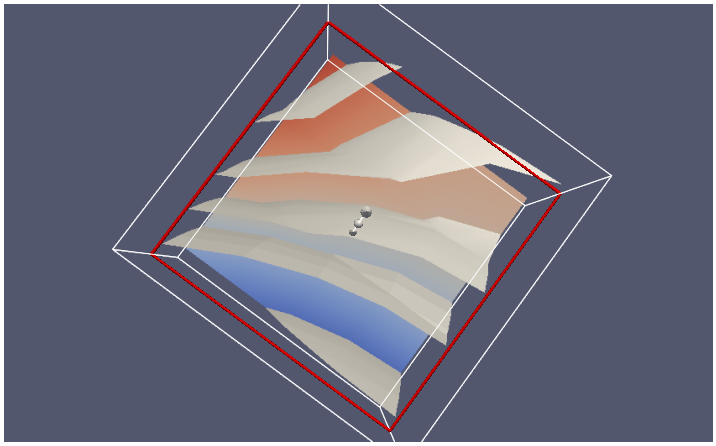
The numerical solution is without approximation errors so we can reuse the unit test from 2D, but it needs an extra `Nz` parameter.

The variation in u is only quadratic so a coarse mesh is okay for visualization. Below is plot from the ParaView (left) and the built-in visualization tool (right). The usage is as in 2D, but now one can use the mouse to rotate the 3D cube.





We can in ParaView add a contour filter and define contour surfaces for $u = -2,1,0,1,2,3$, then add a slice filter to get a slice with colors:



Filename: `poissin_3d_func`.

Chapter 3
A Gallery of finite element solvers

The goal of this chapter is to demonstrate 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 heat equation and continue with a nonlinear Poisson equation, the equations for linear elasticity, the Navier–Stokes equations, and finally look at how to solve systems of nonlinear advection–diffusion–reaction equations. These problems illustrate how to solve time-dependent problems, nonlinear problems, vector-valued problems, and systems of PDE. For each problem, we derive the variational formulation and express the problem in Python in a way that closely resembles the mathematics.

3.1 The heat equation

As a first extension of the Poisson problem from the previous chapter, we consider the time-dependent heat equation, or the time-dependent diffusion equation. This is the natural extension of the Poisson equation describing the stationary distribution of heat in a body to a time-dependent problem.

We will see that by discretizing time into small time intervals and applying standard time-stepping methods, we can solve the heat equation by solving a sequence of variational problems, much like the one we encountered for the Poisson equation.

3.1.1 PDE problem

Our model problem for time-dependent PDEs reads

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

$$u = u_{\text{D}} \text{ on } \partial\Omega, \tag{3.2}$$

$$u = u_0 \text{ at } t = 0\,. \tag{3.3}$$

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_{D} may also vary with space and time. The initial condition u_0 is a function of space only.

3.1.2 Variational formulation

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 sequence of stationary problems, and then turn each stationary problem into a variational formulation.

Let superscript n denote a quantity at time t_n, where n is an integer counting time levels. For example, u^n means u at time level n. A finite difference discretization in time first consists of sampling the PDE at some time level, say t_{n+1}:

$$\left(\frac{\partial u}{\partial t}\right)^{n+1} = \nabla^2 u^{n+1} + f^{n+1}\,. \tag{3.4}$$

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

$$\left(\frac{\partial u}{\partial t}\right)^{n+1} \approx \frac{u^{n+1} - u^n}{\Delta t}, \tag{3.5}$$

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

$$\frac{u^{n+1} - u^n}{\Delta t} = \nabla^2 u^{n+1} + f^{n+1}\,. \tag{3.6}$$

This is our time-discrete version of the heat equation (3.1). This is a so-called *backward Euler* or *implicit Euler* discretization. Alternatively, we may also view this as a finite element discretization in time in the form of the first order dG(0) method, which here is identical to the backward Euler method.

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

$$u^0 = u_0, \tag{3.7}$$

$$u^{n+1} - \Delta t\nabla^2 u^{n+1} = u^n + \Delta t f^{n+1}, \quad n = 0, 1, 2, \ldots \tag{3.8}$$

Given u_0, 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:

$$u^{n+1} - \Delta t\nabla^2 u^{n+1} - u^n - \Delta t f^{n+1} = 0, \quad n = 0, 1, 2, \ldots \tag{3.9}$$

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^{n+1} (which is natural in the program), the resulting weak form arising from formulation (3.8) can be conveniently written in the standard notation:

$$a(u, v) = L_{n+1}(v),$$

where

$$a(u, v) = \int_\Omega (uv + \Delta t\nabla u \cdot \nabla v)\,\mathrm{d}x, \tag{3.10}$$

$$L_{n+1}(v) = \int_\Omega \left(u^n + \Delta t f^{n+1}\right) v\,\mathrm{d}x\,. \tag{3.11}$$

The alternative form (3.9) has an abstract formulation

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

where

$$F(u; v) = \int_\Omega uv + \Delta t\nabla u \cdot \nabla v - (u^n + \Delta t f^{n+1})v\,\mathrm{d}x\,. \tag{3.12}$$

In addition to the variational problem to be solved in each time step, we also need to approximate the initial condition (3.7). This equation can also be turned into a variational problem:

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

with

$$a_0(u, v) = \int_\Omega uv\,\mathrm{d}x, \tag{3.13}$$

$$L_0(v) = \int_\Omega u_0 v\,\mathrm{d}x\,. \tag{3.14}$$

When solving this variational problem, u^0 becomes the L^2 projection of the given initial value u_0 into the finite element space. The alternative is to construct u^0 by just interpolating the initial value u_0; that is, if $u^0 = \sum_{j=1}^{N} U_j^0 \phi_j$, we simply set $U_j = u_0(x_j, y_j)$, 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 projection or interpolation. Both operations are easy to compute in FEniCS through one statement, using either the `project` or `interpolate` function. The most common choice is `project`, which computes an approximation to u_0, but in some applications where we want to verify the code by reproducing exact solutions, one must use `interpolate` (and we use such a test problem!).

In summary, we thus need to solve the following sequence of variational problems to compute the finite element solution to the heat equation: 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 $u^{n+1} \in V$ such that $a(u^{n+1}, v) = L_{n+1}(v)$ for all $v \in \hat{V}$, or alternatively, $F(u^{n+1}, v) = 0$ for all $v \in \hat{V}$, for $n = 0, 1, 2, \ldots$.

3.1.3 FEniCS implementation

Our program needs to implement the time-stepping manually, 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. Just as for the Poisson problem from the previous chapter, we construct a test problem that makes it easy to determine if the calculations are correct. Since we know that our first-order time-stepping scheme is exact for linear functions, we create a test problem which has a linear variation in time. We combine this with a quadratic variation in space. We thus take

$$u = 1 + x^2 + \alpha y^2 + \beta t, \tag{3.15}$$

which 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) into the heat equation (3.1), we find that the right-hand side f must be given by $f(x, y, t) = \beta - 2 - 2\alpha$. The boundary value is $u_{\mathrm{D}}(x, y, t) = 1 + x^2 + \alpha y^2 + \beta t$ and the initial value is $u_0(x, y) = 1 + x^2 + \alpha y^2$.

FEniCS implementation. A new programming issue is how to deal with functions that vary in space *and time*, such as the boundary condition $u_{\mathrm{D}}(x, y, t) = 1 + x^2 + \alpha y^2 + \beta t$. A natural solution is to use a FEniCS `Expression` with time t as a parameter, in addition to the parameters α and β:

```
alpha = 3; beta = 1.2
u_D = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                 degree=2, alpha=alpha, beta=beta, t=0)
```

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

```
u_D.t = t
```

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

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

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

We shall use `u` for the unknown u^{n+1} at the new time level and `u_n` for u^n at the previous time level. The initial value of `u_n` can be computed by either projection or interpolation of u_0. Since we set `t = 0` for the boundary value `u_D`, we can use this to also specify the initial condition. We can then do

```
u_n = project(u_D, V)
# or
u_n = interpolate(u_D, 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 u_0, but by interpolating u_0 so that the degrees of freedom have exact values at $t = 0$ (projection results in approximate 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 of a and L:

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

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

Finally, we perform the time-stepping in a loop:

```
u = Function(V)
t = 0
for n in range(num_steps):
```

```
    # Update current time
    t += dt
    u_D.t = t

    # Solve variational problem
    solve(a == L, u, bc)

    # Update previous solution
    u_n.assign(u)
```

In the last step of the time-stepping loop, we assign the values of the variable `u` (the new computed solution) to the variable `u_n` containing the values at the previous time step. This must be done using the `assign` member function. If we instead try to do `u_n = u`, we will set the `u_n` variable to be the *same* variable as `u` which is not what we want. (We need two variables, one for the values at the previous time step and one for the values at the current time step.)

Remember to update expression objects with the current time!

Inside the time loop, observe that `u_D.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 `u_D` 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 2.3, we compute the difference between the array of nodal values for `u` and the array of nodal values for the interpolated exact solution. This may be done as follows:

```
u_e = interpolate(u_D, V)
error = np.abs(u_e.vector().array() - u.vector().array()).max()
print('error, t=%.2f: %.3g' % (t, error))
```

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

```
from fenics import *
import numpy as np

T = 2.0            # final time
num_steps = 10     # number of time steps
dt = T / num_steps # time step size
alpha = 3          # parameter alpha
beta = 1.2         # parameter beta

# Create mesh and define function space
nx = ny = 8
```

```
mesh = UnitSquareMesh(nx, ny)
V = FunctionSpace(mesh, 'P', 1)

# Define boundary condition
u_D = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                 degree=2, alpha=alpha, beta=beta, t=0)

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u_D, boundary)

# Define initial value
u_n = interpolate(u_D, V)
#u_n = project(u_D, V)

# 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_n + dt*f)*v*dx
a, L = lhs(F), rhs(F)

# Create VTK file for saving solution
vtkfile = File('heat/solution.pvd')
vtkfile << u_n

# Time-stepping
u = Function(V)
t = 0
for n in range(num_steps):

    # Update current time
    t += dt
    u_D.t = t # update for bc

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

    # Save solution to file and plot solution
    vtkfile << u
    plot(u)

    # Compute error at vertices
    u_e = interpolate(u_D, V)
    error = np.abs(u_e.vector().array() - u.vector().array()).max()
    print('t = %.2f: error = %.3g' % (t, error))

    # Update previous solution
    u_n.assign(u)

# Hold plot
interactive()
```

The complete code can be found in the file `ft04_heat.py`.

3.1.4 Diffusion of a Gaussian function

The mathematical problem. Let's solve a more interesting test problem, namely the diffusion of a Gaussian hill. We take the initial value to be given by

$$u_0(x, y) = e^{-ax^2 - ay^2}$$

on the domain $[-2, 2] \times [2, 2]$. We will take $a = 5$. For this problem we will use homogeneous Dirichlet boundary conditions ($u_{\text{D}} = 0$).

FEniCS implementation. Which are the required changes to our previous program? One major change is that the domain is not a unit square anymore. We also want to use much higher resolution. The new domain can be created easily in FEniCS using `RectangleMesh`:

```
nx = ny = 30
mesh = RectangleMesh(Point(-2, -2), Point(2, 2), nx, ny)
```

We also need to redefine the initial condition and boundary condition. Both are easily changed by defining a new `Expression` and by setting $u = 0$ on the boundary. We will also save the solution to file in VTK format in each time step:

```
vtkfile << u
```

The complete program appears below.

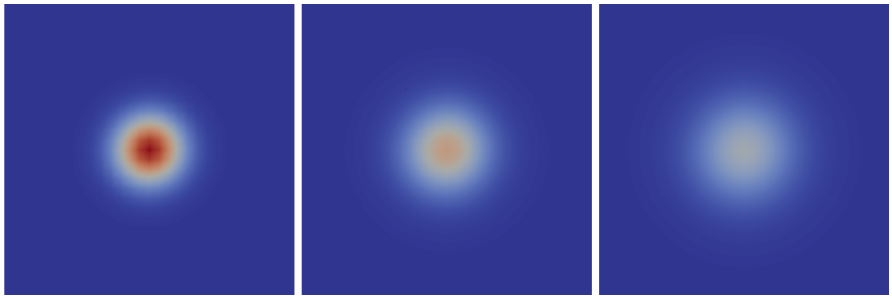
```
from fenics import *
import time

T = 2.0            # final time
num_steps = 50     # number of time steps
dt = T / num_steps # time step size

# 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 condition
def boundary(x, on_boundary):
    return on_boundary

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

# Define initial value
u_0 = Expression('exp(-a*pow(x[0], 2) - a*pow(x[1], 2))',
```

```
                  degree=2, a=5)
u_n = interpolate(u_0, V)

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

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

# Create VTK file for saving solution
vtkfile = File('heat_gaussian/solution.pvd')
vtkfile << u_n

# Time-stepping
u = Function(V)
t = 0
for n in range(num_steps):

    # Update current time
    t += dt

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

    # Save to file and plot solution
    vtkfile << u
    plot(u)

    # Update previous solution
    u_n.assign(u)

# Hold plot
interactive()
```

The complete code can be found in the file `ft05_heat_gaussian.py`.

Visualization in ParaView. To visualize the diffusion of the Gaussian hill, start ParaView, choose **File - Open**, open the file `heat_gaussian/solution.pvd`, click the green **Apply** button on the left to see the initial condition being plotted. 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 have just computed. Choose **File - Save Animation...** to save the animation to the AVI or OGG video format.

Once the animation has been saved to file, you can play the animation offline using a player such as mplayer or VLC, or upload your animation to YouTube. Below is a sequence of snapshots of the solution (first three time steps).



3.2 A nonlinear Poisson equation

We shall now address how to solve nonlinear PDEs. We will see that nonlinear problems can be solved just as easily as linear problems in FEniCS, by simply defining a nonlinear variational problem and calling the `solve` function. When doing so, we will encounter a subtle difference in how the variational problem is defined.

3.2.1 PDE problem

As a sample PDE for the implementation of nonlinear problems, we take the following nonlinear Poisson equation:

$$-\nabla\cdot(q(u)\nabla u) = f, \tag{3.16}$$

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

3.2.2 Variational formulation

As usual, we multiply our PDE by a test function $v \in \hat{V}$, integrate over the domain, and integrate the second-order derivatives by parts. The boundary integral arising from integration by parts vanishes wherever we employ Dirichlet conditions. The resulting variational formulation of our model problem becomes: find $u \in V$ such that

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

where

$$F(u;v) = \int_\Omega q(u)\nabla u \cdot \nabla v - fv \,\mathrm{d}x, \tag{3.18}$$

and

$$V = \{v \in H^1(\Omega) : v = u_{\mathrm{D}} \text{ on } \partial\Omega\},$$
$$\hat{V} = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}.$$

The discrete problem arises as usual by restricting V and $\hat{V}$ to a pair of discrete spaces. As before, we omit any subscript on the discrete spaces and discrete solution. The discrete nonlinear problem is then written as: Find $u \in V$ such that

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

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

3.2.3 FEniCS implementation

Test problem. To solve a test problem, we need to choose the right-hand side f, the coefficient $q(u)$ and the boundary value u_{D}. 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. In particular, we will use the SymPy functions `diff` for symbolic differentiation and `ccode` for C/C++ code generation.

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

```
# Warning: from fenics import * will import both ‘sym‘ and
# ‘q‘ from FEniCS. We therefore import FEniCS first and then
# overwrite these objects.
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)
u_code = sym.printing.ccode(u)
f_code = sym.printing.ccode(f)
print('u =', u_code)
print('f =', f_code)
```

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 have valid syntax for FEniCS `Expression` objects, we must use `x[0]` and `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 FEniCS `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 the present case, 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 value `u_D` as

```
u_D = Expression(u_code)
```

Similarly, we define the right-hand side function as

```
f = Expression(f_code)
```

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` and `q` prior to doing `from fenics import *`,

the latter statement will also import variables with the names `sym` and `q`, overwriting the objects you have previously defined! This may lead to strange errors. The safest solution is to do `import fenics as fe` and then prefix all FEniCS object names by `fe`. The next best solution is to do `from fenics import *` first and then define your own variables that overwrite those imported from `fenics`. This is acceptable if we do not need `sym` and `q` from `fenics`.

FEniCS implementation. 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 to 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):
    return 1 + u**2

mesh = UnitSquareMesh(32, 32)
V = FunctionSpace(mesh, 'P', 1)
u_D = Expression(...)

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u_D, boundary)

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

solve(F == 0, u, bc)
```

The complete code can be found in the file `ft06_poisson_nonlinear.py`.

The major difference from a linear problem is that the unknown function `u` in the variational form in the nonlinear case must be defined as a `Function`, not as a `TrialFunction`. In some sense this is a simplification from the linear case where we must define `u` first as a `TrialFunction` and then as a `Function`.

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

Running the code gives output that tells how the Newton iteration progresses. With $2 \cdot (8 \times 8)$ cells we reach convergence in 8 iterations with a tolerance of 10^{-9}, and the error in the numerical solution is about 10^{-16}. These results bring evidence for a correct implementation. Thinking in terms of finite differences on a uniform mesh, $\mathcal{P}_1$ elements mimic standard second-order differences, which compute the derivative of a linear or quadratic function exactly. Here, ∇u is a constant vector, but then multiplied by $(1+u^2)$, which

is a second-order polynomial in x and y, which the divergence "difference operator" should compute exactly. We can therefore, even with $\mathcal{P}_1$ elements, expect the manufactured u to be reproduced by the numerical method. With a nonlinearity like $1+u^4$, this will not be the case, and we would need to verify convergence rates instead.

The current example shows how easy it is to solve a nonlinear problem in FEniCS. However, experts on the 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 better manual control of the solution process than what we have in the current case. Therefore, we return to this problem in Chapter 3 in [21] 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 see 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 of modern engineering, thus making the PDEs for deformation of elastic bodies likely the most popular PDE model in the world. It takes just one page of code to solve the equations of 2D or 3D elasticity in FEniCS, and the details follow below.

3.3.1 PDE problem

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

$$-\nabla\cdot\sigma = f \text{ in } \Omega, \tag{3.20}$$

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

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

where σ is the stress tensor, f is the body force per unit volume, λ and μ are Lamé's elasticity parameters for the material in Ω, I is the identity tensor, tr is the trace operator on a tensor, ε is the strain tensor (symmetric gradient), and u is the displacement vector field. We have here assumed isotropic elastic conditions.

We combine (3.21) and (3.22) to obtain

$$\sigma = \lambda(\nabla \cdot u)I + \mu(\nabla u + (\nabla u)^\top). \tag{3.23}$$

Note that (3.20)–(3.22) can easily be transformed to a single vector PDE for u, which is the governing PDE for the unknown u (Navier's equation). In the derivation of the variational formulation, however, it is convenient to keep the splitting of the equations as above.

3.3.2 Variational formulation

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 vector-valued test function space, and integrating over the domain Ω:

$$-\int_\Omega (\nabla \cdot \sigma) \cdot v \,\mathrm{d}x = \int_\Omega f \cdot v \,\mathrm{d}x.$$

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

$$-\int_\Omega (\nabla \cdot \sigma) \cdot v \,\mathrm{d}x = \int_\Omega \sigma : \nabla v \,\mathrm{d}x - \int_{\partial\Omega} (\sigma \cdot n) \cdot v \,\mathrm{d}s,$$

where the colon operator is the inner product between tensors (summed pairwise product of all elements), 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 as $\sigma \cdot n = T$. On the remaining part of the boundary, we assume that the value of the displacement is given as a Dirichlet condition. We then have

$$\int_\Omega \sigma : \nabla v \,\mathrm{d}x = \int_\Omega f \cdot v \,\mathrm{d}x + \int_{\partial\Omega_T} T \cdot v \,\mathrm{d}s.$$

Inserting the expression (3.23) for σ gives the variational form with u as unknown. Note that the boundary integral on the remaining part $\partial\Omega \setminus \Omega_T$ vanishes due to the Dirichlet condition ($v = 0$).

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

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

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

$$L(v) = \int_\Omega f \cdot v \,\mathrm{d}x + \int_{\partial\Omega_T} T \cdot v \,\mathrm{d}s\,. \tag{3.27}$$

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

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

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

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

The formulation (3.28) is what naturally arises from minimization of elastic potential energy and is a more popular formulation than (3.25).

3.3.3 FEniCS implementation

Test problem. As a test example, we may look at a clamped beam deformed under its own weight. Then $f = (0, 0, -\varrho g)$ is the body force per unit volume with ϱ the density of the beam and g the acceleration of gravity. The beam is box-shaped with length L and has a square cross section of width W. We set $u = u_{\mathrm{D}} = (0,0,0)$ at the clamped end, $x = 0$. The rest of the boundary is traction free; that is, we set $T = 0$.

The code. We first list the code and then comment upon the new constructions compared to the Poisson equation case.

```
from fenics import *

# Scaled variables
L = 1; W = 0.2
mu = 1
rho = 1
delta = W/L
gamma = 0.4*delta**2
beta = 1.25
lambda_ = 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 condition
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)

# Define strain and stress

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 = Constant((0, 0, rho*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
plot(u, title='Displacement', mode='displacement')

# Plot stress
s = sigma(u) - (1./3)*tr(sigma(u))*Identity(d)  # deviatoric stress
von_Mises = sqrt(3./2*inner(s, s))
V = FunctionSpace(mesh, 'P', 1)
von_Mises = project(von_Mises, V)
plot(von_Mises, title='Stress intensity')

# Compute magnitude of displacement
u_magnitude = sqrt(dot(u, u))
u_magnitude = project(u_magnitude, V)
plot(u_magnitude, 'Displacement magnitude')
print('min/max u:', u_magnitude.vector().array().min(),
      u_magnitude.vector().array().max())
```

The complete code can be found in the file `ft07_elasticity.py`.

We comment below on some of the key features of this example that we have not seen in previous examples.

Vector function spaces. The primary unknown is now a vector field u and not a scalar field, so we need to work with a vector function space:

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

With `u = Function(V)` we get `u` as a vector-valued finite element function.

Constant vectors. In the boundary condition $u = 0$, we must set a vector value to zero, not just a scalar, and a constant zero vector is specified as `Constant((0, 0, 0))` in FEniCS. The corresponding 2D code would use `Constant((0, 0))`. Later in the code, we also need `f` as a vector and specify it as `Constant((0, 0, rho*g))`.

`nabla_grad`. The gradient and divergence operators now have a prefix `nabla_`. This is strictly not necessary in the present problem, but recommended in general for vector PDEs arising from continuum mechanics, if you interpret ∇ as a vector in the PDE notation; see the box about `nabla_grad` in Section 3.4.2.

Stress computation. As soon as `u` is computed, we can compute various stress measures, here the von Mises stress defined as $\sigma_M = \sqrt{\frac{3}{2}s : s}$ where s is the deviatoric stress tensor

$$s = \sigma - \frac{1}{3}\mathrm{tr}\,(\sigma)\,I\,.$$

There is a one to one mapping between these formulas and the FEniCS code:

```
s = sigma(u) - (1./3)*tr(sigma(u))*Identity(d)
von_Mises = sqrt(3./2*inner(s, s))
```

The `von_Mises` variable is now an expression that must be projected to a finite element space before we can visualize it.

Scaling. Before doing simulations for a specific problem, it is often advantageous to scale the problem as it reduces the need for setting physical parameters, and one obtains dimensionsless numbers that reflect the competition of parameters and physical effects. We develop the code for the original model with dimensions, and run the scaled problem by tweaking parameters appropriately. Scaling reduces the number of active parameters from 6 to 2 in the present application.

In Navier's equation for u, arising from inserting (3.21) and (3.22) in (3.20),

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

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

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

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

$$\gamma = \frac{\varrho g L^2}{\mu U}$$

is also a dimensionless variable reflecting the ratio of the load ϱg and the shear stress term $\mu\nabla^2 u \sim \mu U/L^2$ in the PDE.

Sometimes, one will argue to chose U to make γ unity ($U = \varrho g L^2/\mu$). However, in elasticity, this leads us to displacements of the size of the geometry, which makes plots look very strange. We therefore want the characteristic displacement to be a small fraction of the characteristic length of the geometry. This can be achieved by choosing U equal to the maximum deflection of a clamped beam, for which there actually exists an formula: $U = \frac{3}{2}\varrho g L^2 \delta^2/E$, where $\delta = L/W$ is a parameter reflecting how slender the beam is, and E is the modulus of elasticity. Thus, the dimensionless parameter δ is very important in the problem (as expected, since $\delta \gg 1$ is what gives beam theory!). Taking E to be of the same order as μ, which is the case for many materials, we realize that $\gamma \sim \delta^{-2}$ is an appropriate choice. Experimenting with the code to find a displacement that "looks right" in plots of the deformed geometry, points to $\gamma = 0.4\delta^{-2}$ as our final choice of γ.

The simulation code implements the problem with dimensions and physical parameters λ, μ, ϱ, g, L, and W. However, we can easily reuse this code for a scaled problem: just set $\mu = \varrho = L = 1$, W as W/L (δ^{-1}), $g = \gamma$, and $\lambda = \beta$.

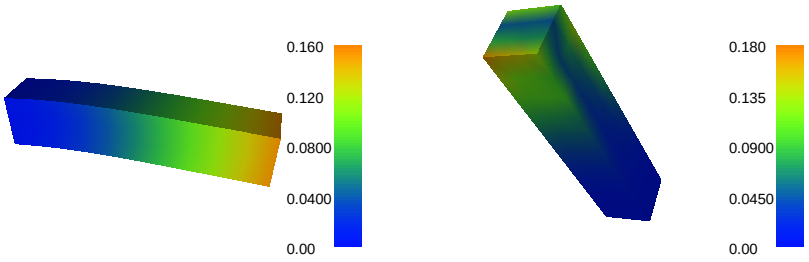


Fig. 3.1 Gravity-induced deformation of a clamped beam: deflection (left) and stress intensity seen from below (right).

3.4 The Navier–Stokes equations

As our next example in this chapter, we will solve the incompressible Navier–Stokes equations. This problem combines many of the challenges from our previously studied problems: time-dependence, nonlinearity, and vector-valued variables. We shall touch on a number of FEniCS topics, many of them quite

advanced. But you will see that even a relatively complex algorithm such as a second-order splitting method for the incompressible Navier–Stokes equations, can be implemented with relative ease in FEniCS.

3.4.1 PDE problem

The incompressible Navier–Stokes equations are a system of equations for the velocity u and pressure p in an incompressible fluid:

$$\varrho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) = \nabla\cdot\sigma(u,p) + f, \tag{3.29}$$

$$\nabla\cdot u = 0. \tag{3.30}$$

The right-hand side f is a given force per unit volume and just as for the equations of linear elasticity, $\sigma(u,p)$ denotes the stress tensor which for a Newtonian fluid is given by

$$\sigma(u,p) = 2\mu\epsilon(u) - pI, \tag{3.31}$$

where $\epsilon(u)$ is the strain-rate tensor

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

The parameter μ is the dynamic viscosity. Note that the momentum equation (3.29) is very similar to the elasticity equation (3.20). The difference is in the two additional terms $\varrho(\partial u/\partial t + u\cdot\nabla u)$ and the different expression for the stress tensor. The two extra terms express the acceleration balanced by the force $F = \nabla\cdot\sigma + f$ per unit volume in Newton's second law of motion.

3.4.2 Variational formulation

The Navier–Stokes equations are different from the time-dependent heat equation in that we need to solve a system of equations and this system is of a special type. If we apply the same technique as for the heat equation; that is, replacing the time derivative with a simple difference quotient, we obtain a nonlinear system of equations. This in itself is not a problem for FEniCS as we saw in Section 3.2, but the system has a so-called *saddle point structure* and requires special techniques (preconditioners and iterative methods) to be solved efficiently.

Instead, we will apply a simpler and often very efficient approach, known as a *splitting method*. The idea is to consider the two equations (3.29) and

(3.30) separately. There exist many splitting strategies for the incompressible Navier–Stokes equations. One of the oldest is the method proposed by Chorin [6] and Temam [28], often referred to as *Chorin's method*. We will use a modified version of Chorin's method, the so-called incremental pressure correction scheme (IPCS) due to [13] which gives improved accuracy compared to the original scheme at little extra cost.

The IPCS scheme involves three steps. First, we compute a *tentative velocity* $u^\star$ by advancing the momentum equation (3.29) by a midpoint finite difference scheme in time, but using the pressure p^n from the previous time interval. We will also linearize the nonlinear convective term by using the known velocity u^n from the previous time step: $u^n \cdot \nabla u^n$. The variational problem for this first step is:

$$\begin{aligned}&\langle \varrho(u^\star - u^n)/\Delta t, v\rangle + \langle \varrho u^n \cdot \nabla u^n, v\rangle + \\ &\langle \sigma(u^{n+\frac{1}{2}}, p^n), \epsilon(v)\rangle + \langle p^n n, v\rangle_{\partial\Omega} - \\ &\langle \mu \nabla u^{n+\frac{1}{2}} \cdot n, v\rangle_{\partial\Omega} = \langle f^{n+1}, v\rangle. \end{aligned} \tag{3.32}$$

This notation, suitable for problems with many terms in the variational formulations, requires some explanation. First, we use the short-hand notation

$$\langle v, w\rangle = \int_\Omega vw \,\mathrm{d}x, \quad \langle v, w\rangle_{\partial\Omega} = \int_{\partial\Omega} vw \,\mathrm{d}s.$$

This allows us to express the variational problem in a more compact way. Second, we use the notation $u^{n+\frac{1}{2}}$. This notation means the value of u at the midpoint of the interval, usually approximated by an arithmetic mean

$$u^{n+\frac{1}{2}} \approx (u^n + u^{n+1})/2.$$

Third, we notice that the variational problem (3.32) arises from the integration by parts of the term $\langle -\nabla \cdot \sigma, v\rangle$. Just as for the elasticity problem in Section 3.3, we obtain

$$\langle -\nabla \cdot \sigma, v\rangle = \langle \sigma, \epsilon(v)\rangle - \langle T, v\rangle_{\partial\Omega},$$

where $T = \sigma \cdot n$ is the boundary traction. If we solve a problem with a free boundary, we can take $T = 0$ on the boundary. However, if we compute the flow through a channel or a pipe and want to model flow that continues into an "imaginary channel" at the outflow, we need to treat this term with some care. The assumption we then make is that the derivative of the velocity in the direction of the channel is zero at the outflow, corresponding to a flow that is "fully developed" or doesn't change significantly downstream of the outflow. Doing so, the remaining boundary term at the outflow becomes $pn - \mu \nabla u \cdot n$, which is the term appearing in the variational problem (3.32).

`grad(u)` vs. `nabla_grad(u)`

For scalar functions ∇u has a clear meaning as the vector

$$\nabla u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z} \right).$$

However, if u is vector-valued, the meaning is less clear. Some sources define ∇u as the matrix with elements $\partial u_j / \partial x_i$, while other sources prefer $\partial u_i / \partial x_j$. In FEniCS, `grad(u)` is defined as the matrix with elements $\partial u_i / \partial x_j$, which is the natural definition of ∇u if we think of this as the *gradient* or *derivative* of u. This way, the matrix ∇u can be applied to a differential $\mathrm{d}x$ to give an increment $\mathrm{d}u = \nabla u \, \mathrm{d}x$. Since the alternative interpretation of ∇u as the matrix with elements $\partial u_j / \partial x_i$ is very common, in particular in continuum mechanics, FEniCS provides the operator `nabla_grad` for this purpose. For the Navier–Stokes equations, it is important to consider the term $u \cdot \nabla u$ which should be interpreted as the vector w with elements $w_i = \sum_j \left(u_j \frac{\partial}{\partial x_j} \right) u_i = \sum_j u_j \frac{\partial u_i}{\partial x_j}$. This term can be implemented in FEniCS either as `grad(u)*u`, since this is expression becomes $\sum_j \partial u_i / \partial x_j u_j$, or as `dot(u, nabla_grad(u))` since this expression becomes $\sum_i u_i \partial u_j / \partial x_i$. We will use the notation `dot(u, nabla_grad(u))` below since it corresponds more closely to the standard notation $u \cdot \nabla u$.

To be more precise, there are three different notations used for PDEs involving gradient, divergence, and curl operators. One employs $\operatorname{grad} u$, $\operatorname{div} u$, and $\operatorname{curl} u$ operators. Another employs ∇u as a synonym for $\operatorname{grad} u$, $\nabla \cdot u$ means $\operatorname{div} u$, and $\nabla \times u$ is the name for $\operatorname{curl} u$. The third operates with ∇u, $\nabla \cdot u$, and $\nabla \times u$ in which ∇ is a *vector* and, e.g., ∇u is a dyadic expression: $(\nabla u)_{i,j} = \partial u_j / \partial x_i = (\operatorname{grad} u)^\top$. The latter notation, with ∇ as a vector operator, is often handy when deriving equations in continuum mechanics, and if this interpretation of ∇ is the foundation of your PDE, you must use `nabla_grad`, `nabla_div`, and `nabla_curl` in FEniCS code as these operators are compatible with dyadic computations. From the Navier–Stokes equations we can easily see what ∇ means: if the convective term has the form $u \cdot \nabla u$ (actually meaning $(u \cdot \nabla) u$), ∇ is a vector operator, reading `dot(u, nabla_grad(u))` in FEniCS, but if we see $\nabla u \cdot u$ or $(\operatorname{grad} u) \cdot u$, the corresponding FEniCS expression is `dot(grad(u), u)`.

We now move on to the second step in our splitting scheme for the incompressible Navier–Stokes equations. In the first step, we computed the tentative velocity $u^\star$ based on the pressure from the previous time step. We may now use the computed tentative velocity to compute the new pressure p^n:

$$\langle \nabla p^{n+1}, \nabla q \rangle = \langle \nabla p^n, \nabla q \rangle - \Delta t^{-1} \langle \nabla \cdot u^\star, q \rangle. \tag{3.33}$$

Note here that q is a scalar-valued test function from the pressure space, whereas the test function v in (3.32) is a vector-valued test function from the velocity space.

One way to think about this step is to subtract the Navier–Stokes momentum equation (3.29) expressed in terms of the tentative velocity $u^\star$ and the pressure p^n from the momentum equation expressed in terms of the velocity u^n and pressure p^n. This results in the equation

$$(u^n - u^\star)/\Delta t + \nabla p^{n+1} - \nabla p^n = 0. \tag{3.34}$$

Taking the divergence and requiring that $\nabla \cdot u^n = 0$ by the Navier–Stokes continuity equation (3.30), we obtain the equation $-\nabla \cdot u^\star/\Delta t + \nabla^2 p^{n+1} - \nabla^2 p^n = 0$, which is a Poisson problem for the pressure p^{n+1} resulting in the variational problem (3.33).

Finally, we compute the corrected velocity u^{n+1} from the equation (3.34). Multiplying this equation by a test function v, we obtain

$$\langle u^{n+1}, v \rangle = \langle u^\star, v \rangle - \Delta t \langle \nabla (p^{n+1} - p^n), v \rangle. \tag{3.35}$$

In summary, we may thus solve the incompressible Navier–Stokes equations efficiently by solving a sequence of three linear variational problems in each time step.

3.4.3 FEniCS implementation

Test problem 1: Channel flow. As a first test problem, we compute the flow between two infinite plates, so-called channel or Poiseuille flow, since this problem has a known analytical solution. Let H be the distance between the plates and L the length of the channel. There are no body forces.

We may scale the problem first to get rid of seemingly independent physical parameters. The physics of this problem is governed by viscous effects only, in the direction perpendicular to the flow, so a time scale should be based on diffusion accross the channel: $t_c = H^2/\nu$. We let U, some characteristic inflow velocity, be the velocity scale and H the spatial scale. The pressure scale is taken as the characteristic shear stress, $\mu U/H$, since this is a primary example of shear flow. Inserting $\bar{x} = x/H$, $\bar{y} = y/H$, $\bar{z} = z/H$, $\bar{u} = u/U$, $\bar{p} = Hp/(\mu U)$, and $\bar{t} = H^2/\nu$ in the equations results in the scaled Navier–Stokes equations (dropping bars after the scaling):

$$\frac{\partial u}{\partial t} + \mathrm{Re}\, u \cdot \nabla u = -\nabla p + \nabla^2 u,$$
$$\nabla \cdot u = 0\,.$$

Here, $\mathrm{Re} = \varrho U H/\mu$ is the Reynolds number. Because of the time and pressure scale, which are different from convection-dominated fluid flow, the Reynolds number is associated with the convective term and not the viscosity term. Note that the last term in the first equation is zero, but we included this term as it arises naturally from the original $\nabla \cdot \sigma$ term.

The exact solution is derived by assuming $u = (u_x(x,y,z),0,0)$, with the x axis pointing along the channel. Since $\nabla \cdot u = 0$, u cannot depend on x. The physics of channel flow is also two-dimensional so we can omit the z coordinate (more precisely: $\partial/\partial z = 0$). Inserting $u = (u_x,0,0)$ in the (scaled) governing equations gives $u_x''(y) = \partial p/\partial x$. Differentiating this equation with respect to x shows that $\partial^2 p/\partial^2 x = 0$ so $\partial p/\partial x$ is a constant, here called $-\beta$. This is the driving force of the flow and can be specified as a known parameter in the problem. Integrating $u_x''(y) = -\beta$ over the width of the channel, $[0,1]$, and requiring $u = 0$ at the channel walls, results in $u_x = \frac{1}{2}\beta y(1-y)$. The characteristic inlet flow in the channel, U, can be taken as the maximum inflow at $y = 1/2$, implying that $\beta = 8$. The length of the channel, L/H in the scaled model, has no impact on the result, so for simplicity we just compute on the unit square. Mathematically, the pressure must be prescribed at a point, but since p does not depend on y, we can set p to a known value, e.g. zero, along the outlet boundary $x = 1$. The result is $p(x) = 8(1-x)$ and $u_x = 4y(1-y)$.

The boundary conditions can be set as $p = 1$ at $x = 0$, $p = 0$ at $x = 1$ and $u = 0$ on the walls $y = 0,1$. This defines the pressure drop and should result in unit maximum velocity at the inlet and outlet and a parabolic velocity profile without further specifications. Note that it is only meaningful to solve the Navier–Stokes equations in 2D or 3D geometries, although the underlying mathematical problem collapses to two 1D problems, one for $u_x(y)$ and one for $p(x)$.

The scaled model is not so easy to simulate using a standard Navier–Stokes solver with dimensions. However, one can argue that the convection term is zero, so the Re coefficient in front of this term in the scaled PDEs is not important and can be set to unity. In that case, setting $\varrho = \mu = 1$ in the original Navier–Stokes equations resembles the scaled model.

For a specific engineering problem one wants to simulate a specific fluid and set corresponding parameters. A general solver is most naturally implemented with dimensions and the original physical parameters. However, the scaled problem simplifies numerical simulations a lot. First of all, it tells that all fluids flow in the same way: it does not matter whether we have oil, gas, or water flowing between two plates, and it does not matter how fast the flow is (up to some criticial value of the Reynolds number where the flow becomes unstable and goes over to a complicated turbulent flow of totally different na-

ture). This means that one simulation is enough to cover all types of channel flows! In other applications scaling tells us that it might be necessary to set just the fraction of some parameters (dimensionless numbers) rather than the parameters themselves. This simplifies exploring the input parameter space which is often the purpose of simulation. Frequently, the scaled problem is run by setting some of the input parameters with dimension to fixed values (often unity).

FEniCS implementation. Our previous examples have all started out with the creation of a mesh and then the definition of a `FunctionSpace` on the mesh. For the splitting scheme we will use to solve the Navier–Stokes equations we need to define two function spaces, one for the velocity and one for the pressure:

```
V = VectorFunctionSpace(mesh, 'P', 2)
Q = FunctionSpace(mesh, 'P', 1)
```

The first space `V` is a vector-valued function space for the velocity and the second space `Q` is a scalar-valued function space for the pressure. We use piecewise quadratic elements for the velocity and piecewise linear elements for the pressure. When creating a `VectorFunctionSpace` in FEniCS, the value-dimension (the length of the vectors) will be set equal to the geometric dimension of the finite element mesh. One can easily create vector-valued function spaces with other dimensions in FEniCS by adding the keyword parameter `dim`:

```
V = VectorFunctionSpace(mesh, 'P', 2, dim=10)
```

Stable finite element spaces for the Navier–Stokes equations

It is well-known that certain finite element spaces are not *stable* for the Navier–Stokes equations, or even for the simpler Stokes equations. The prime example of an unstable pair of finite element spaces is to use first degree continuous piecewise polynomials for both the velocity and the pressure. Using an unstable pair of spaces typically results in a solution with *spurious* (unwanted, non-physical) oscillations in the pressure solution. The simple remedy is to use piecewise continuous piecewise quadratic elements for the velocity and continuous piecewise linear elements for the pressure. Together, these elements form the so-called *Taylor-Hood* element. Spurious oscillations may occur also for splitting methods if an unstable element pair is used.

Since we have two different function spaces, we need to create two sets of trial and test functions:

```
u = TrialFunction(V)
```

```
v = TestFunction(V)
p = TrialFunction(Q)
q = TestFunction(Q)
```

As we have seen in previous examples, boundaries may be defined in FEniCS by defining Python functions that return `True` or `False` depending on whether a point should be considered part of the boundary, for example

```
def boundary(x, on_boundary):
    return near(x[0], 0)
```

This function defines the boundary to be all points with x-coordinate equal to (near) zero. The `near` function comes from FEniCS and performs a test with tolerance: `abs(x[0]-0) < 3E-16` so we do not run into rounding troubles. Alternatively, we may give the boundary definition as a string of C++ code, much like we have previously defined expressions such as `u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')`. The above definition of the boundary in terms of a Python function may thus be replaced by a simple C++ string:

```
boundary = 'near(x[0], 0)'
```

This has the advantage of moving the computation of which nodes belong to the boundary from Python to C++, which improves the efficiency of the program.

For the current example, we will set three different boundary conditions. First, we will set $u = 0$ at the walls of the channel; that is, at $y = 0$ and $y = 1$. Second, we will set $p = 1$ at the inflow ($x = 0$) and, finally, $p = 0$ at the outflow ($x = 1$). This will result in a pressure gradient that will accelerate the flow from an initial stationary state. These boundary conditions may be defined as follows:

```
# Define boundaries
inflow   = 'near(x[0], 0)'
outflow  = 'near(x[0], 1)'
walls    = 'near(x[1], 0) || near(x[1], 1)'

# Define boundary conditions
bcu_noslip  = DirichletBC(V, Constant((0, 0)), walls)
bcp_inflow  = DirichletBC(Q, Constant(8), inflow)
bcp_outflow = DirichletBC(Q, Constant(0), outflow)
bcu = [bcu_noslip]
bcp = [bcp_inflow, bcp_outflow]
```

At the end, we collect the boundary conditions for the velocity and pressure in Python lists so we can easily access them in the following computation.

We now move on to the definition of the variational forms. There are three variational problems to be defined, one for each step in the IPCS scheme. Let us look at the definition of the first variational problem. We start with some constants:

```
U   = 0.5*(u_n + u)
n   = FacetNormal(mesh)
f   = Constant((0, 0))
k   = Constant(dt)
mu  = Constant(mu)
rho = Constant(rho)
```

The next step is to set up the variational form for the first step (3.32) in the solution process. Since the variational problem contains a mix of known and unknown quantities we have introduced a naming convention to be used throughout the book: `u` is the unknown (mathematically u^{n+1}) as a trial function in the variational form, `u_` is the most recently computed approximation (u^{n+1} available as a finite element FEniCS `Function` object), `u_n` is u^n, and the same convention goes for `p`, `p_` (p^{n+1}), and `p_n` (p^n).

```
def epsilon(u):
    return sym(nabla_grad(u))

# Define stress tensor
def sigma(u, p):
    return 2*mu*epsilon(u) - p*Identity(len(u))

# Define variational problem for step 1
F1 = rho*dot((u - u_n) / k, v)*dx + \
     rho*dot(dot(u_n, nabla_grad(u_n)), v)*dx \
   + inner(sigma(U, p_n), epsilon(v))*dx \
   + dot(p_n*n, v)*ds - dot(mu*nabla_grad(U)*n, v)*ds \
   - rho*dot(f, v)*dx
a1 = lhs(F1)
L1 = rhs(F1)
```

Note that we, in the definition of the variational problem, take advantage of the Python programming language to define our own operators `sigma` and `epsilon`. Using Python this way makes it easy to extend the mathematical language of FEniCS with special operators and constitutive laws.

Also note that FEniCS can sort out the bilinear form $a(u,v)$ and linear form $L(v)$ forms by the `lhs` and `rhs` functions. This is particularly convenient in longer and more complicated variational forms.

The splitting scheme requires the solution of a sequence of three variational problems in each time step. We have previously used the built-in FEniCS function `solve` to solve variational problems. Under the hood, when a user calls `solve(a == L, u, bc)`, FEniCS will perform the following steps:

```
A = assemble(A)
b = assemble(L)
bc.apply(A, b)
solve(A, u.vector(), b)
```

In the last step, FEniCS uses the overloaded `solve` function to solve the linear system `AU = b` where `U` is the vector of degrees of freedom for the function $u(x) = \sum_{j=1} U_j \phi_j(x)$.

In our implementation of the splitting scheme, we will make use of these low-level commands to first assemble and then call solve. This has the advantage that we may control when we assemble and when we solve the linear system. In particular, since the matrices for the three variational problems are all time-independent, it makes sense to assemble them once and for all outside of the time-stepping loop:

```
A1 = assemble(a1)
A2 = assemble(a2)
A3 = assemble(a3)
```

Within the time-stepping loop, we may then assemble only the right-hand side vectors, apply boundary conditions, and call the solve function as here for the first of the three steps:

```
# Time-stepping
t = 0
for n in range(num_steps):

    # Update current time
    t += dt

    # Step 1: Tentative velocity step
    b1 = assemble(L1)
    [bc.apply(b1) for bc in bcu]
    solve(A1, u_.vector(), b1)
```

Notice the Python *list comprehension* `[bc.apply(b1) for bc in bcu]` which iterates over all `bc` in the list `bcu`. This is a convenient and compact way to construct a loop that applies all boundary conditions in a single line. Also, the code works if we add more Dirichlet boundary conditions in the future.

Finally, let us look at an important detail in how we use parameters such as the time step `dt` in the definition of our variational problems. Since we might want to change these later, for example if we want to experiment with smaller or larger time steps, we wrap these using a FEniCS `Constant`:

```
k = Constant(dt)
```

The assembly of matrices and vectors in FEniCS is based on code generation. This means that whenever we change a variational problem, FEniCS will have to generate new code, which may take a little time. New code will also be generated when a float value for the time step is changed. By wrapping this parameter using `Constant`, FEniCS will treat the parameter as a generic constant and not a specific numerical value, which prevents repeated code generation. In the case of the time step, we choose a new name `k` instead of `dt` for the `Constant` since we also want to use the variable `dt` as a Python float as part of the time-stepping.

The complete code for simulating 2D channel flow with FEniCS looks as follows:

```
from fenics import *
```

```
import numpy as np

T = 10.0           # final time
num_steps = 500    # number of time steps
dt = T / num_steps # time step size
mu = 1             # kinematic viscosity
rho = 1            # density

# Create mesh and define function spaces
mesh = UnitSquareMesh(16, 16)
V = VectorFunctionSpace(mesh, 'P', 2)
Q = FunctionSpace(mesh, 'P', 1)

# Define boundaries
inflow  = 'near(x[0], 0)'
outflow = 'near(x[0], 1)'
walls   = 'near(x[1], 0) || near(x[1], 1)'

# Define boundary conditions
bcu_noslip = DirichletBC(V, Constant((0, 0)), walls)
bcp_inflow = DirichletBC(Q, Constant(8), inflow)
bcp_outflow = DirichletBC(Q, Constant(0), outflow)
bcu = [bcu_noslip]
bcp = [bcp_inflow, bcp_outflow]

# Define trial and test functions
u = TrialFunction(V)
v = TestFunction(V)
p = TrialFunction(Q)
q = TestFunction(Q)

# Define functions for solutions at previous and current time steps
u_n = Function(V)
u_  = Function(V)
p_n = Function(Q)
p_  = Function(Q)

# Define expressions used in variational forms
U   = 0.5*(u_n + u)
n   = FacetNormal(mesh)
f   = Constant((0, 0))
k   = Constant(dt)
mu  = Constant(mu)
rho = Constant(rho)

# Define strain-rate tensor
def epsilon(u):
    return sym(nabla_grad(u))

# Define stress tensor
def sigma(u, p):
    return 2*mu*epsilon(u) - p*Identity(len(u))

# Define variational problem for step 1
```

```
F1 = rho*dot((u - u_n) / k, v)*dx + \
     rho*dot(dot(u_n, nabla_grad(u_n)), v)*dx \
   + inner(sigma(U, p_n), epsilon(v))*dx \
   + dot(p_n*n, v)*ds - dot(mu*nabla_grad(U)*n, v)*ds \
   - rho*dot(f, v)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# Define variational problem for step 2
a2 = dot(nabla_grad(p), nabla_grad(q))*dx
L2 = dot(nabla_grad(p_n), nabla_grad(q))*dx - (1/k)*div(u_)*q*dx

# Define variational problem for step 3
a3 = dot(u, v)*dx
L3 = dot(u_, v)*dx - k*dot(nabla_grad(p_ - p_n), v)*dx

# Assemble matrices
A1 = assemble(a1)
A2 = assemble(a2)
A3 = assemble(a3)

# Apply boundary conditions to matrices
[bc.apply(A1) for bc in bcu]
[bc.apply(A2) for bc in bcp]

# Time-stepping
t = 0
for n in range(num_steps):

    # Update current time
    t += dt

    # Step 1: Tentative velocity step
    b1 = assemble(L1)
    [bc.apply(b1) for bc in bcu]
    solve(A1, u_.vector(), b1)

    # Step 2: Pressure correction step
    b2 = assemble(L2)
    [bc.apply(b2) for bc in bcp]
    solve(A2, p_.vector(), b2)

    # Step 3: Velocity correction step
    b3 = assemble(L3)
    solve(A3, u_.vector(), b3)

    # Plot solution
    plot(u_)

    # Compute error
    u_e = Expression(('4*x[1]*(1.0 - x[1])', '0'), degree=2)
    u_e = interpolate(u_e, V)
    error = np.abs(u_e.vector().array() - u_.vector().array()).max()
    print('t = %.2f: error = %.3g' % (t, error))
```

```
    print('max u:', u_.vector().array().max())

    # Update previous solution
    u_n.assign(u_)
    p_n.assign(p_)

# Hold plot
interactive()
```

The complete code can be found in the file `ft08_navier_stokes_channel.py`.

Verification. We compute the error at the nodes as we have done before to verify that our implementation is correct. Our Navier–Stokes solver computes the solution to the time-dependent incompressible Navier–Stokes equations, starting from the initial condition $u = (0, 0)$. We have not specified the initial condition explicitly in our solver which means that FEniCS will initialize all variables, in particular the previous and current velocities `u_n` and `u_`, to zero. Since the exact solution is quadratic, we expect the solution to be exact to within machine precision at the nodes at infinite time. For our implementation, the error quickly approaches zero and is approximately 10^{-6} at time $T = 10$.

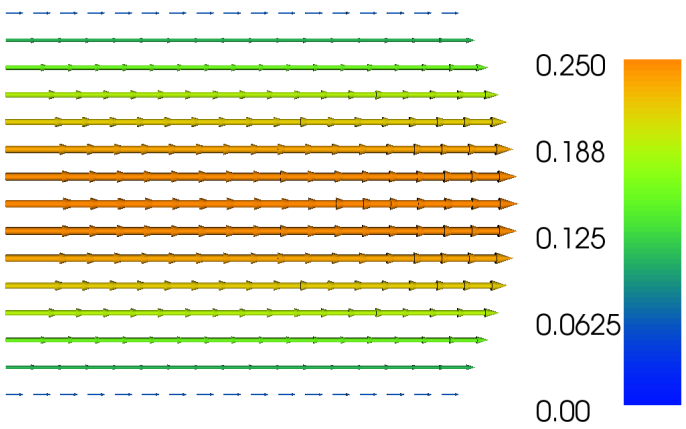


Fig. 3.2 Plot of the velocity profile at the final time for the Navier–Stokes Poiseuille flow example.

Exercise 3.1: Simulate channel flow in a 3D geometry

FEniCS solvers typically have the number of space dimensions parameterized, so a 1D, 2D, and 3D code all look the same. We shall demonstrate what this

means by extending the 2D solver `navier_stokes_channel.py` to a simulator where the domain is a box (the unit cube in the scaled model).

a) Set up boundary conditions for u at all points on the boundary. Set up boundary conditions for p at all points on the boundary as this is required by our Poisson equation for p (but not in the original mathematical model – there, knowing p at one point throughout time is sufficient).

Solution. At the inlet $x = 0$ we have the velocity completely described: $(u_x, 0, 0)$. At the channel walls, $y = 0$ and $y = 1$, we also have the velocity completely described: $u = (0, 0, 0)$ because of no-slip. At the outlet x=1 we do not specify anything. This means that the boundary integrals in Step 1 vanish and that $p = 0$ and $\partial u/\partial n = 0$, with n as the x direction, implying "no change" with x, which is reasonable (since we know that $\partial/\partial x = 0$ because of incompressibility). For the pressure we set $p = 8$ at $x = 0$ and $p = 0$ at $x = 1$ to represent a scaled pressure gradient equal to 8 (which leads to a unit maximum velocity). At $y = 0$ and $y = 1$ we do not specify anything, which implies $\partial p/\partial y = 0$. This is a condition much discussed in the literature, but it works perfectly in channel flow with straight walls.

The two remaining boundaries, $z = 0$ and $z = 1$, requires attention. For the pressure, "nothing happens" in the z direction so $\partial p/\partial z = \partial p/\partial n = 0$ is the condition. This is automatically implemented by the finite element method. For the velocity we also have a "nothing happens" criterion in the 3rd direction, and we can in addition use the assumption of $u_z = 0$, if needed. The derivative criterion means $\partial u/\partial z = \partial u/\partial n = 0$ in the boundary integrals. There is also an integral involving pn_z in a component PDE with u_z in all terms.

b) Modify the `navier_stokes_channel.py` file so it computes 3D channel flow.

Solution. We must switch the domain from `UnitSquareMesh` to `UnitCubeMesh`. We must also switch all 3-vectors to 2-vectors, such as replacing going from `(0,0)` to `(0,0,0)` in `bcu_noslip`. Similarly, `f` and `u_e` must extend their 2-vectors to 3-vectors.

```
from fenics import *
import numpy as np

T = 10.0           # final time
num_steps = 500    # number of time steps
dt = T / num_steps # time step size
mu = 1             # kinematic viscosity
rho = 1            # density

# Create mesh and define function spaces
mesh = UnitCubeMesh(4, 8, 4)
V = VectorFunctionSpace(mesh, 'P', 2)
Q = FunctionSpace(mesh, 'P', 1)
```

```
# Define boundaries
inflow  = 'near(x[0], 0)'
outflow = 'near(x[0], 1)'
walls   = 'near(x[1], 0) || near(x[1], 1)'

# Define boundary conditions
bcu_noslip = DirichletBC(V, Constant((0, 0, 0)), walls)
bcp_inflow = DirichletBC(Q, Constant(8), inflow)
bcp_outflow = DirichletBC(Q, Constant(0), outflow)
bcu = [bcu_noslip]
bcp = [bcp_inflow, bcp_outflow]

# Define trial and test functions
u = TrialFunction(V)
v = TestFunction(V)
p = TrialFunction(Q)
q = TestFunction(Q)

# Define functions for solutions at previous and current time steps
u0 = Function(V)
u1 = Function(V)
p0 = Function(Q)
p1 = Function(Q)

# Define expressions used in variational forms
U   = 0.5*(u0 + u)
n   = FacetNormal(mesh)
f   = Constant((0, 0, 0))
k   = Constant(dt)
mu  = Constant(mu)
rho = Constant(rho)

# Define strain-rate tensor
def epsilon(u):
    return sym(nabla_grad(u))

# Define stress tensor
def sigma(u, p):
    return 2*mu*epsilon(u) - p*Identity(len(u))

# Define variational problem for step 1
F1 = rho*dot((u - u0) / k, v)*dx + \
     rho*dot(dot(u0, nabla_grad(u0)), v)*dx \
   + inner(sigma(U, p0), epsilon(v))*dx \
   + dot(p0*n, v)*ds - dot(mu*nabla_grad(U)*n, v)*ds \
   - rho*dot(f, v)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# Define variational problem for step 2
a2 = dot(nabla_grad(p), nabla_grad(q))*dx
L2 = dot(nabla_grad(p0), nabla_grad(q))*dx - (1/k)*div(u1)*q*dx

# Define variational problem for step 3
```

```
a3 = dot(u, v)*dx
L3 = dot(u1, v)*dx - k*dot(nabla_grad(p1 - p0), v)*dx

# Assemble matrices
A1 = assemble(a1)
A2 = assemble(a2)
A3 = assemble(a3)

# Apply boundary conditions to matrices
[bc.apply(A1) for bc in bcu]
[bc.apply(A2) for bc in bcp]

# Time-stepping
t = 0
for n in xrange(num_steps):

    # Update current time
    t += dt

    # Step 1: Tentative velocity step
    b1 = assemble(L1)
    [bc.apply(b1) for bc in bcu]
    solve(A1, u1.vector(), b1)

    # Step 2: Pressure correction step
    b2 = assemble(L2)
    [bc.apply(b2) for bc in bcp]
    solve(A2, p1.vector(), b2)

    # Step 3: Velocity correction step
    b3 = assemble(L3)
    solve(A3, u1.vector(), b3)

    # Plot solution
    plot(u1)

    # Compute error
    u_e = Expression(('4*x[1]*(1.0 - x[1])', '0', '0'), degree=2)
    u_e = interpolate(u_e, V)
    error = np.abs(u_e.vector().array() - u1.vector().array()).max()
    print('t = %.2f: error = %.3g' % (t, error))
    print('max u:', u1.vector().array().max())

    # Update previous solution
    u0.assign(u1)
    p0.assign(p1)

# Hold plot
interactive()
```

3.4.4 Flow past a cylinder

We now turn our attention to a more challenging physical example: flow past a circular cylinder. The geometry and parameters are taken from problem DFG 2D-2 in the FEATFLOW/1995-DFG benchmark suite and is illustrated in Figure 3.3. The kinematic viscosity is given by $\nu = 0.001 = \mu/\varrho$ and the inflow velocity profile is specified as

$$u(x,y,t) = \left(1.5 \cdot \frac{4y(1-y)}{0.41^2}, 0\right),$$

which has a maximum magnitude of 1.5 at $y = 0.41/2$. We do not scale anything in this benchmark since exact parameters in the case we want to simulate are known.

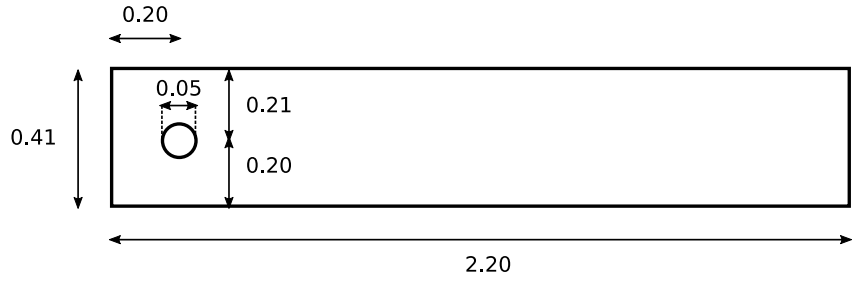


Fig. 3.3 Geometry for the flow past a cylinder test problem. Notice the slightly perturbed and unsymmetric geometry.

FEniCS implementation. So far all our domains have been simple shapes such as a unit square or a rectangular box. A number of such simple meshes may be created in FEniCS using the built-in meshes (`UnitIntervalMesh`, `UnitSquareMesh`, `UnitCubeMesh`, `IntervalMesh`, `RectangleMesh`, and `BoxMesh`). FEniCS supports the creation of more complex meshes via a technique called *constructive solid geometry* (CSG), which lets us define geometries in terms of simple shapes (primitives) and set operations: union, intersection, and set difference. The set operations are encoded in FEniCS using the operators `+` (union), `*` (intersection), and `-` (set difference). To access the CSG functionality in FEniCS, one must import the FEniCS module `mshr` which provides the extended meshing functionality of FEniCS.

The geometry for the cylinder flow test problem can be defined easily by first defining the rectangular channel and then subtracting the circle:

```
channel = Rectangle(Point(0, 0), Point(2.2, 0.41))
cylinder = Circle(Point(0.2, 0.2), 0.05)
geometry = channel - cylinder
```

We may then create the mesh by calling the function `generate_mesh`:

```
mesh = generate_mesh(geometry, 64)
```

To solve the cylinder test problem, we only need to make a few minor changes to the code we wrote for the Poiseuille flow test case. Besides defining the new mesh, the only change we need to make is to modify the boundary conditions and the time step size. The boundaries are specified as follows:

```
inflow   = 'near(x[0], 0)'
outflow  = 'near(x[0], 2.2)'
walls    = 'near(x[1], 0) || near(x[1], 0.41)'
cylinder = 'on_boundary && x[0]>0.1 && x[0]<0.3 && x[1]>0.1 && x[1]<0.3'
```

The last line may seem cryptic before you catch the idea: we want to pick out all boundary points (`on_boundary`) that also lie within the 2D domain $[0.1, 0.3] \times [0.1, 0.3]$, see Figure 3.3. The only possible points are then the points on the circular boundary!

In addition to these essential changes, we will make a number of small changes to improve our solver. First, since we need to choose a relatively small time step to compute the solution (a time step that is too large will make the solution blow up) we add a progress bar so that we can follow the progress of our computation. This can be done as follows:

```
progress = Progress('Time-stepping')
set_log_level(PROGRESS)

t = 0.0
for n in range(num_steps):

    # Update current time
    t += dt

    # Place computation here

    # Update progress bar
    progress.update(t / T)
```

Log levels and printing in FEniCS

Notice the call to `set_log_level(PROGRESS)` which is essential to make FEniCS actually display the progress bar. FEniCS is actually quite informative about what is going on during a computation but the amount of information printed to screen depends on the current log level. Only messages with a priority higher than or equal to the current log level will be displayed. The predefined log levels in FEniCS are `DBG`, `TRACE`, `PROGRESS`, `INFO`, `WARNING`, `ERROR`, and `CRITICAL`. By default, the log level is set to `INFO` which means that messages at level `DBG`, `TRACE`, and `PROGRESS` will not be printed. Users may print messages using the FEniCS functions `info`, `warning`, and `error` which will print messages at

the obvious log level (and in the case of `error` also throw an exception and exit). One may also use the call `log(level, message)` to print a message at a specific log level.

Since the system(s) of linear equations are significantly larger than for the simple Poiseuille flow test problem, we choose to use an iterative method instead of the default direct (sparse) solver used by FEniCS when calling `solve`. Efficient solution of linear systems arising from the discretization of PDEs requires the choice of both a good iterative (Krylov subspace) method and a good preconditioner. For this problem, we will simply use the biconjugate gradient stabilized method (BiCGSTAB). This can be done by adding the keyword `bicgstab` in the call to `solve`. We also add a preconditioner, `ilu` to further speed up the computations:

```
solve(A1, u1.vector(), b1, 'bicgstab', 'ilu')
solve(A2, p1.vector(), b2, 'bicgstab', 'ilu')
solve(A3, u1.vector(), b3, 'bicgstab')
```

Finally, to be able to postprocess the computed solution in Paraview, we store the solution to file in each time step. To avoid cluttering our working directory with a large number of solution files, we make sure to store the solution in a subdirectory:

```
vtkfile_u = File('navier_stokes_cylinder/velocity.pvd')
vtkfile_p = File('navier_stokes_cylinder/pressure.pvd')
```

Note that one does not need to create the directory before running the program. It will be created automatically by FEniCS.

We also store the solution using a FEniCS `TimeSeries`. This allows us to store the solution not for visualization (as when using VTK files), but for later reuse in a computation as we will see in the next section. Using a `TimeSeries` it is easy and efficient to read in solutions from certain points in time during a simulation. The `TimeSeries` class uses a binary HDF5 file for efficient storage and access to data.

Figures 3.4 and 3.5 show the velocity and pressure at final time visualized in Paraview. For the visualization of the velocity, we have used the **Glyph** filter to visualize the vector velocity field. For the visualization of the pressure, we have used the **Warp By Scalar** filter.

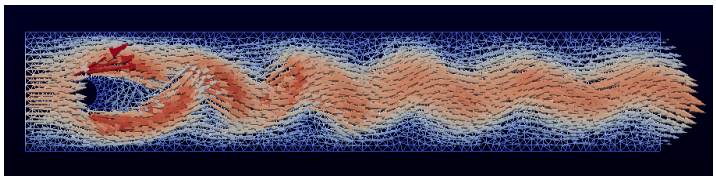


Fig. 3.4 Plot of the velocity for the cylinder test problem at final time.

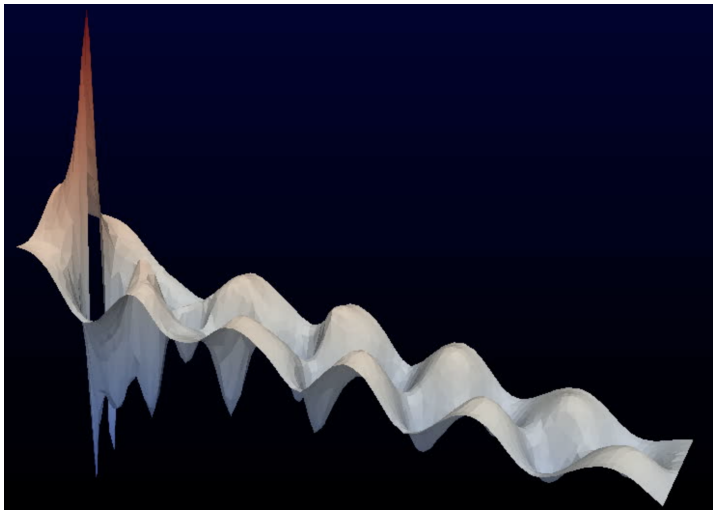


Fig. 3.5 Plot of the pressure for the cylinder test problem at final time.

The complete code for the cylinder test problem looks as follows:

```
from fenics import *
from mshr import *
import numpy as np

T = 5.0            # final time
num_steps = 5000   # number of time steps
dt = T / num_steps # time step size
mu = 0.001         # dynamic viscosity
rho = 1            # density

# Create mesh
channel = Rectangle(Point(0, 0), Point(2.2, 0.41))
cylinder = Circle(Point(0.2, 0.2), 0.05)
geometry = channel - cylinder
mesh = generate_mesh(geometry, 64)

# Define function spaces
V = VectorFunctionSpace(mesh, 'P', 2)
Q = FunctionSpace(mesh, 'P', 1)

# Define boundaries
inflow   = 'near(x[0], 0)'
outflow  = 'near(x[0], 2.2)'
walls    = 'near(x[1], 0) || near(x[1], 0.41)'
cylinder = 'on_boundary && x[0]>0.1 && x[0]<0.3 && x[1]>0.1 && x[1]<0.3'

# Define inflow profile
inflow_profile = ('4.0*1.5*x[1]*(0.41 - x[1]) / pow(0.41, 2)', '0')

# Define boundary conditions
```

```
bcu_inflow = DirichletBC(V, Expression(inflow_profile, degree=2), inflow)
bcu_walls = DirichletBC(V, Constant((0, 0)), walls)
bcu_cylinder = DirichletBC(V, Constant((0, 0)), cylinder)
bcp_outflow = DirichletBC(Q, Constant(0), outflow)
bcu = [bcu_inflow, bcu_walls, bcu_cylinder]
bcp = [bcp_outflow]

# Define trial and test functions
u = TrialFunction(V)
v = TestFunction(V)
p = TrialFunction(Q)
q = TestFunction(Q)

# Define functions for solutions at previous and current time steps
u_n = Function(V)
u_  = Function(V)
p_n = Function(Q)
p_  = Function(Q)

# Define expressions used in variational forms
U   = 0.5*(u_n + u)
n   = FacetNormal(mesh)
f   = Constant((0, 0))
k   = Constant(dt)
mu  = Constant(mu)

# Define symmetric gradient
def epsilon(u):
    return sym(nabla_grad(u))

# Define stress tensor
def sigma(u, p):
    return 2*mu*epsilon(u) - p*Identity(len(u))

# Define variational problem for step 1
F1 = rho*dot((u - u_n) / k, v)*dx \
   + rho*dot(dot(u_n, nabla_grad(u_n)), v)*dx \
   + inner(sigma(U, p_n), epsilon(v))*dx \
   + dot(p_n*n, v)*ds - dot(mu*nabla_grad(U)*n, v)*ds \
   - rho*dot(f, v)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# Define variational problem for step 2
a2 = dot(nabla_grad(p), nabla_grad(q))*dx
L2 = dot(nabla_grad(p_n), nabla_grad(q))*dx - (1/k)*div(u_)*q*dx

# Define variational problem for step 3
a3 = dot(u, v)*dx
L3 = dot(u_, v)*dx - k*dot(nabla_grad(p_ - p_n), v)*dx

# Assemble matrices
A1 = assemble(a1)
A2 = assemble(a2)
```

```
A3 = assemble(a3)

# Apply boundary conditions to matrices
[bc.apply(A1) for bc in bcu]
[bc.apply(A2) for bc in bcp]

# Create VTK files for visualization output
vtkfile_u = File('navier_stokes_cylinder/velocity.pvd')
vtkfile_p = File('navier_stokes_cylinder/pressure.pvd')

# FIXME: mpi_comm_world should not be needed here, fix in FEniCS!

# Create time series for saving solution for later
timeseries_u = TimeSeries('navier_stokes_cylinder/velocity')
timeseries_p = TimeSeries('navier_stokes_cylinder/pressure')

# Save mesh to file for later
File('cylinder.xml.gz') << mesh

# Create progress bar
progress = Progress('Time-stepping')
set_log_level(PROGRESS)

# Time-stepping
t = 0
for n in range(num_steps):

    # Update current time
    t += dt

    # Step 1: Tentative velocity step
    b1 = assemble(L1)
    [bc.apply(b1) for bc in bcu]
    solve(A1, u_.vector(), b1, 'bicgstab', 'ilu')

    # Step 2: Pressure correction step
    b2 = assemble(L2)
    [bc.apply(b2) for bc in bcp]
    solve(A2, p_.vector(), b2, 'bicgstab', 'ilu')

    # Step 3: Velocity correction step
    b3 = assemble(L3)
    solve(A3, u_.vector(), b3, 'bicgstab')

    # Plot solution
    plot(u_, title='Velocity')
    plot(p_, title='Pressure')

    # Save solution to file (VTK)
    vtkfile_u << (u_, t)
    vtkfile_p << (p_, t)

    # Save solution to file (HDF5)
    timeseries_u.store(u_.vector(), t)
```

```
    timeseries_p.store(p_.vector(), t)

    # Update previous solution
    u_n.assign(u_)
    p_n.assign(p_)

    # Update progress bar
    progress.update(t / T)
    print('u max:', u_.vector().array().max())

# Hold plot
interactive()
```

The complete code can be found in the file `ft09_navier_stokes_cylinder.py`.

3.5 A system of advection–diffusion–reaction equations

The problems we have encountered so far—with the notable exception of the Navier–Stokes equations—all share a common feature: they all involve models expressed by a *single* scalar or vector PDE. In many situations the model is instead expressed as a system of PDEs, describing different quantities and with possibly (very) different physics. As we saw for the Navier–Stokes equations, one way to solve a system of PDEs in FEniCS is to use a splitting method where we solve one equation at a time and feed the solution from one equation into the next. However, one of the strengths with FEniCS is the ease by which one can instead define variational problems that couple several PDEs into one compound system. In this section, we will look at how to use FEniCS to write solvers for such systems of coupled PDEs. The goal is to demonstrate how easy it is to implement fully implicit, also known as monolithic, solvers in FEniCS.

3.5.1 PDE problem

Our model problem is the following system of advection–diffusion–reaction equations:

$$\frac{\partial u_1}{\partial t} + w \cdot \nabla u_1 - \nabla \cdot (\epsilon \nabla u_1) = f_1 - K u_1 u_2, \tag{3.36}$$

$$\frac{\partial u_2}{\partial t} + w \cdot \nabla u_2 - \nabla \cdot (\epsilon \nabla u_2) = f_2 - K u_1 u_2, \tag{3.37}$$

$$\frac{\partial u_3}{\partial t} + w \cdot \nabla u_3 - \nabla \cdot (\epsilon \nabla u_3) = f_3 + K u_1 u_2 - K u_3. \tag{3.38}$$

This system models the chemical reaction between two species A and B in some domain Ω:

$$A + B \to C.$$

We assume that the equation is *first-order*, meaning that the reaction rate is proportional to the concentrations $[A]$ and $[B]$ of the two species A and B:

$$\frac{\mathrm{d}}{\mathrm{d}t}[C] = K[A][B].$$

We also assume that the formed species C spontaneously decays with a rate proportional to the concentration $[C]$. In the PDE system (3.36)–(3.38), we use the variables u_1, u_2, and u_3 to denote the concentrations of the three species:

$$u_1 = [A], \quad u_2 = [B], \quad u_3 = [C].$$

We see that the chemical reactions are accounted for in the right-hand sides of the PDE system (3.36)–(3.38).

The chemical reactions take part at each point in the domain Ω. In addition, we assume that the species A, B, and C diffuse throughout the domain with diffusivity ϵ (the terms $-\nabla \cdot (\epsilon \nabla u_i)$) and are advected with velocity w (terms like $w \cdot \nabla u_i$).

To make things visually and physically interesting, we shall let the chemical reaction take place in the velocity field computed from the solution of the incompressible Navier–Stokes equations around a cylinder from the previous section. In summary, we will thus be solving the following coupled system of nonlinear PDEs:

$$\varrho \left(\frac{\partial w}{\partial t} + w \cdot \nabla w \right) = \nabla \cdot \sigma(w, p) + f, \tag{3.39}$$

$$\nabla \cdot w = 0, \tag{3.40}$$

$$\frac{\partial u_1}{\partial t} + w \cdot \nabla u_1 - \nabla \cdot (\epsilon \nabla u_1) = f_1 - K u_1 u_2, \tag{3.41}$$

$$\frac{\partial u_2}{\partial t} + w \cdot \nabla u_2 - \nabla \cdot (\epsilon \nabla u_2) = f_2 - K u_1 u_2, \tag{3.42}$$

$$\frac{\partial u_3}{\partial t} + w \cdot \nabla u_3 - \nabla \cdot (\epsilon \nabla u_3) = f_3 + K u_1 u_2 - K u_3. \tag{3.43}$$

We assume that $u_1 = u_2 = u_3 = 0$ at $t = 0$ and inject the species A and B into the system by specifying nonzero source terms f_1 and f_2 close to the corners at the inflow, and take $f_3 = 0$. The result will be that A and B are convected by advection and diffusion throughout the channel, and when they mix the species C will be formed.

Since the system is one-way coupled from the Navier–Stokes subsystem to the advection–diffusion–reaction subsystem, we do not need to recompute the solution to the Navier–Stokes equations, but can just read back the previously computed velocity field w and feed it into our equations. But we *do* need to learn how to read and write solutions from time-dependent PDE problems.

3.5.2 Variational formulation

We obtain the variational formulation of our system by multiplying each equation by a test function, integrating the second-order terms $-\nabla\cdot(\epsilon\nabla u_i)$ by parts, and summing up the equations. When working with FEniCS it is convenient to think of the PDE system as a vector of equations. The test functions are collected in a vector too, and the variational formulation is the inner product of the vector PDE and the vector test function.

We also need introduce some discretization in time. We will use the backward Euler method as before when we solved the heat equation and approximate the time derivatives by $(u_i^{n+1} - u_i^n)/\Delta t$. Let v_1, v_2, and v_3 be the test functions, or the components of the test vector function. The inner product results in

$$\int_\Omega (\Delta t^{-1}(u_1^{n+1} - u_1^n)v_1 + w\cdot\nabla u_1^{n+1} v_1 + \epsilon\nabla u_1^{n+1}\cdot\nabla v_1)\,\mathrm{d}x \tag{3.44}$$

$$+\int_\Omega (\Delta t^{-1}(u_2^{n+1} - u_2^n)v_2 + w\cdot\nabla u_2^{n+1} v_2 + \epsilon\nabla u_2^{n+1}\cdot\nabla v_2)\,\mathrm{d}x \tag{3.45}$$

$$+\int_\Omega (\Delta t^{-1}(u_3^{n+1} - u_3^n)v_3 + w\cdot\nabla u_3^{n+1} v_3 + \epsilon\nabla u_3^{n+1}\cdot\nabla v_3)\,\mathrm{d}x \tag{3.46}$$

$$-\int_\Omega (f_1 v_1 + f_2 v_2 + f_3 v_3)\,\mathrm{d}x \tag{3.47}$$

$$-\int_\Omega (-K u_1^{n+1} u_2^{n+1} v_1 - K u_1^{n+1} u_2^{n+1} v_2 + K u_1^{n+1} u_2^{n+1} v_3 - K u_3^{n+1} v_3)\,\mathrm{d}x = 0. \tag{3.48}$$

For this problem it is natural to assume homogeneous Neumann boundary conditions on the entire boundary for u_1, u_2, and u_3; that is, $\partial u_i/\partial n = 0$ for $i = 1, 2, 3$. This means that the boundary terms vanish when we integrate by parts.

3.5.3 FEniCS implementation

The first step is to read the mesh from file. Luckily, we made sure to save the mesh to file in the Navier–Stokes example and can now easily read it back from file:

```
mesh = Mesh(cylinder.xml.gz')
```

The mesh is stored in the native FEniCS XML format (with additional gzipping to decrease the file size).

Next, we need to define the finite element function space. For this problem, we need to define several spaces. The first space we create is the space for the velocity field w from the Navier–Stokes simulation. We call this space W and define the space by

```
W = VectorFunctionSpace(mesh, 'P', 2)
```

It is important that this space is exactly the same as the space we used for the velocity field in the Navier–Stokes solver. To read the values for the velocity field, we use a `TimeSeries`:

```
timeseries_w = TimeSeries('navier_stokes_cylinder/velocity')
```

This will initialize the object `timeseries_w` which we will call later in the time-stepping loop to retrieve values from the file `velocity.h5` (in binary HDF5 format).

For the three concentrations u_1, u_2, and u_3, we want to create a *mixed space* with functions that represent the full system (u_1, u_2, u_3) as a single entity. To do this, we need to define a `MixedElement` as the product space of three simple finite elements and then used the mixed element to define the function space:

```
P1 = FiniteElement('P', 'triangle', 1)
element = MixedElement([P1, P1, P1])
V = FunctionSpace(mesh, element)
```

Mixed elements as products of elements

FEniCS also allows finite elements to be defined as products of simple elements (or mixed elements). For example, the well-known Taylor–Hood element, with quadratic velocity components and linear pressure functions, may be defined as follows:

```
P2 = VectorElement('P', 'triangle', 2)
P1 = FiniteElement('P', 'triangle', 1)
TH = P2 * P1
```

This syntax works great for two elements, but for three or more elements we meet a subtle issue in how the Python interpreter handles the `*` operator. For the reaction system, we create the mixed element by `element = MixedElement([P1, P1, P1])` and one would be tempted to write

```
element = P1 * P1 * P1
```

However, this is equivalent to writing `element = (P1 * P1) * P1` so the result will be a mixed element consisting of two subsystems, the first of which in turn consists of two scalar subsystems.

Finally, we remark that for the simple case of a mixed system consisting of three scalar elements as for the reaction system, the definition is in fact equivalent to using a standard vector-valued element:

```
element = VectorElement('P', 'triangle', 1, dim=3)
V = FunctionSpace(mesh, element)
```

Once the space has been created, we need to define our test functions and finite element functions. Test functions for a mixed function space can be created by replacing `TestFunction` by `TestFunctions`:

```
v_1, v_2, v_3 = TestFunctions(V)
```

Since the problem is nonlinear, we need to work with functions rather than trial functions for the unknowns. This can be done by using the corresponding `Functions` construction in FEniCS. However, as we will need to access the `Function` for the entire system itself, we first need to create that function and then access its components:

```
u = Function(V)
u_1, u_2, u_3 = split(u)
```

These functions will be used to represent the unknowns u_1, u_2, and u_3 at the new time level $n+1$. The corresponding values at the previous time level n are denoted by `u_n1`, `u_n2`, and `u_n3` in our program.

When now all functions and test functions have been defined, we can express the nonlinear variational problem (3.44):

```
F = ((u_1 - u_n1) / k)*v_1*dx + dot(w, grad(u_1))*v_1*dx \
  + eps*dot(grad(u_1), grad(v_1))*dx + K*u_1*u_2*v_1*dx  \
  + ((u_2 - u_n2) / k)*v_2*dx + dot(w, grad(u_2))*v_2*dx \
  + eps*dot(grad(u_2), grad(v_2))*dx + K*u_1*u_2*v_2*dx  \
  + ((u_3 - u_n3) / k)*v_3*dx + dot(w, grad(u_3))*v_3*dx \
  + eps*dot(grad(u_3), grad(v_3))*dx - K*u_1*u_2*v_3*dx + K*u_3*v_3*dx \
  - f_1*v_1*dx - f_2*v_2*dx - f_3*v_3*dx
```

The time-stepping simply consists of solving this variational problem in each time step by a call to the `solve` function:

```
t = 0
for n in range(num_steps):
    t += dt
    timeseries_w.retrieve(w.vector(), t)
    solve(F == 0, u)
    u_n.assign(u)
```

In each time step, we first read the current value for the velocity field from the time series we have previously stored. We then solve the nonlinear system, and assign the computed values to the left-hand side values for the next time interval.

The solution at the final time is shown in Figure 3.6. We clearly see the advection of the species A and B and the formation of C along the center of the channel where A and B meet.

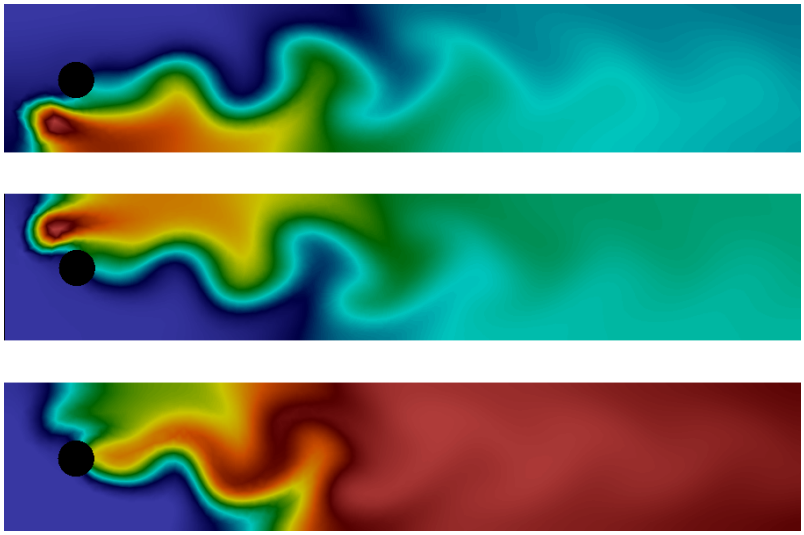


Fig. 3.6 Plot of the concentrations of the three species A, B, and C (from top to bottom) at final time.

The complete code is presented below.

```
from fenics import *

T = 5.0            # final time
num_steps = 500    # number of time steps
dt = T / num_steps # time step size
eps = 0.01         # diffusion coefficient
K = 10.0           # reaction rate

# Read mesh from file
mesh = Mesh('cylinder.xml.gz')
```

```
# Define function space for velocity
W = VectorFunctionSpace(mesh, 'P', 2)

# Define function space for system of concentrations
P1 = FiniteElement('P', 'triangle', 1)
element = MixedElement([P1, P1, P1])
V = FunctionSpace(mesh, element)

# Define test functions
v_1, v_2, v_3 = TestFunctions(V)

# Define functions for velocity and concentrations
w = Function(W)
u = Function(V)
u_n = Function(V)

# Split system functions to access components
u_1, u_2, u_3 = split(u)
u_n1, u_n2, u_n3 = split(u_n)

# Define source terms
f_1 = Expression('pow(x[0]-0.1,2)+pow(x[1]-0.1,2)<0.05*0.05 ? 0.1 : 0',
                 degree=1)
f_2 = Expression('pow(x[0]-0.1,2)+pow(x[1]-0.3,2)<0.05*0.05 ? 0.1 : 0',
                 degree=1)
f_3 = Constant(0)

# Define expressions used in variational forms
k = Constant(dt)
K = Constant(K)
eps = Constant(eps)

# Define variational problem
F = ((u_1 - u_n1) / k)*v_1*dx + dot(w, grad(u_1))*v_1*dx \
  + eps*dot(grad(u_1), grad(v_1))*dx + K*u_1*u_2*v_1*dx  \
  + ((u_2 - u_n2) / k)*v_2*dx + dot(w, grad(u_2))*v_2*dx \
  + eps*dot(grad(u_2), grad(v_2))*dx + K*u_1*u_2*v_2*dx  \
  + ((u_3 - u_n3) / k)*v_3*dx + dot(w, grad(u_3))*v_3*dx \
  + eps*dot(grad(u_3), grad(v_3))*dx - K*u_1*u_2*v_3*dx + K*u_3*v_3*dx \
  - f_1*v_1*dx - f_2*v_2*dx - f_3*v_3*dx

# Create time series for reading velocity data
timeseries_w = TimeSeries('navier_stokes_cylinder/velocity')

# Create VTK files for visualization output
vtkfile_u_1 = File('reaction_system/u_1.pvd')
vtkfile_u_2 = File('reaction_system/u_2.pvd')
vtkfile_u_3 = File('reaction_system/u_3.pvd')

# Create progress bar
progress = Progress('Time-stepping')
set_log_level(PROGRESS)

# Time-stepping
```

```
t = 0
for n in range(num_steps):

    # Update current time
    t += dt

    # Read velocity from file
    timeseries_w.retrieve(w.vector(), t)

    # Solve variational problem for time step
    solve(F == 0, u)

    # Save solution to file (VTK)
    _u_1, _u_2, _u_3 = u.split()
    vtkfile_u_1 << _u_1
    vtkfile_u_2 << _u_2
    vtkfile_u_3 << _u_3

    # Update previous solution
    u_n.assign(u)

    # Update progress bar
    progress.update(t / T)

# Hold plot
interactive()
```

The complete code can be found in the file `ft10_reaction_system.py`.

Finally, we comment on three important techniques that are very useful when working with systems of PDEs: setting initial conditions, setting boundary conditions, and extracting components of the system for plotting or postprocessing.

3.5.4 Setting initial conditions for mixed systems

In our example, we did not need to worry about setting an initial condition, since we start with $u_1 = u_2 = u_3 = 0$. This happens automatically in the code when we set `u_n = Function(V)`. This creates a `Function` for the whole system and all degrees of freedom are set to zero.

If we want to set initial conditions for the components of the system separately, the easiest solution is to define the initial conditions as a vector-valued `Expression` and then project this to the `Function` representing the whole system. For example,

```
u_0 = Expression(('sin(x[0])', 'cos(x[0]*x[1])', 'exp(x[1])'), degree=1)
u_n = project(u_0, V)
```

This defines u_1, u_2, and u_2 to be the projections of $\sin x$, $\cos(xy)$, and $\exp(y)$, respectively.

3.5.5 Setting boundary conditions for mixed systems

In our example, we also did not need to worry about setting boundary conditions since we used a natural Neumann condition. If we want to set Dirichlet conditions for individual components of the system, this can be done as usual by the class `DirichletBC`, but we must specify for which subsystem we set the boundary condition. For example, to specify that u_2 should be equal to xy on the boundary defined by `boundary`, we do

```
u_D = Expression('x[0]*x[1]', degree=1)
bc = DirichletBC(V.sub(1), u_D, boundary)
```

The object `bc` or a list of such objects containing different boundary conditions, can then be passed to the `solve` function as usual. Note that numbering starts at 0 in FEniCS so the subspace corresponding to u_2 is `V.sub(1)`.

3.5.6 Accessing components of mixed systems

If `u` is a `Function` defined on a mixed function space in FEniCS, there are several ways in which `u` can be *split* into components. Above we already saw an example of the first of these:

```
u_1, u_2, u_3 = split(u)
```

This extracts the components of `u` as *symbols* that can be used in a variational problem. The above statement is in fact equivalent to

```
u_1 = u[0]
u_2 = u[1]
u_3 = u[2]
```

Note that `u[0]` is not really a `Function` object, but merely a symbolic expression, just like `grad(u)` in FEniCS is a symbolic expression and not a `Function` representing the gradient. This means that `u_1`, `u_2`, `u_3` can be used in a variational problem, but cannot be used for plotting or postprocessing.

To access the components of `u` for plotting and saving the solution to file, we need to use a different variant of the `split` function:

```
_u_1, _u_2, _u_3 = u.split()
```

This returns three subfunctions as actual objects with access to the common underlying data stored in `u`, which makes plotting and saving to file possible. Alternatively, we can do

```
_u_1, _u_2, _u_3 = u.split(deepcopy=True)
```

which will create `_u_1`, `_u_2`, and `u_3` as stand-alone `Function` objects, each holding a copy of the subfunction data extracted from `u`. This is useful in many situations but is not necessary for plotting and saving solutions to file.

Chapter 4
Subdomains and boundary conditions

So far, we have only looked briefly at how to specify boundary conditions. In this chapter, we look more closely at how to specify boundary conditions on specific parts (subdomains) of the boundary and how to combine multiple boundary conditions. We will also look at how to generate meshes with subdomains and how to define coefficients and variational problems that look different in different subdomains.

4.1 Combining Dirichlet and Neumann conditions

Let's return to our Poisson solver from Chapter 2 and see how to extend the mathematics and the implementation to handle a Dirichlet condition in combination with a Neumann condition. The domain is still the unit square, but now we set the Dirichlet condition $u = u_{\text{D}}$ 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 $y = 1$.

4.1.1 PDE problem

Let Γ_{D} and Γ_{N} denote the parts of the boundary $\partial\Omega$ where the Dirichlet and Neumann conditions apply, respectively. The complete boundary-value problem can be written as

$$-\nabla^2 u = f \quad \text{in } \Omega, \tag{4.1}$$

$$u = u_{\mathrm{D}} \text{ on } \Gamma_{\mathrm{D}}, \tag{4.2}$$

$$-\frac{\partial u}{\partial n} = g \quad \text{on } \Gamma_{\mathrm{N}}. \tag{4.3}$$

Again we choose $u = 1 + x^2 + 2y^2$ as the exact solution and adjust f, g, and u_{D} accordingly:

$$\begin{aligned} f &= -6, \\ g &= \begin{cases} 0, & y = 0 \\ 4, & y = 1 \end{cases} \\ u_{\mathrm{D}} &= 1 + x^2 + 2y^2. \end{aligned}$$

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

$$g(x, y) = 4y.$$

4.1.2 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

$$-\int_\Omega (\nabla^2 u) v \,\mathrm{d}x = \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x - \int_{\partial\Omega} \frac{\partial u}{\partial n} v \,\mathrm{d}s,$$

and since $v = 0$ on Γ_{D},

$$-\int_{\partial\Omega} \frac{\partial u}{\partial n} v \,\mathrm{d}s = -\int_{\Gamma_{\mathrm{N}}} \frac{\partial u}{\partial n} v \,\mathrm{d}s = \int_{\Gamma_{\mathrm{N}}} g v \,\mathrm{d}s,$$

by applying the boundary condition on Γ_{N}. The resulting weak form reads

$$\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g v \,\mathrm{d}s. \tag{4.4}$$

Expressing this equation in the standard notation $a(u, v) = L(v)$ is straightforward with

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x, \tag{4.5}$$

$$L(v) = \int_\Omega f v \,\mathrm{d}x - \int_{\Gamma_\mathrm{N}} g v \,\mathrm{d}s\,. \tag{4.6}$$

4.1.3 FEniCS implementation

How does the Neumann condition impact the implementation? Let us revisit our previous implementation `ft01_poisson.py` from Section 2.2 and examine which changes we need to make to incorporate the Neumann condition. It turns out that only two are necessary.

- The function `boundary` defining the Dirichlet boundary must be modified.
- The new boundary term must be added to the expression for `L`.

The first adjustment can be coded as

```
tol = 1E-14

def boundary_D(x, on_boundary):
    if on_boundary:
        if near(x[0], 0, tol) or near(x[0], 1, tol):
            return True
        else:
            return False
    else:
        return False
```

A more compact implementation reads

```
def boundary_D(x, on_boundary):
    return on_boundary and (near(x[0], 0, tol) or near(x[0], 1, tol))
```

The second adjustment of our program concerns the definition of `L`, which needs to include the Neumann condition:

```
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 other modifications are necessary.

Note that the integration `*ds` is carried out over the entire boundary, including the Dirichlet boundary. However, since the test function `v` vanishes on the Dirichlet boundary (as a result specifying a `DirichletBC`), the integral will only include the contribution from the Neumann boundary.

4.2 Setting multiple Dirichlet conditions

In the previous section, we used a single function $u_{\mathrm{D}}(x,y)$ for setting Dirichlet conditions at two parts of the boundary. Often it is more practical to use multiple functions, one for each subdomain of the boundary. Let us return to the case from Section 4.1 and redefine the problem in terms of two Dirichlet conditions:

$$\begin{aligned} -\nabla^2 u &= f \quad \text{in } \Omega, \\ u &= u_{\mathrm{L}} \quad \text{on } \Gamma_{\mathrm{D}}^{\mathrm{L}}, \\ u &= u_{\mathrm{R}} \quad \text{on } \Gamma_{\mathrm{D}}^{\mathrm{R}}, \\ -\frac{\partial u}{\partial n} &= g \quad \text{on } \Gamma_{\mathrm{N}}. \end{aligned}$$

Here, $\Gamma_{\mathrm{D}}^{\mathrm{L}}$ is the left boundary $x=0$, while $\Gamma_{\mathrm{D}}^{\mathrm{R}}$ is the right boundary $x=1$. We note that $u_{\mathrm{L}} = 1+2y^2$, $u_{\mathrm{R}} = 2+2y^2$, and $g = 4y$.

For the boundary condition on $\Gamma_{\mathrm{D}}^{\mathrm{L}}$, we define the usual triple of an expression for the boundary value, a function defining the location of the boundary, and a `DirichletBC` object:

```
u_L = Expression('1 + 2*x[1]*x[1]')

def boundary_L(x, on_boundary):
    tol = 1E-14
    return on_boundary and near(x[0], 0, tol)

bc_L = DirichletBC(V, u_L, boundary_L)
```

For the boundary condition on $\Gamma_{\mathrm{D}}^{\mathrm{R}}$, we write a similar code snippet:

```
u_R = Expression('2 + 2*x[1]*x[1]')

def boundary_R(x, on_boundary):
    tol = 1E-14
    return on_boundary and near(x[0], 1, tol)

bc_R = DirichletBC(V, u_R, boundary_R)
```

We collect the two boundary conditions in a list which we can pass to the `solve` function to compute the solution:

```
bcs = [bc_L, bc_R]
...
solve(a == L, u, bcs)
```

Note that for boundary values that do not depend on x or y, we might replace the `Expression` objects by `Constant` objects.

4.3 Defining subdomains for different materials

Solving PDEs in domains made up of different materials is a frequently encountered task. In FEniCS, these kinds of problems are handled by defining subdomains inside the domain. A simple example with two materials (subdomains) in 2D will demonstrate the idea.

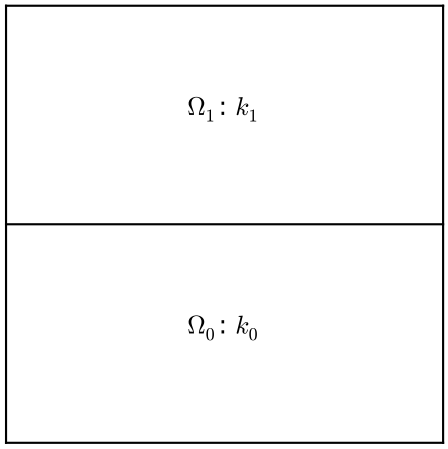


Fig. 4.1 Medium with discontinuous material properties.

Suppose we want to solve

$$\nabla \cdot [\kappa(x,y)\nabla u(x,y)] = 0, \tag{4.7}$$

in a domain Ω consisting of two subdomains where κ takes on a different value in each subdomain. We take $\Omega = [0,1] \times [0,1]$ and divide it into two equal subdomains, as depicted in Figure 4.1,

$$\Omega_0 = [0,1] \times [0,1/2], \quad \Omega_1 = [0,1] \times (1/2,1]\,.$$

We define $\kappa(x,y) = \kappa_0$ in Ω_0 and $\kappa(x,y) = \kappa_1$ in Ω_1, where $\kappa_0 > 0$ and $\kappa_1 > 0$ are given constants.

Physically, this problem may be viewed as a model of heat conduction, where the heat conduction in Ω_1 is more efficient than in Ω_0. An alternative interpretation is flow in porous media with two geological layers, where the layers' ability to transport the fluid differ.

4.3.1 Using expressions to define subdomains

The simplest way of implementing a variable coefficient κ is to define an `Expression` object where we return the appropriate κ 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, k_0, k_1):
        self.k_0, self.k_1 = k_0, k_1

    def eval(self, value, x):
        "Set value[0] to value at point x"
        tol = 1E-14
        if x[1] <= 0.5 + tol:
            value[0] = self.k_0
        else:
            value[0] = self.k_1

# Initialize k
k = K()
k.set_k_values(1, 0.01)
```

The `eval` method gives great flexibility in defining functions, but a downside is that FEniCS will call `eval` in Python for each node `x`, which is a slow process.

An alternative method is to use a C++ string expression as we have seen before, which is much more efficient in FEniCS. This can be done using inline if tests in C++:

```
tol = 1E-14
k_0 = 1.0
k_1 = 0.01
k = Expression('x[1] <= 0.5 + tol ? k_0 : k_1',
               tol=tol, k_0=k_0, k_1=k_1)
```

This method of defining variable coefficients works if the subdomains are simple shapes that can be expressed in terms of geometric inequalities. However, for more complex subdomains, we will need to use a more general technique, as we will see next.

4.3.2 Using mesh functions to define subdomains

We now address how to specify the subdomains Ω_0 and Ω_1 using a more general technique. This technique involves the use of two classes that are essential

in FEniCS when working with subdomains: `SubDomain` and `MeshFunction`. Consider the following definition of the boundary $x = 0$:

```
def boundary(x, on_boundary):
    tol = 1E-14
    return on_boundary and near(x[0], 0, tol)
```

This boundary definition is actually a shortcut to the more general FEniCS concept `SubDomain`. A `SubDomain` is a class which defines a region in space (a subdomain) in terms of a member function `inside` which returns `True` for points that belong to the subdomain and `False` for points that don't belong to the subdomain. Here is how to specify the boundary $x = 0$ as a `SubDomain`:

```
class Boundary(SubDomain):
    def inside(self, x, on_boundary):
        tol = 1E-14
        return on_boundary and near(x[0], 0, tol)

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

We notice that the `inside` function of the class `Boundary` is (almost) identical to the previous boundary definition in terms of the `boundary` function. Technically, our class `Boundary` is a *subclass* of the FEniCS class `SubDomain`.

We will use two `SubDomain` subclasses to define the two subdomains Ω_0 and Ω_1:

```
tol = 1E-14

class Omega_0(SubDomain):
    def inside(self, x, on_boundary):
        return x[1] <= 0.5 + tol

class Omega_1(SubDomain):
    def inside(self, x, on_boundary):
        return x[1] >= 0.5 - tol
```

Notice the use of `<=` and `>=` in both tests. FEniCS will call the `inside` function for each vertex in a cell to determine whether or not the cell belongs to a particular subdomain. For this reason, it is important that the test holds for all vertices in cells aligned with the boundary. In addition, we use a tolerance to make sure that vertices on the internal boundary at $y = 0.5$ will belong to *both* subdomains. This is a little counter-intuitive, but is necessary to make the cells both above and below the internal boundary belong to either Ω_0 or Ω_1.

To define the variable coefficient κ, we will use a powerful tool in FEniCS called a `MeshFunction`. A `MeshFunction` is a discrete function that can be evaluated at a set of so-called *mesh entities*. A mesh entity in FEniCS is either a vertex, an edge, a face, or a cell (triangle or tetrahedron). A `MeshFunction` over cells is suitable to represent subdomains (materials), while a `MeshFunction` over facets (edges or faces) is used to represent pieces

of external or internal boundaries. A `MeshFunction` over cells can also be used to represent boundary markers for mesh refinement. A FEniCS `MeshFunction` is parameterized both over its data type (like integers or booleans) and its dimension (0 = vertex, 1 = edge etc.). Special subclasses `VertexFunction`, `EdgeFunction` etc. are provided for easy definition of a `MeshFunction` of a particular dimension.

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, `'size_t'` for non-negative (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 (`'size_t'`) for numbering the subdomains:

```
materials = CellFunction('size_t', mesh)
```

Next, we use the two subdomains to *mark* the cells belonging to each subdomain:

```
# Mark subdomains with numbers 0 and 1
subdomain0 = Omega_0()
subdomain1 = Omega_1()
subdomain0.mark(materials, 0)
subdomain1.mark(materials, 1)
```

This will set the values of the mesh function `materials` to 0 on each cell belonging to Ω_0 and 1 on all cells belonging to Ω_1. Alternatively, we can use the following equivalent code to mark the cells:

```
materials.set_all(0)
subdomain1.mark(materials, 1)
```

To examine the values of the mesh function and see that we have indeed defined our subdomains correctly, we can simply plot the mesh function:

```
plot(materials, interactive=True)
```

We may also wish to store the values of the mesh function for later use:

```
File('materials.xml.gz') << materials
```

which can later be read back from file as follows:

```
File('materials.xml.gz') >> materials
```

Now, to use the values of the mesh function `materials` to define the variable coefficient κ, we create a FEniCS `Expression`:

```
class K(Expression):
    def __init__(self, materials, k_0, k_1, **kwargs):
        self.materials = materials
        self.k_0 = k_0
```

```
        self.k_1 = k_1

def eval_cell(self, values, x, cell):
        if self.materials[cell.index] == 0:
            values[0] = self.k_0
        else:
            values[0] = self.k_1

k = K(materials, k_0, k_1, degree=0)
```

This is similar to the `Expression` subclass we defined above, but we make use of the member function `eval_cell` in place of the regular `eval` function. This version of the evaluation function has an addition `cell` argument which we can use to check on which cell we are currently evaluating the function.

Since we make use of geometric tests to define the two `SubDomains` for Ω_0 and Ω_1, the `MeshFunction` method may seem like an unnecessary complication of the simple method using an `Expression` with an if-test. However, in general the definition of subdomains may be available as a `MeshFunction` (from a data file), perhaps generated as part of the mesh generation process, and not as a simple geometric test. In such cases the method demonstrated here is the recommended way to define subdomains.

4.3.3 Vectorized version of subdomain definitions

To speed up this code, we can vectorize the expressions:

```
materials = CellFunction('size_t', mesh)
materials.set_all(0)  # "the rest"
for m, subdomain in enumerate(subdomains[1:], 1):
    subdomain.mark(materials, m)

kappa_values = kappa
V0 = FunctionSpace(mesh, 'DG', 0)
kappa = Function(V0)
help = np.asarray(materials.array(), dtype=np.int32)
kappa.vector()[:] = np.choose(help, kappa_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.

4.3.4 Using C++ code snippets to define subdomains

The `SubDomain` and `Expression` Python classes are very convenient, but their use leads to function calls from C++ to Python for each node in the

mesh. Since this involves a significant cost, we need to make use of C++ code for large-scale computational problems.

Instead of writing the `SubDomain` subclass in Python, we may instead use the `CompiledSubDomain` tool in FEniCS to specify the subdomain in C++ code and thereby speed up our code. Consider the definition of the classes `Omega_0` and `Omega_1` above in Python. The key strings that define these subdomains can be expressed in C++ syntax and fed to `CompiledSubDomain` as follows:

```
tol = 1E-14
subdomain0 = CompiledSubDomain('x[1] <= 0.5 + tol', tol=tol)
subdomain1 = CompiledSubDomain('x[1] >= 0.5 - tol', tol=tol)
```

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:

```
boundary_R = CompiledSubDomain('on_boundary && near(x[0], 1, tol)',
                               tol=1E-14)
```

It is also 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[0], 1, tol)')
```

Python `Expression` classes may also be redefined using C++ for more efficient code. Consider again the definition of the class `K` above for the variable coefficient $\kappa = \kappa(x)$. This may be redefined using a C++ code snippet and the keyword `cppcode` to the regular FEniCS `Expression` class:

```
cppcode = """
class K : public Expression
{
public:

  void eval(Array<double>& values,
            const Array<double>& x,
            const ufc::cell& cell) const
  {
    if ((*materials)[cell.index] == 0)
      values[0] = k_0;
    else
      values[0] = k_1;
  }

  std::shared_ptr<MeshFunction<std::size_t>> materials;
  double k_0;
  double k_1;
```

```
};
"""

k = Expression(cppcode=cppcode, degree=0)
k.materials = materials
k.k_0 = k_0
k.k_1 = k_1
```

Exercise 4.1: Efficiency of Python vs C++ expressions

Consider a cube mesh with N cells in each spatial direction. We want to define a `Function` on this mesh where the values are given by the mathematical function $f(x,y,z) = a\sin(bxyz)$, where a and b are two parameters. Write a `class SineXYZ`:

```
class SineXYZ(Expression):
    def __init__(self, a, b):
        self.a, self.b = a, b

    def eval(self, value, x):
        value[0] = self.a*sin(self.b*x[0]*x[1]*x[2])
```

Create an alternative `Expression` based on giving the formula for $f(x,y,z)$ as a C++ code string. Compare the computational efficiency of the two implementations (e.g., using `time.clock()` to measure the CPU time).

The `sin` function used in class `SineXYZ.eval` can mean many things. This is an advanced FEniCS function if imported from `fenics`. Much more efficient versions for sin of numbers are found in `math.sin` and `numpy.sin`. Compare the use `sin` from `fenics`, `math`, `numpy`, and `sympy` (note that `sin` from `sympy` is very slow).

Solution. Here is an appropriate program:

```
from __future__ import print_function
from fenics import *
import time

def make_sine_Function(N, method):
    """Fill a Function with sin(x*y*z) values."""
    mesh = UnitCubeMesh(N, N, N)
    V = FunctionSpace(mesh, 'Lagrange', 2)

    if method.startswith('Python'):
        if method.endswith('fenics.sin'):
            # Need sin as local variable in this function
            from fenics import sin
        elif method.endswith('math.sin'):
            from math import sin
        elif method.endswith('numpy.sin'):
```

```
            from numpy import sin
        elif method.endswith('sympy.sin'):
            from sympy import sin
        else:
            raise NotImplementedError('method=%s' % method)
        print('sin:', sin, type(sin))

        class SineXYZ(Expression):
            def __init__(self, a, b):
                self.a, self.b = a, b

            def eval(self, value, x):
                value[0] = self.a*sin(self.b*x[0]*x[1]*x[2])

        expr = SineXYZ(a=1, b=2)

    elif method == 'C++':
        expr = Expression('a*sin(b*x[0]*x[1]*x[2])', a=1, b=2)

    t0 = time.clock()
    u = interpolate(expr, V)
    t1 = time.clock()
    return u, t1-t0

def main(N):
    u, cpu_py_fenics  = make_sine_Function(N, 'Python-fenics.sin')
    u, cpu_py_math    = make_sine_Function(N, 'Python-math.sin')
    u, cpu_py_numpy   = make_sine_Function(N, 'Python-numpy.sin')
    u, cpu_py_sympy   = make_sine_Function(N, 'Python-sympy.sin')
    u, cpu_cpp = make_sine_Function(N, 'C++')
    print("""DOFs: %d
Python:
fenics.sin: %.2f
math.sin:   %.2f
numpy.sin:  %.2f
sympy.sin:  %.2f
C++:        %.2f
Speed-up:   math: %.2f  sympy: %.2f""" %
          (u.function_space().dim(),
           cpu_py_fenics, cpu_py_math,
           cpu_py_numpy, cpu_py_sympy,
           cpu_cpp,
           cpu_py_math/float(cpu_cpp),
           cpu_py_sympy/float(cpu_cpp)))

def profile():
    import cProfile
    prof = cProfile.Profile()
    prof.runcall(main)
    prof.dump_stats("tmp.profile")
    # http://docs.python.org/2/library/profile.html

main(20)
#profile()
```

Running the program shows that `sin` from `math` is the most efficient choice, but a string C++ runs 40 times faster. Note that `fenics.sin`, which is a sine function in the UFL language that can work with symbolic expressions in finite element forms, is (naturally) less efficient than the `sin` functions for numbers in `math` and `numpy`.
Filename: `Expression_efficiency`.

4.4 Setting multiple Dirichlet, Neumann, and Robin conditions

Consider again the model problem from Section 4.2 where we had both Dirichlet and Neumann conditions. The term `g*v*ds` in the expression for `L` implies a boundary integral over the complete boundary, or in FEniCS terms, an integral over all *exterior facets*. This means that the boundary integral extends also over the part of the boundary Γ_{D} where we have Dirichlet conditions. However, only the integral over Γ_{N} will contribute since $v = 0$ on Γ_{D} (which happens when we apply the Dirichlet boundary condition).

From an efficiency point of view, we would ideally like to compute the integral `g*v*ds` only over the part of the boundary where we actually have Neumann conditions. More importantly, in other problems one may have different Neumann conditions or other conditions like the Robin type condition. This can be handled in FEniCS by defining a `MeshFunction` that marks different portions of the boundary. The same technique can also be used to treat multiple Dirichlet conditions.

4.4.1 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 Γ_{D}^0, Γ_{D}^1, ..., of the boundary:

$$u_{\mathrm{D}}^0 \text{ on } \Gamma_{\mathrm{D}}^0, \quad u_{\mathrm{D}}^1 \text{ on } \Gamma_{\mathrm{D}}^1, \quad \ldots$$

where u_{D}^i are prescribed functions, $i = 0, 1, \ldots$ On other parts, Γ_{N}^0, Γ_{N}^1, and so on, we have Neumann conditions:

$$-\kappa \frac{\partial u}{\partial n} = g_0 \text{ on } \Gamma_{\mathrm{N}}^0, \quad -\kappa \frac{\partial u}{\partial n} = g_1 \text{ on } \Gamma_{\mathrm{N}}^1, \quad \ldots$$

Finally, we have *Robin conditions*:

$$-\kappa\frac{\partial u}{\partial n} = r(u-s),$$

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 Γ_{R}^0, Γ_{R}^1, and so forth:

$$-\kappa\frac{\partial u}{\partial n} = r_0(u-s_0) \text{ on } \Gamma_{\mathrm{R}}^0, \quad -\kappa\frac{\partial u}{\partial n} = r_1(u-s_1) \text{ on } \Gamma_{\mathrm{R}}^1, \quad \ldots$$

4.4.2 PDE problem

With the notation above, the model problem to be solved with multiple Dirichlet, Neumann, and Robin conditions can be formulated as follows:

$$-\nabla\cdot(\kappa\nabla u) = -f, \text{ in } \Omega, \tag{4.8}$$

$$u = u_{\mathrm{D}}^i \text{ on } \Gamma_{\mathrm{D}}^i, \quad i = 0,1,\ldots \tag{4.9}$$

$$-\kappa\frac{\partial u}{\partial n} = g_i \text{ on } \Gamma_{\mathrm{N}}^i, \quad i = 0,1,\ldots \tag{4.10}$$

$$-\kappa\frac{\partial u}{\partial n} = r_i(u-s_i) \text{ on } \Gamma_{\mathrm{R}}^i, \quad i = 0,1,\ldots \tag{4.11}$$

4.4.3 Variational formulation

As usual, we multiply by a test function v and integrate by parts:

$$-\int_\Omega \nabla\cdot(\kappa\nabla u)v\,\mathrm{d}x = \int_\Omega \kappa\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega}\kappa\frac{\partial u}{\partial n}v\,\mathrm{d}s\,.$$

On the Dirichlet part of the boundary (Γ_{D}^i), the boundary integral vanishes since $v = 0$. On the remaining part of the boundary, we split the boundary integral into contributions from the Neumann part (Γ_{N}^i) and Robin part (Γ_{R}^i). Inserting the boundary conditions, we obtain

$$\begin{aligned}-\int_{\partial\Omega}\kappa\frac{\partial u}{\partial n}v\,\mathrm{d}s &= -\sum_i\int_{\Gamma_{\mathrm{N}}^i}\kappa\frac{\partial u}{\partial n}\,\mathrm{d}s - \sum_i\int_{\Gamma_{\mathrm{R}}^i}\kappa\frac{\partial u}{\partial n}\,\mathrm{d}s\\ &= \sum_i\int_{\Gamma_{\mathrm{N}}^i} g_i\,\mathrm{d}s + \sum_i\int_{\Gamma_{\mathrm{R}}^i} r_i(u-s_i)\,\mathrm{d}s\,.\end{aligned}$$

We thus obtain the following variational problem:

$$F = \int_\Omega \kappa \nabla u \cdot \nabla v \,\mathrm{d}x + \sum_i \int_{\Gamma_{\mathrm{N}}^i} g_i v \,\mathrm{d}s + \sum_i \int_{\Gamma_{\mathrm{R}}^i} r_i (u - s_i) v \,\mathrm{d}s - \int_\Omega f v \,\mathrm{d}x = 0\,. \tag{4.12}$$

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 integrals from the Robin condition must for this reason be split in two parts:

$$\int_{\Gamma_{\mathrm{R}}^i} r_i (u - s_i) v \,\mathrm{d}s = \int_{\Gamma_{\mathrm{R}}^i} r_i u v \,\mathrm{d}s - \int_{\Gamma_{\mathrm{R}}^i} r_i s_i v \,\mathrm{d}s\,.$$

We then have

$$a(u,v) = \int_\Omega \kappa \nabla u \cdot \nabla v \,\mathrm{d}x + \sum_i \int_{\Gamma_{\mathrm{R}}^i} r_i u v \,\mathrm{d}s, \tag{4.13}$$

$$L(v) = \int_\Omega f v \,\mathrm{d}x - \sum_i \int_{\Gamma_{\mathrm{N}}^i} g_i v \,\mathrm{d}s + \sum_i \int_{\Gamma_{\mathrm{R}}^i} r_i s_i v \,\mathrm{d}s\,. \tag{4.14}$$

Alternatively, we may keep the formulation (4.12) and either solve the variational problem as a nonlinear problem (`F == 0`) in FEniCS or use the FEniCS functions `lhs` and `rhs` to extract the bilinear and linear parts of `F`:

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

Note that if we choose the solve this linear problem as a nonlinear problem, the Newton iteration will converge in a single iteration.

4.4.4 FEniCS implementation

Let us examine how to extend our Poisson solver to handle general combinations of Dirichlet, Neumann, and Robin boundary conditions. Compared to our previous code, we must consider the following extensions:

- Defining markers for the different parts of the boundary.
- Splitting the boundary integral into parts using the markers.

A general approach to the first task is to mark each of the desired boundary parts 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

markers will be defined using a `MeshFunction`, but contrary to Section 4.3, this is not a function over cells, but a function over the facets of the mesh. We use a `FacetFunction` for this purpose:

```
boundary_markers = FacetFunction('size_t', mesh)
```

As in Section 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):
    tol = 1E-14
    def inside(self, x, on_boundary):
        return on_boundary and near(x[0], 0, tol)

bx0 = BoundaryX0()
bx0.mark(boundary_markers, 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': u_D},
                       1: {'Robin':     (r, s)},
                       2: {'Neumann':   g},
                       3: {'Neumann',   0}}
```

specifies

- a Dirichlet condition $u = u_{\mathrm{D}}$ for $x = 0$;
- a Robin condition $-\kappa\partial_n u = r(u - s)$ for $x = 1$;
- a Neumann condition $-\kappa\partial_n u = g$ for $y = 0$;
- a Neumann condition $-\kappa\partial_n u = 0$ for $y = 1$.

As explained in Section 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 code snippet:

```
bcs = []
for i in boundary_conditions:
    if 'Dirichlet' in boundary_conditions[i]:
        bc = DirichletBC(V, boundary_conditions[i]['Dirichlet'],
                         boundary_markers, i))
        bcs.append(bc)
```

A new aspect of the variational problem is the two distinct boundary integrals over Γ_{N}^i and Γ_{R}^i. Having a mesh function over exterior cell facets (our `boundary_markers` object), where subdomains (boundary parts) are numbered as $0, 1, 2, \ldots$, 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.

To express integrals over the boundary parts using `ds(i)`, we must first redefine the measure `ds` in terms of our boundary markers:

```
ds = Measure('ds', domain=mesh, subdomain_data=boundary_markers)
```

Similarly, if we want integration over different parts of the domain, we redefine `dx` as

```
dx = Measure('dx', domain=mesh, subdomain_data=domain_markers)
```

where `domain_markers` 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 then be written

```
a = kappa*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 following code snippet:

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

Applying `sum(integrals_N)` will apply the `+` operator to the variational forms in the `integrals_N` 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:

```
integrals_R_a = []
integrals_R_L = []
for i in boundary_conditions:
    if 'Robin' in boundary_conditions[i]:
        r, s = boundary_conditions[i]['Robin']
        integrals_R_a.append(r*u*v*ds(i))
        integrals_R_L.append(r*s*v*ds(i))
```

We are now in a position to define the `a` and `L` expressions in the variational formulation:

```
a = kappa*dot(grad(u), grad(v))*dx + sum(integrals_R_a)
L = f*v*dx - sum(integrals_N) + sum(integrals_R_L)
```

Alternatively, we may use the FEniCS functions `lhs` and `rhs` as mentioned above to simplify the extraction of terms for the Robin integrals:

```
integrals_R = []
for i in boundary_conditions:
    if 'Robin' in boundary_conditions[i]:
        r, s = boundary_conditions[i]['Robin']
        integrals_R.append(r*(u - s)*v*ds(i))

F = kappa*dot(grad(u), grad(v))*dx + \
    sum(integrals_R) - f*v*dx + sum(integrals_N)
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(i)`:

The complete code for this example can be found in the function `solver_bc` in the program `ft11_poisson_bcs.py`.

4.4.5 Test problem

We will use the same exact solution $u_e = 1 + x^2 + 2y^2$ as in Chapter 2, and thus take $\kappa = 1$ and $f = -6$. 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 $-\partial u/\partial n = -\partial u/\partial y = 4y = 4$, 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 specify $r \neq 0$ arbitrarily in the Robin condition. We will set $r = 1000$ and $s = u$.

The boundary parts are thus Γ_{D}^0: $x = 0$, Γ_{D}^1: $x = 1$, Γ_{R}^0: $y = 0$, and Γ_{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 the exact solution 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.

```
# Define manufactured solution in sympy and derive f, g, etc.
import sympy as sym
x, y = sym.symbols('x[0], x[1]')            # needed by UFL
u = 1 + x**2 + 2*y**2                       # exact solution
u_e = u                                     # exact solution
u_00 = u.subs(x, 0)                         # restrict to x = 0
```

```
u_01 = u.subs(x, 1)                          # restrict to x = 1
f = -sym.diff(u, x, 2) - sym.diff(u, y, 2)   # -Laplace(u)
f = sym.simplify(f)                          # simplify f
g = -sym.diff(u, y).subs(y, 1)               # compute g = -du/dn
r = 1000                                     # Robin data, arbitrary
s = u                                        # Robin data, u = s
# Collect variables
variables = [u_e, u_00, u_01, f, g, r, s]
# Turn into C/C++ code strings
variables = [sym.printing.ccode(var) for var in variables]
# Turn into FEniCS Expression
variables = [Expression(var, degree=2) for var in variables]
# Extract variables
u_e, u_00, u_01, f, g, r, s = variables
# Define boundary conditions
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
```

This simple test problem is turned into a real unit test for different function spaces in the function `test_solver_bc`.

4.4.6 Debugging 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 (P_1) elements, add the corresponding vertex coordinate to the output.

```
if debug:
    # Print all vertices that belong to the boundary parts
    for x in mesh.coordinates():
        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('Number of Dirichlet conditions:', len(bcs))
    if V.ufl_element().degree() == 1:  # P1 elements
        d2v = dof_to_vertex_map(V)
        coor = mesh.coordinates()
    for i, bc in enumerate(bcs):
        print('Dirichlet condition %d' % i)
        boundary_values = bc.get_boundary_values()
        for dof in boundary_values:
            print('   dof %2d: u=%g' % (dof, boundary_values[dof]))
```

```
            if V.ufl_element().degree() == 1:
                print('    at point %s' %
                      (str(tuple(coor[d2v[dof]].tolist()))))
```

Calls to the `inside` method

In the code snippet above, we call the inside method for each `mesh.coordinate()`; i.e., for each vertex. We could also place a printout inside the `inside` method. Then it will be surprising to see that this method is called not only for the points assoicated with degrees of freedom. For P1 elements the method is also called for each midpoint on each facet of the cells. This is because a Dirichlet condition is by default set only if the entire facet can be said to be subject to such a condition.

4.5 Generating meshes with subdomains

So far, we have worked mostly with simple meshes (the unit square) and defined boundaries and subdomains in terms of simple geometric tests like $x = 0$ or $y \leq 0.5$. For more complex geometries, it is not realistic to specify boundaries and subdomains in this way. Instead, the boundaries and subdomains must be defined as part of the mesh generation process. We will now look at how to use the FEniCS mesh generation tool `mshr` to generate meshes and define subdomains.

4.5.1 PDE problem

We will again solve the Poisson equation, but this time for a different application. Consider an iron cylinder with copper wires wound around the cylinder as in Figure 4.2. Through the copper wires a static current $J = 1\,\mathrm{A}$ is flowing and we want to compute the magnetic field B in the iron cylinder, the copper wires, and the surrounding vacuum.

First, we simplify the problem to a 2D problem. We can do this by assuming that the cylinder extends far along the z-axis and as a consequence the field is virtually independent of the z-coordinate. Next, we consider Maxwell's equation to derive a Poisson equation for the magnetic field (or rather its potential):

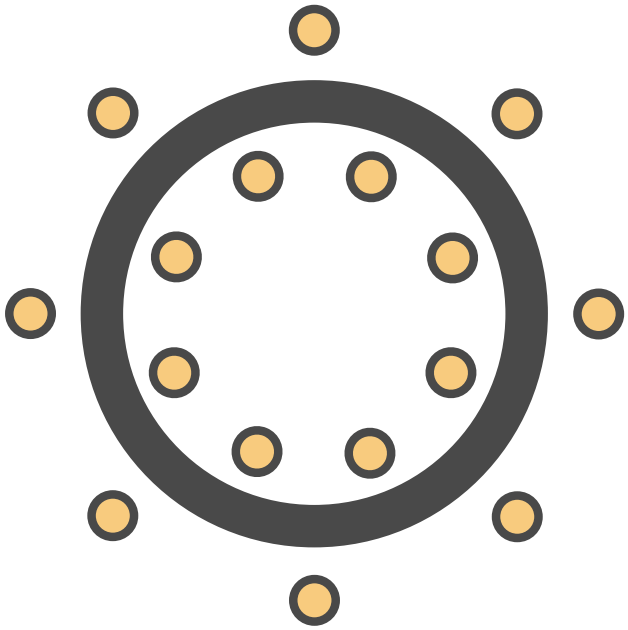


Fig. 4.2 Cross-section of an iron cylinder with copper wires wound around the cylinder, here with $n = 8$ windings. The inner circles are cross-sections of the copper wire coming up ("north") and the outer circles are cross-sections of the copper wire going down into the plane ("south").

$$\nabla \cdot D = \varrho, \tag{4.15}$$

$$\nabla \cdot B = 0, \tag{4.16}$$

$$\nabla \times E = -\frac{\partial B}{\partial t}, \tag{4.17}$$

$$\nabla \times H = \frac{\partial D}{\partial t} + J. \tag{4.18}$$

Here, D is the displacement field, B is the magnetic field, E is the electric field, and H is the magnetizing field. In addition to Maxwell's equations, we also need a constitutive relation between B and H,

$$B = \mu H, \tag{4.19}$$

which holds for an isotropic linear magnetic medium. Here, μ is the magnetic permeability of the material. Now, since B is solenoidal (divergence free) according to Maxwell's equations, we know that B must be the curl of some vector field A. This field is called the magnetic vector potential. Since $\partial D/\partial t = 0$, it follows that

$$J = \nabla \times H = \nabla \times (\mu^{-1} B) = \nabla \times (\mu^{-1} \nabla \times A) = -\nabla \cdot (\mu^{-1} \nabla A). \tag{4.20}$$

In the last step, we have expanded the second derivatives and used the gauge freedom of A to simplify the equations to a simple vector-valued Poisson problem for the magnetic vector potential; if $B = \nabla \times A$, then $B = \nabla \times (A + \nabla\psi)$ for any scalar field ψ (the gauge function). For the current problem, we thus need to solve the following 2D Poisson problem for the z-component A_z of the magnetic vector potential:

$$-\nabla \cdot (\mu^{-1} \nabla A_z) = J_z \quad \text{in } \mathbb{R}^2, \tag{4.21}$$

$$\lim_{|(x,y)| \to \infty} A_z = 0. \tag{4.22}$$

Since we cannot solve this problem on an infinite domain, we will truncate the domain using a large disk and set $A_z = 0$ on the boundary. The current J_z is set to $+1\,\mathrm{A}$ in the interior set of circles (copper wire cross-sections) and to $-1\,\mathrm{A}$ in the exterior set of circles in Figure 4.2.

Once the magnetic vector potential has been computed, we can compute the magnetic field $B = B(x, y)$ by

$$B(x, y) = \left(\frac{\partial A_z}{\partial y}, -\frac{\partial A_z}{\partial x} \right). \tag{4.23}$$

4.5.2 Variational formulation

The variational problem is derived as before by multiplying the PDE with a test function v and integrating by parts. Since the boundary integral vanishes due to the Dirichlet condition, we obtain

$$\int_\Omega \mu^{-1} \nabla A_z \cdot \nabla v \,\mathrm{d}x = \int_\Omega J_z v \,\mathrm{d}x, \tag{4.24}$$

or, in other words, $a(A_z, v) = L(v)$ with

$$a(A_z, v) = \int_\Omega \mu^{-1} \nabla A_z \cdot \nabla v \,\mathrm{d}x, \tag{4.25}$$

$$L(v) = \int_\Omega J_z v \,\mathrm{d}x. \tag{4.26}$$

4.5.3 FEniCS implementation

The first step is to generate a mesh for the geometry described in Figure 4.2. We let a and b be the inner and outer radii of the iron cylinder and let c_1 and c_2 be the radii of the two concentric distributions of copper wire cross-sections. Furthermore, we let r be the radius of a copper wire, R be the radius of our domain, and n be the number of windings (giving a total of $2n$ copper-wire cross-sections). This geometry can be described easily using `mshr` and a little bit of Python programming:

```
# Define geometry for background
domain = Circle(Point(0, 0), R)

# Define geometry for iron cylinder
cylinder = Circle(Point(0, 0), b) - Circle(Point(0, 0), a)

# Define geometry for wires (N = North (up), S = South (down))
angles_N = [i*2*pi/n for i in range(n)]
angles_S = [(i + 0.5)*2*pi/n for i in range(n)]
wires_N = [Circle(Point(c_1*cos(v), c_1*sin(v)), r) for v in angles_N]
wires_S = [Circle(Point(c_2*cos(v), c_2*sin(v)), r) for v in angles_S]
```

The mesh that we generate will be a mesh of the entire disk with radius R but we need the mesh generation to respect the internal boundaries defined by the iron cylinder and the copper wires. We also want `mshr` to label the subdomains so that we can easily specify material parameters (μ) and currents. To do this, we use the `mshr` function `set_subdomain` as follows:

```
# Set subdomain for iron cylinder
domain.set_subdomain(1, cylinder)

# Set subdomains for wires
for (i, wire) in enumerate(wires_N):
    domain.set_subdomain(2 + i, wire)
for (i, wire) in enumerate(wires_S):
    domain.set_subdomain(2 + n + i, wire)
```

Once the subdomains have been created, we can generate the mesh:

```
mesh = generate_mesh(domain, 32)
```

A detail of the mesh is shown in Figure 4.3.

The mesh generated with `mshr` will contain information about the subdomains we have defined. To use this information in the definition of our variational problem and subdomain-dependent parameters, we will need to create a `MeshFunction` that marks the subdomains. This can be easily created by a call to the member function `mesh.domains()`, which holds the subdomain data generated by `mshr`:

```
markers = MeshFunction('size_t', mesh, 2, mesh.domains())
```

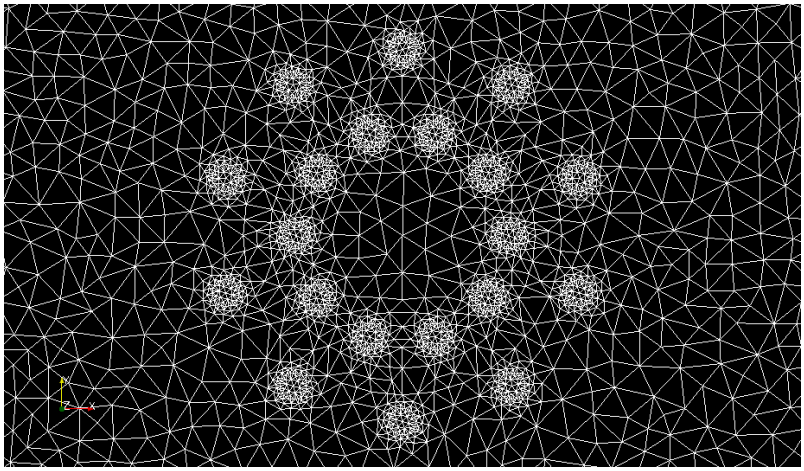


Fig. 4.3 Plot of the mesh generated for the magnetostatics test problem. The subdomains for the iron cylinder and copper wires are clearly visible

This line creates a `MeshFunction` with unsigned integer values (the subdomain numbers) with dimension 2, which is the cell dimension for this 2D problem.

We can now use the markers as we have done before to redefine the integration measure `dx`:

```
dx = Measure('dx', domain=mesh, subdomain_data=markers)
```

Integrals over subdomains can then be expressed by `dx(0)`, `dx(1)`, and so on. We use this to define the current $J_z = \pm 1\,\mathrm{A}$ in the coppper wires:

```
J_N = Constant(1.0)
J_S = Constant(-1.0)
A_z = TrialFunction(V)
v = TestFunction(V)
a = (1 / mu)*dot(grad(A_z), grad(v))*dx
L_N = sum(J_N*v*dx(i) for i in range(2, 2 + n))
L_S = sum(J_S*v*dx(i) for i in range(2 + n, 2 + 2*n))
L = L_N + L_S
```

The permeability is defined as an `Expression` that depends on the subdomain number:

```
class Permeability(Expression):
    def __init__(self, mesh, **kwargs):
        self.markers = markers
    def eval_cell(self, values, x, ufc_cell):
        if markers[ufc_cell.index] == 0:
            values[0] = 4*pi*1e-7 # vacuum
        elif markers[ufc_cell.index] == 1:
            values[0] = 1e-5      # iron (should really be 2.5e-1)
```

```
        else:
            values[0] = -6.4e-6   # copper

mu = Permeability(mesh, degree=1)
```

As seen in this code snippet, we have used a somewhat less extreme value for the magnetic permeability of iron. This is to make the solution a little more interesting. It would otherwise be completely dominated by the field in the iron cylinder.

Finally, when A_z has been computed, we can compute the magnetic field:

```
W = VectorFunctionSpace(mesh, 'P', 1)
B = project(as_vector((A_z.dx(1), -A_z.dx(0))), W)
```

We use `as_vector()` to interpret the tuple `(A_z.dx(1), -A_z.dx(0))` as a vector. The resulting plots of the magnetic vector potential and magnetic field are shown in Figures 4.4 and 4.5.

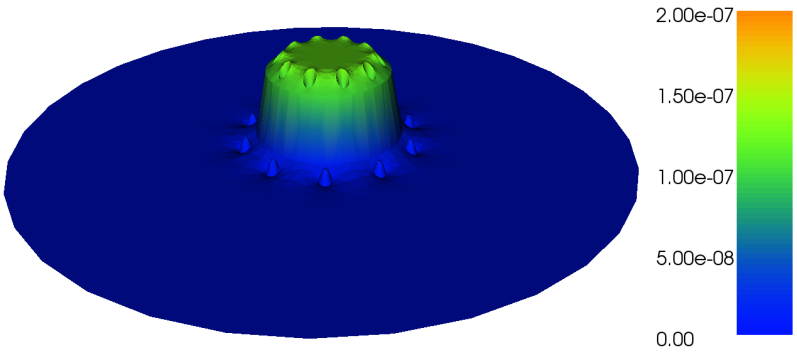


Fig. 4.4 Plot of the z-component A_z of the magnetic vector potential.

The complete code for computing the magnetic field follows below.

```
from fenics import *
from mshr import *
from math import sin, cos, pi

a = 1.0   # inner radius of iron cylinder
b = 1.2   # outer radius of iron cylinder
c_1 = 0.8 # radius for inner circle of copper wires
c_2 = 1.4 # radius for outer circle of copper wires
r = 0.1   # radius of copper wires
R = 5.0   # radius of domain
n = 10    # number of windings

# FIXME: Use 'domain' instead of 'geometry' in other examples

# Define geometry for background
```

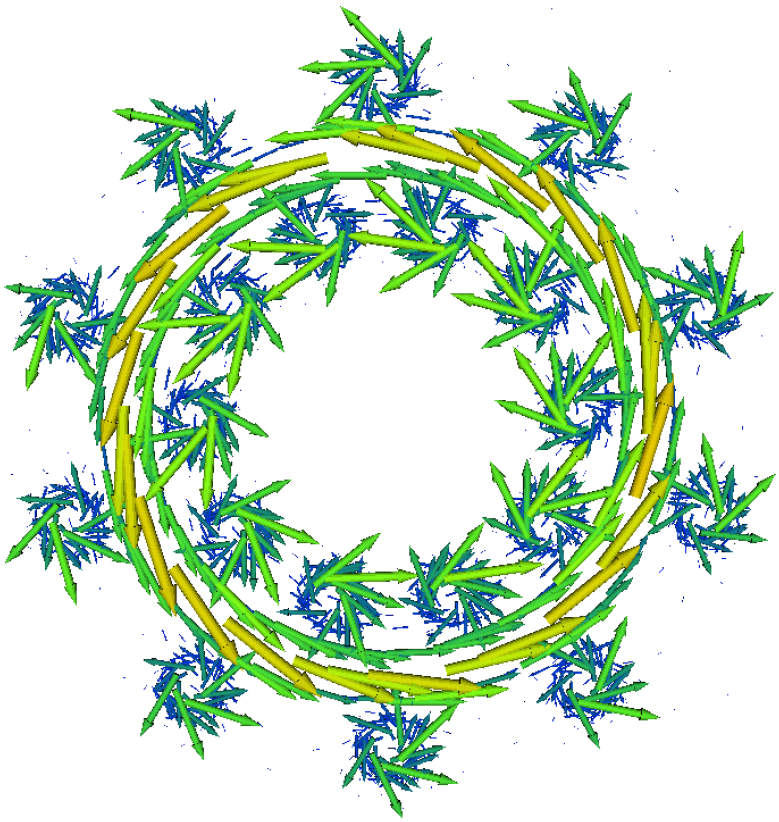


Fig. 4.5 Plot of the magnetic field B in the xy-plane.

```
domain = Circle(Point(0, 0), R)

# Define geometry for iron cylinder
cylinder = Circle(Point(0, 0), b) - Circle(Point(0, 0), a)

# Define geometry for wires (N = North (up), S = South (down))
angles_N = [i*2*pi/n for i in range(n)]
angles_S = [(i + 0.5)*2*pi/n for i in range(n)]
wires_N = [Circle(Point(c_1*cos(v), c_1*sin(v)), r) for v in angles_N]
wires_S = [Circle(Point(c_2*cos(v), c_2*sin(v)), r) for v in angles_S]

# Set subdomain for iron cylinder
domain.set_subdomain(1, cylinder)

# Set subdomains for wires
for (i, wire) in enumerate(wires_N):
    domain.set_subdomain(2 + i, wire)
for (i, wire) in enumerate(wires_S):
    domain.set_subdomain(2 + n + i, wire)
```

```
# Create mesh
mesh = generate_mesh(domain, 32)

# FIXME: Remove when working
#File('magnetostatics.xml.gz') << mesh
#mesh = Mesh('magnetostatics.xml.gz')

# Define function space
V = FunctionSpace(mesh, 'P', 1)

# Define boundary condition
bc = DirichletBC(V, Constant(0), 'on_boundary')

# Define subdomain markers and integration measure
markers = MeshFunction('size_t', mesh, 2, mesh.domains())
dx = Measure('dx', domain=mesh, subdomain_data=markers)

# Define current densities
J_N = Constant(1.0)
J_S = Constant(-1.0)

# Define magnetic permeability
class Permeability(Expression):
    def __init__(self, mesh, **kwargs):
        self.markers = markers
    def eval_cell(self, values, x, ufc_cell):
        if markers[ufc_cell.index] == 0:
            values[0] = 4*pi*1e-7 # vacuum
        elif markers[ufc_cell.index] == 1:
            values[0] = 1e-5      # iron (should really be 2.5e-1)
        else:
            values[0] = -6.4e-6   # copper

mu = Permeability(mesh, degree=1)

# Define variational problem
A_z = TrialFunction(V)
v = TestFunction(V)
a = (1 / mu)*dot(grad(A_z), grad(v))*dx
L_N = sum(J_N*v*dx(i) for i in range(2, 2 + n))
L_S = sum(J_S*v*dx(i) for i in range(2 + n, 2 + 2*n))
L = L_N + L_S

# Solve variational problem
A_z = Function(V)
solve(a == L, A_z, bc)

# Compute magnetic field (B = curl A)
W = VectorFunctionSpace(mesh, 'P', 1)
B = project(as_vector((A_z.dx(1), -A_z.dx(0))), W)

# Plot solution
plot(A_z)
```

```
plot(B)

# Save solution to file
vtkfile_A_z = File('magneticpotential.pvd')
vtkfile_B = File('magneticfield.pvd')
vtkfile_A_z << A_z
vtkfile_B << B

interactive()
```

The complete code can be found in the file `ft12_magnetostatics.py`.

Chapter 5
Extensions: Improving the Poisson solver

The FEniCS programs we have written so far have been designed as flat Python scripts. This works well for solving simple demo problems. However, when you build a solver for an advanced application, you will quickly find the need for more structured programming. In particular, you may want to reuse your solver to solve a large number of problems where you vary the boundary conditions, the domain, and coefficients such as material parameters. In this chapter, we will see how to write general solver functions to improve the usability of FEniCS programs. We will also discuss how to utilize iterative solvers with preconditioners for solving linear systems and how to compute derived quantities, such as, e.g., the flux on a part of the boundary.

5.1 Refactoring the Poisson solver

All programs created in this book so far are "flat"; that is, they are not organized into logical, reusable units in terms of Python functions. Such flat programs are useful for quickly testing out some software, but not well suited for serious problem solving. We shall therefore look at how to *refactor* the Poisson solver from Chapter 2. For a start, this means splitting the code into functions, but this is just a reordering of the existing statements. During refactoring, we also try make the functions we create as reusable as possible in other contexts. We will also encapsulate statements specific to a certain problem into (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) are often mixed together, which tends to give a blurred understanding of the problem at hand.

5.1.1 A more general solver function

We consider the flat program developed in Section 2.2. 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 $u = u_{\mathrm{D}}$ on the boundary, while other statements arise from our simple test problem. Let us collect the general, reusable code in a function called `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 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_{D}, 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 also add the polynomial degree of the finite element function space as an argument to `solver`.

```
from fenics import *

def solver(f, u_D, 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 = u_D (Expresssion) on
    the boundary.
    """

    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

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

    bc = DirichletBC(V, u_D, 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
```

The remaining tasks of our initial program, such as calling the `solve` function with problem-specific parameters and plotting, can be placed in a separate function. Here we choose to put this code in a function named `run_solver`:

```
def run_solver():
    "Run solver to compute and post-process solution"

    # Set up problem parameters and call solver
    u_D = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    f = Constant(-6.0)
    u = solver(f, u_D, 8, 8, 1)

    # Plot solution and mesh
    u.rename('u', 'solution')
    plot(u)
    plot(u.function_space().mesh())

    # Save solution to file in VTK format
    vtkfile = File('poisson_solver/solution.pvd')
    vtkfile << u
```

The solution can now be computed, plotted, and saved to file by simply calling the `run_solver` function.

5.1.2 Writing the solver as a Python module

The refactored code is put in a file `ft03_poisson_solver.py`. We should make sure that such a file can be imported (and hence reused) in other programs. This means that all statements in the main program that are not inside functions should appear within 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 `ft03_poisson_solver.py`, the main program is simply a call to `run_solver()` followed by a call `interactive()` to hold the plot:

```
if __name__ == '__main__':
    run_solver()
    interactive()
```

The complete code can be found in the file `ft03_poisson_solver.py`.

5.1.3 Verification and unit tests

The remaining part of our first program is to compare the numerical and the exact solutions. 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 module `unittest`, but here we are going to use pytest (or nose) since that will result in shorter and clearer code.

Mathematically, our unit test is that the finite element solution of our problem when $f = -6$ equals the exact solution $u = u_{\mathrm{D}} = 1 + x^2 + 2y^2$ at the vertices of the mesh. We have already created a code that finds the error at the vertices for our numerical solution. Because of rounding errors, we cannot demand this 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. If we want to test that the `solver` function works for meshes up to $2 \times (20 \times 20)$ elements and cubic Lagrange elements, 10^{-10} is an appropriate tolerance for testing that the maximum error vanishes (see Section 2.3).

To make our test case work together with pytest and nose, we have to make a couple of small adjustments to our program. The simple rule is that each test must be placed in a function that

- has a name starting with `test_`,
- has no arguments, and
- implements a test expressed 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, and otherwise runs silently. The `msg` string is optional, so `assert success` is the minimal test. In our case, we will write `assert max_error < tol`, where `tol` is the tolerance 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():
    "Test solver by reproducing u = 1 + x^2 + 2y^2"

    # Set up parameters for testing
    tol = 1E-10
    u_D = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    f = Constant(-6.0)

    # Iterate over mesh sizes and degrees
    for Nx, Ny in [(3, 3), (3, 5), (5, 3), (20, 20)]:
        for degree in 1, 2, 3:
            print('Solving on a 2 x (%d x %d) mesh with P%d elements.'
                  % (Nx, Ny, degree))

            # Compute solution
            u = solver(f, u_D, Nx, Ny, degree)

            # Extract the mesh
```

```
            mesh = u.function_space().mesh()

            # Compute maximum error at vertices
            vertex_values_u_D = u_D.compute_vertex_values(mesh)
            vertex_values_u  = u.compute_vertex_values(mesh)
            import numpy as np
            error_max = np.max(np.abs(vertex_values_u_D - \
                                      vertex_values_u))

            # Check maximum error
            msg = 'error_max = %g' % error_max
            assert error_max < tol, msg

if __name__ == '__main__':
    run_solver()
    interactive()
```

To run the test, we type the following command:

Terminal

```
Terminal> py.test ft03_poisson_solver.py
```

This will run all functions `test_*()` (currently only the `test_solver` function) found in the file and report the results. For more verbose output, add the flags `-s -v`.

We shall make it a habit in the following test 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.

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.

5.1.4 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.py` or `ft03_poisson_solver.py` and change the mesh construction from `UnitSquareMesh(16, 16)` to `UnitCubeMesh(16, 16, 16)`. Now the domain is the unit cube partitioned into $16 \times 16 \times 16$ boxes, and

each box is divided into six tetrahedron-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.

If we want to parameterize the creation of unit interval, unit square, or unit cube over dimension, we can do so by encapsulating this part of the code in a function. Given a list or tuple with the divisions into cells in the various spatial coordinates, the following function returns the mesh for a d-dimensional cube:

```
def UnitHyperCube(divisions):
    mesh_classes = [UnitIntervalMesh, UnitSquareMesh, UnitCubeMesh]
    d = len(divisions)
    mesh = mesh_classes[d-1](*divisions)
    return 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 components of the list `divisions` as separate arguments to the constructor of the mesh construction class picked out by `mesh_class[d-1]`. 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])
```

The `solver` function from `ft03_poisson_solver.py` may be modified to solve d-dimensional problems by replacing the `Nx` and `Ny` parameters by `divisions`, and calling the function `UnitHyperCube` to create the mesh. Note that `UnitHyperCube` is a *function* and not a *class*, but we have named it with *CamelCase* to make it look like a class:

```
mesh = UnitHyperCube(divisions)
```

Exercise 5.1: Solve a Poisson problem

Solve the following problem

$$\nabla^2 u = 2e^{-2x}\sin(\pi y)((4-5\pi^2)\sin(2\pi x) - 8\pi\cos(2\pi x)) \text{ in } \Omega = [0,1]\times[0,1] \tag{5.1}$$

$$u = 0 \quad \text{on } \partial\Omega \tag{5.2}$$

The exact solution is given by

$$u(x,y) = 2e^{-2x}\sin(\pi x)\sin(\pi y)\,.$$

Compute the maximum numerical approximation error in a mesh with $2(N_x \times N_y)$ elements and in a mesh with double resolution: $4(N_x \times N_y)$ elements. Show that the doubling the resolution reduces the error by a factor 4 when using Lagrange elements of degree one. Make an illustrative plot of the solution too.

a) Base your implementation on editing the program `ft01_poisson.py`.

Hint 1. In the string for an `Expression` object, `pi` is the value of π. Also note that π^2 must be expressed with syntax `pow(pi,2)` and not (the common Python syntax) `pi**2`.

FEniCS will abort with a compilation error if you type the expressions in a wrong way syntax-wise. Search for *error:* in the `/very/long/path/compile.log` file mentioned in the error message to see what the C++ compiler reported as error in the expressions.

Hint 2. The result that with P1 elements, doubling the resolution reduces the error with a factor of four, is an asymptotic result so it requires a sufficiently fine mesh. Here one may start with $N_x = N_y = 20$.
Filename: `poisson_fsin_flat`.

Solution. Looking at the `ft01_poisson.py` code, we realize that the following edits are required:

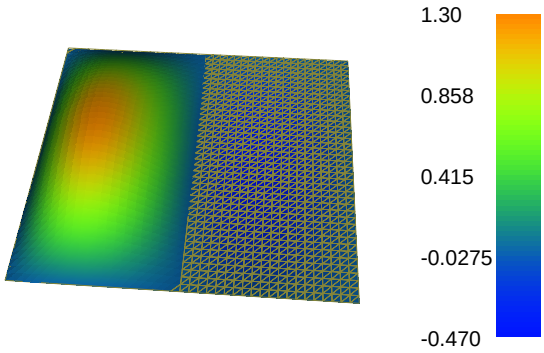
- Modify the `mesh` computation.
- Modify `u_b` and `f`.
- Add expression for the exact solution.
- Modify the computation of the numerical error.
- Insert a loop to enable solving the problem twice.
- Put the error reduction computation and the plot statements after the loop.

Here is the modified code:

```
from fenics import *

Nx = Ny = 20
error = []
for i in range(2):
    Nx *= (i+1)
    Ny *= (i+1)

    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'Lagrange', 1)

    # Define boundary conditions
    u0 = Constant(0)
```

```
    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 = Expression('-2*exp(-2*x[0])*sin(pi*x[1])*('
                   '(4-5*pow(pi,2))*sin(2*pi*x[0]) '
                   ' - 8*pi*cos(2*pi*x[0]))')
    # Note: no need for pi=DOLFIN_PI in f, pi is valid variable
    a = inner(nabla_grad(u), nabla_grad(v))*dx
    L = f*v*dx

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

    u_e = Expression(
        '2*exp(-2*x[0])*sin(2*pi*x[0])*sin(pi*x[1])')

    u_e_Function = interpolate(u_e, V)         # exact solution
    u_e_array = u_e_Function.vector().array()  # dof values
    max_error = (u_e_array - u.vector().array()).max()
    print('max error:', max_error, '%dx%d mesh' % (Nx, Ny))
    error.append(max_error)

print('Error reduction:', error[1]/error[0])

# Plot solution and mesh
plot(u)

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

# Hold plot
interactive()
```

The number π has the symbol `M_PI` in C and C++, but in C++ strings in `Expression` objects, the symbol `pi` can be used directly (or one can use the less readable `DOLFIN_PI`).



b) Base your implementation on a new file that imports functionality from the module `ft03_poisson_solver.py`. Embed the check of the reduction of the numerical approximation error in a unit test. Filename: `poisson_fsin_func`.

Solution. Solving the two problems is a matter of calling `solver` with different sets of arguments. To compute the numerical error, we need code that is close to what we have in `test_solver`.

```
from poisson_solver import (
    solver, Expression, Constant, interpolate, File, plot,
    interactive)

def data():
    """Return data for this Poisson problem."""
    u0 = Constant(0)
    u_e = Expression(
        '2*exp(-2*x[0])*sin(2*pi*x[0])*sin(pi*x[1])')
    f = Expression('-2*exp(-2*x[0])*sin(pi*x[1])*('
                   '(4-5*pow(pi,2))*sin(2*pi*x[0]) '
                   ' - 8*pi*cos(2*pi*x[0]))')
    return u0, f, u_e

def test_solver():
    """Check convergence rate of solver."""
    u0, f, u_e = data()
    Nx = 20
    Ny = Nx
    error = []
    # Loop over refined meshes
    for i in range(2):
        Nx *= i+1
        Ny *= i+1
        print('solving on 2(%dx%d) mesh' % (Nx, Ny))
```

```
        u = solver(f, u0, Nx, Ny, degree=1)
        # Make a finite element function of the exact u_e
        V = u.function_space()
        u_e_array = interpolate(u_e, V).vector().array()
        max_error = (u_e_array - u.vector().array()).max()  # Linf norm
        error.append(max_error)
        print('max error:', max_error)
    for i in range(1, len(error)):
        error_reduction = error[i]/error[i-1]
        print('error reduction:', error_reduction)
        assert abs(error_reduction - 0.25) < 0.1

def application():
    """Plot the solution."""
    u0, f, u_e = data()
    Nx = 40
    Ny = Nx
    u = solver(f, u0, Nx, Ny, 1)
    # Dump solution to file in VTK format
    file = File("poisson.pvd")
    file << u
    # Plot solution and mesh
    plot(u)

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

The unit test is embedded in a proper test function `test_solver` for the pytest or nose testing frameworks. Visualization of the solution is encapsulated in the `application` function. Since we need `u_e`, `u_b`, and `f` in two functions, we place the definitions in a function `data` to avoid copies of these expressions.

Remarks. This exercise demonstrates that changing a flat program to solve a new problem requires careful editing of statements scattered around in the file, while the solution in b), based on the `solver` function, requires *no modifications* of the `ft03_poisson_solver.py` file, just *minimalistic additional new code* in a separate file. The Poisson solver remains in one place (`ft03_poisson_solver.py`) while in a) we got two Poisson solvers. If you decide to switch to an iterative solution method for linear systems, you can do so in one place in b), and all applications can take advantage of the extension. Hopefully, with this exercise you realize that embedding PDE solvers in functions (or classes) makes more reusable software than flat programs.

Exercise 5.2: Refactor the code for membrane deflection

The `ft02_poisson_membrane.py` program simulates the deflection of a membrane. Refactor this code such that we have a `solver` function as in the program with name `ft03_poisson_solver.py`. Let the user have the option to choose a direct or iterative solver for the linear system. Also implement a unit test where you have $p = 4$ (constant) and use P2 and P3 elements. In this case, the exact solution is quadratic in x and y and will be "exactly" reproduced by P2 and higher-order elements.

Solution. We can use the `solver` function from `ft03_poisson_solver.py` right away. The major difference is that the domain is now a circle and not a square. We change the `solver` function by letting the mesh be an argument `mesh` (instead of `Nx` and `Ny`):

```
def solver(
    f, u_b, mesh, degree=1,
    linear_solver='Krylov', # Alt: 'direct'
    ...):
    V = FunctionSpace(mesh, 'P', degree)
    # code as before
```

The complete code becomes

```
def application(beta, R0, num_elements_radial_dir):
    # Scaled pressure function
    p = Expression(
        '4*exp(-pow(beta,2)*(pow(x[0], 2) + pow(x[1]-R0, 2)))',
        beta=beta, R0=R0)

    # Generate mesh over the unit circle
    domain = Circle(Point(0.0, 0.0), 1.0)
    mesh = generate_mesh(domain, num_elements_radial_dir)

    w = solver(p, Constant(0), mesh, degree=1,
               linear_solver='direct')
    w.rename('w', 'deflection')  # set name and label (description)

    # Plot scaled solution, mesh and pressure
    plot(mesh, title='Mesh over scaled domain')
    plot(w, title='Scaled ' + w.label())
    V = w.function_space()
    p = interpolate(p, V)
    p.rename('p', 'pressure')
    plot(p, title='Scaled ' + p.label())

    # Dump p and w to file in VTK format
    vtkfile1 = File('membrane_deflection.pvd')
    vtkfile1 << w
    vtkfile2 = File('membrane_load.pvd')
    vtkfile2 << p
```

The key function to simulate membrane deflection is named `application`.

For $p = 4$, we have $w = 1 - x^2 - y^2$ as exact solution. The unit test for P2 and P3 goes as follows:

```
def test_membrane():
    """Verification for constant pressure."""
    p = Constant(4)
    # Generate mesh over the unit circle
    domain = Circle(Point(0.0, 0.0), 1.0)
    for degree in 2, 3:
        print('********* P%d elements:' % degree)
        n = 5
        for i in range(4):  # Run some resolutions
            n *= (i+1)
            mesh = generate_mesh(domain, n)
            #info(mesh)
            w = solver(p, Constant(0), mesh, degree=degree,
                       linear_solver='direct')
            print('max w: %g, w(0,0)=%g, h=%.3E, dofs=%d' %
                  (w.vector().array().max(), w((0,0)),
                   1/np.sqrt(mesh.num_vertices()),
                   w.function_space().dim()))

            w_exact = Expression('1 - x[0]*x[0] - x[1]*x[1]')
            w_e = interpolate(w_exact, w.function_space())
            error = np.abs(w_e.vector().array() -
                           w.vector().array()).max()
            print('error: %.3E' % error)
            assert error < 9.61E-03

def application2(
    beta, R0, num_elements_radial_dir):
    """Explore more built-in visulization features."""
    # Scaled pressure function
    p = Expression(
        '4*exp(-pow(beta,2)*(pow(x[0], 2) + pow(x[1]-R0, 2)))',
        beta=beta, R0=R0)

    # Generate mesh over the unit circle
    domain = Circle(Point(0.0, 0.0), 1.0)
    mesh = generate_mesh(domain, num_elements_radial_dir)

    w = solver(p, Constant(0), mesh, degree=1,
               linear_solver='direct')
    w.rename('w', 'deflection')

    # Plot scaled solution, mesh and pressure
    plot(mesh, title='Mesh over scaled domain')
    viz_w = plot(w,
                 wireframe=False,
                 title='Scaled membrane deflection',
                 axes=False,
                 interactive=False,
                 )
    viz_w.elevate(-10) # adjust (lift) camera from default view
```

```
    viz_w.plot(w)      # bring new settings into action
    viz_w.write_png('deflection')
    viz_w.write_pdf('deflection')

    V = w.function_space()
    p = interpolate(p, V)
    p.rename('p', 'pressure')
    viz_p = plot(p, title='Scaled pressure', interactive=False)
    viz_p.elevate(-10)
    viz_p.plot(p)
    viz_p.write_png('pressure')
    viz_p.write_pdf('pressure')

    # Dump w and p to file in VTK format
    vtkfile1 = File('membrane_deflection.pvd')
    vtkfile1 << w
    vtkfile2 = File('membrane_load.pvd')
    vtkfile2 << p
```

The striking feature is that the solver does not reproduce the solution to an accuracy more than about 0.01 (!), regardless of the resolution and type of element.
Filename: `membrane_func`.

5.2 Working with linear solvers

Sparse LU decomposition (Gaussian elimination) is used by default to solve linear systems of equations in FEniCS programs. This is a very robust and simple method. It is the recommended method for systems with up to a few thousand unknowns and may hence be the method of choice for many 2D and smaller 3D problems. However, sparse LU decomposition becomes slow and one quickly runs out of memory for larger problems. For large problems, we instead need to use *iterative methods* which are faster and require much less memory. We will now look at how to take advantage of state-of-the-art iterative solution methods in FEniCS.

5.2.1 Controlling the solution process

Choosing a linear solver and preconditioner. 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 system 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.

Choosing a linear algebra backend. The actual GMRES and ILU implementations that are brought into action depend 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. If PETSc is not available, then FEniCS falls back to using the Eigen backend. The linear algebra backend in FEniCS can be set using the following command:

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

where `backendname` is a string. To see which linear algebra backends are available, you can call the FEniCS function `list_linear_algebra_backends()`. Similarly, one may check which linear algebra backend is currently being used by the following command:

```
print parameters['linear_algebra_backend']

# Alternative syntax for Python 3
print(parameters['linear_algebra_backend'])
```

Setting solver parameters. We will normally want to control the tolerance in the stopping criterion and the maximum number of iterations when running an iterative method. Such parameters can be controlled at both a *global* and a *local* level. We will start by looking at how to set global parameters. For more advanced programs, one may want to use a number of different linear solvers and set different tolerances and other parameters. Then it becomes important to control the parameters at a *local* level. We will return to this issue in Section 5.2.3.

Changing a parameter in the global FEniCS parameter database affects all linear solvers (created *after* the parameter has been set). The global FEniCS parameter database is simply called `parameters` and it 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.

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 file (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. We may extend the previous solver function from `ft03_poisson_solver.py` in Section 5.1.1 such that it also offers the GMRES+ILU preconditioned Krylov solver:

```
def solver(
    f, u_b, Nx, Ny,
    degree=1,               # Polynomial degree of function space
    linear_solver='Krylov', # Linear solver method (alt: 'direct')
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,           # Relative tolerance in Krylov solver
    max_iter=1000,          # Max iterations in Krylov solver
    log_level=PROGRESS,     # Amount of solver output
    print_parameters=False, # Print solver parameters to screen?
    ):
    ...
    # Set up variational problem: a, L, declare u, etc.

    if linear_solver == 'Krylov':
        prm = parameters['krylov_solver']
        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 print_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
```

This new `solver` function, found in the file `ft14_poisson_iterative.py`, replaces the one in `ft03_poisson_solver.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.

A remark regarding unit tests. Regarding verification of the new `solver` function in terms of unit tests, it turns out that unit testing for a problem where the approximation error vanishes 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 P_2 elements, it is hard to force the linear solver error below 10^{-6}. Consequently, tolerances in tests depend on the numerical method being used. The interested reader is referred to the `test_solver` function in `ft14_poisson_iterative.py` for details: this 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 List of linear solver methods and preconditioners

Which linear solvers and preconditioners that are available in FEniCS depends on how FEniCS has been configured and which linear algebra backend is currently active. The following table shows an example of which linear solvers that can be available through FEniCS when the PETSc backend is active:

Name	Method
`'bicgstab'`	Biconjugate gradient stabilized method
`'cg'`	Conjugate gradient method
`'gmres'`	Generalized minimal residual method
`'minres'`	Minimal residual method
`'petsc'`	PETSc built in LU solver
`'richardson'`	Richardson method
`'superlu_dist'`	Parallel SuperLU
`'tfqmr'`	Transpose-free quasi-minimal residual method
`'umfpack'`	UMFPACK

The set of available preconditioners also depends on configuration and linear algebra backend. The following table shows an example of which preconditioners may be available:

Name	Method
`'icc'`	Incomplete Cholesky factorization
`'ilu'`	Incomplete LU factorization
`'petsc_amg'`	PETSc algebraic multigrid
`'sor'`	Successive over-relaxation

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

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

5.2.3 Linear variational problem and solver objects

The FEniCS interface allows different ways to access the core functionality, ranging from very high-level to low-level access. So far, we have mostly used the high-level call `solve(a == L, u, bc)` to solve a variational problem `a == L` with a certain boundary condition `bc`. However, sometimes you may need more fine-grained control over the solution process. In particular, the call to `solve` will create certain objects that are thrown away after the solution has been computed, and it may be practical or efficient to *reuse* those objects.

In this section, we will look at an alternative interface to solving linear variational problems in FEniCS, which may be preferable in many situations compared to the high-level `solve` function interface. This interface uses the two classes `LinearVariationalProblem` and `LinearVariationalSolver`. Using this interface, the equivalent of `solve(a == L, u, bc)` looks as follows:

```
u = Function(V)
problem = LinearVariationalProblem(a, L, u, bc)
```

```
solver = LinearVariationalSolver(problem)
solver.solve()
```

Many FEniCS 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 the 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 above. Note that global parameter values can only affect local parameter values if set before the time of creation of the local object. Thus, changing the value of the tolerance in the global parameter database will not affect the parameters for already created solvers.

The linear variational problem and solver objects as outlined above are incorporated in an alternative solver function, named `solver_objects`, in `ft14_poisson_iterative.py`. Otherwise, this function is similar to the previously shown `solver` function.

5.2.4 Explicit assembly and solve

As we saw already in Section 3.4, linear variational problems can be assembled explicitly in FEniCS into matrices and vectors using the `assemble` function. This allows even more fine-grained control of the solution process compared to using the high-level `solve` function or using the classes `LinearVariationalProblem` and `LinearVariationalSolver`. We will now look more closely into how to use the `assemble` function and how to combine this with low-level calls for solving the assembled linear systems.

Given a variational problem $a(u,v) = L(v)$, 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 $\hat{\phi}_1, \ldots, \hat{\phi}_N$. This implies

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

which is nothing but a linear system,

$$AU = b,$$

where the entries of 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 sides 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-hand side vector b, and then solve the linear system $AU = b$ for the vector U. 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 the same as before; that is, `a` refers to the bilinear form involving a `TrialFunction` object `u` and a `TestFunction` object `v`, and `L` involves the same `TestFunction` object `v`. From `a` and `L`, the `assemble` function can compute A and b.

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.

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`, we must apply each condition in `bcs` to the system:

```
for bc in bcs:
    bc.apply(A, b)

# Alternative syntax using list comprehension
[bc.apply(A, b) for bc in bcs]
```

Alternatively, we can use the function `assemble_system`, which takes the boundary conditions into account during the assembly of the matrix and vector:

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

The `assemble_system` function is preferable to the combination of `assemble` and `bc.apply` when the linear system is symmetric, since `assemble_system` will incorporate the boundary conditions in a symmetric way. Even if the matrix `A` that comes out of the call to `assemble` is symmetric (for a symmetric bilinear form `a`), the call to `bc.apply` will break the symmetry.

Once the linear system has been assembled, we need to compute the solution $U = A^{-1}b$ and store the solution U in the vector `U = u.vector()`. In the same way as linear variational problems can be programmed using different interfaces in FEniCS—the high-level `solve` function, the class `LinearVariationalSolve`, and the low-level `assemble` function—linear systems can also be programmed using different interfaces in FEniCS. The high-level interface to solving a linear system in FEniCS is also named `solve`:

```
solve(A, U, b)
```

By default, `solve(A, U, b)` uses sparse LU decomposition to compute the solution. Specification of an iterative solver and preconditioner can be made through two optional arguments:

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

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

This high-level interface is useful for many applications, but sometimes more fine-grained control is needed. One can then create one or more `KrylovSolver` objects that are then used to solve linear systems. Each different solver object can have its own set of parameters and selection of iterative method and preconditioner. Here is an example:

```
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()
solver.solve(A, U, b)
```

The function `solver_linalg` in the program file `ft14_poisson_iterative.py` implements a solver function where the user can choose between different types of assembly. The function `demo_linalg` runs a test problem on a sequence of meshes and solves the problem with symmetric and non-symmetric modification of the system matrix. One can monitor the number of Krylov method iterations 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` for this problem.

The choice of start vector for the iterations in a linear solver is often important. By default, the values of `u` and thus the vector `U = u.vector()`

will be initialized to zero. If we instead wanted to initialize `U` with random numbers in the interval $[-100, 100]$ this can be done as follows:

```
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 both turn off the default behavior of setting the start vector ("initial guess") to zero, and also set the values of the vector `U` to nonzero values.

Using a nonzero initial guess can be particularly important for time-dependent problems or when solving a linear system as part of a nonlinear iteration, since then the previous solution vector `U` will often be a good initial guess for the solution in the next time step or iteration. In this case, the values in the vector `U` will naturally be initialized with the previous solution vector (if we just used it to solve a linear system), so the only extra step necessary is to set the parameter `nonzero_initial_guess` to `True`.

5.2.5 Examining matrix and vector values

When calling `A = assemble(a)` and `b = assemble(L)`, the object `A` will be of type `Matrix`, while `b` and `u.vector()` are of type `Vector`. To examine the values, we may convert the matrix and vector data to `numpy` arrays by calling the `array()` method as shown before. For example, if you wonder how essential boundary conditions are incorporated into linear systems, 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 the preferred tool for computing the eigenvalues of large, sparse matrices of the type encountered in PDE problems (see `demo/documented/eigenvalue` in the FEniCS source code tree for a demo).

5.2.6 Examining the degrees of freedom

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

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

For a finite element function from a standard continuous piecewise linear function space (P_1 Lagrange elements), these values will be the same as the values we get by the following statement:

```
vertex_values = u.compute_vertex_values(mesh)
```

Both `nodal_values` and `vertex_values` will be `numpy` arrays and they will be of the same length and contain the same values, but with possibly different ordering. The array `vertex_values` will have the same ordering as the vertices of the mesh, while `nodal_values` will be ordered in a way that (nearly) minimizes the bandwidth of the system matrix and thus improves the efficiency of linear solvers.

A fundamental question is: what are the coordinates of the vertex whose value is `nodal_values[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.

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)
>>> coordinates = mesh.coordinates()
>>> coordinates
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. ]])
```

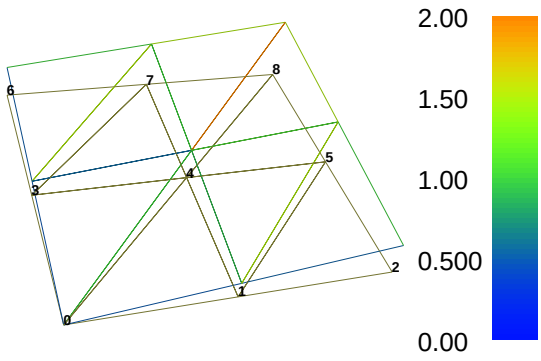
We see from this output that for this particular mesh, the vertices are first numbered along $y = 0$ with increasing x coordinate, then along $y = 0.5$, and so on.

Next we compute a function `u` on this mesh. Let's take $u = x + y$:

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

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

Note that we may examine the vertex numbering in the plot window. We type `w` to turn on wireframe instead of a fully colored surface, `m` to show the mesh, and then `v` to show the numbering of the vertices.



Let's instead examine the values we get by calling `u.compute_vertex_values()`:

```
>>> vertex_values = u.compute_vertex_values()
>>> for i, x in enumerate(coordinates):
...     print('vertex %d: vertex_values[%d] = %g\tu(%s) = %g' %
...           (i, i, vertex_values[i], x, u(x)))
vertex 0: vertex_values[0] = 0      u([ 0.  0.]) = 8.46545e-16
vertex 1: vertex_values[1] = 0.5    u([ 0.5  0. ]) = 0.5
```

```
vertex 2: vertex_values[2] = 1          u([ 1.  0.]) = 1
vertex 3: vertex_values[3] = 0.5    u([ 0.   0.5]) = 0.5
vertex 4: vertex_values[4] = 1          u([ 0.5  0.5]) = 1
vertex 5: vertex_values[5] = 1.5    u([ 1.   0.5]) = 1.5
vertex 6: vertex_values[6] = 1          u([ 0.  1.]) = 1
vertex 7: vertex_values[7] = 1.5    u([ 0.5  1. ]) = 1.5
vertex 8: vertex_values[8] = 2          u([ 1.  1.]) = 2
```

We can ask FEniCS to give us the mapping from vertices to degrees of freedom for a certain function space V:

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

Now, `nodal_values[v2d[i]]` will give us the value of the degree of freedom in `u` corresponding to vertex `i` (`v2d[i]`). In particular, `nodal_values[v2d]` is an array with all the elements in the same (vertex numbered) order as `coordinates`. The inverse map, from degrees of freedom number to vertex number is given by `dof_to_vertex_map(V)`. This means that we may call `coordinates[dof_to_vertex_map(V)]` to get an array of all the coordinates in the same order as the degrees of freedom. Note that these mappings are only available in FEniCS for P_1 elements.

For Lagrange elements of degree larger than 1, there are degrees of freedom (nodes) that do not correspond to vertices. For these elements, we may get the vertex values by calling `u.compute_vertex_values(mesh)`, and we can get the degrees of freedom by calling `u.vector().array()`. To get the coordinates associated with all degrees of freedom, we need to iterate over the elements of the mesh and ask FEniCS to return the coordinates and dofs associated with each cell. This information is stored in the `FiniteElement` and `DofMap` object of a `FunctionSpace`. The following code illustrates how to iterate over all elements of a mesh and print the degrees of freedom and coordinates associated with the element.

```
element = V.element()
dofmap = V.dofmap()
for cell in cells(mesh):
    print(element.tabulate_dof_coordinates(cell))
    print(dofmap.cell_dofs(cell.index()))
```

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 expensive while the other two are very efficient (but limited to certain points).

To demonstrate the use of point evaluation 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 = u_D(center) - u(center)
print('Error at %s: %g' % (center, error))
```

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

```
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 `u_D` is a quadratic function. When the center point is a node, as in a $2 \times (2 \times 2)$ or $2 \times (4 \times 4)$ 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 solution by dividing by max(|u|)."""
    nodal_values = u.vector().array()
    u_max = np.abs(nodal_values).max()
    nodal_values /= u_max
    u.vector()[:] = nodal_values
    #u.vector().set_local(dofs) # alternative
```

The `/=` operator implies an in-place modification of the object on the left-hand side: all elements of the array `nodal_values` are divided by the value `u_max`. Alternatively, we could do `nodal_values = nodal_values / u_max`, which implies creating a new array on the right-hand side and assigning this array to the name `nodal_values`.

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 use `u.set_local(...)`.

All the code in this can be found in the file `ft14_poisson_iterative.py` (Poission solver with use of iterative methods).

5.3 Postprocessing computations

As the final theme in this chapter, we will look at how to *postprocess computations*; that is, how to compute various derived quantities from the computed solution of a PDE. The solution u itself may be of interest for visualizing general features of the solution, but sometimes one is interested in computing the solution of a PDE to compute a specific quantity that derives from the solution, such as, e.g., the flux, a point-value, or some average of the solution.

5.3.1 A variable-coefficient Poisson problem

As a test problem, we will extend the Poisson problem from Chapter 2 with a variable coefficient $\kappa(x,y)$ in the Laplace operator:

$$-\nabla\cdot[\kappa(x,y)\nabla u(x,y)] = f(x,y) \qquad \text{in } \Omega, \tag{5.3}$$

$$u(x,y) = u_{\mathrm{D}}(x,y) \quad \text{on } \partial\Omega\,. \tag{5.4}$$

Let us continue to use our favorite solution $u(x,y) = 1+x^2+2y^2$ and then prescribe $\kappa(x,y) = x+y$. It follows that $u_{\mathrm{D}}(x,y) = 1+x^2+2y^2$ and $f(x,y) = -8x-10y$.

We shall quickly demonstrate that this simple extension of our model problem only requires an equally simple extension of the FEniCS program. The following simple changes must be made to the previously shown codes:

- the `solver` function must take `k` (κ) as an argument,
- a new `Expression k` must be defined for the variable coefficient,
- the right-hand side `f` must be an `Expression` since it is no longer a constant,
- the formula for $a(u,v)$ in the variational problem must be updated.

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

$$\int_\Omega \kappa\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega}\kappa\frac{\partial u}{\partial n}v\,\mathrm{d}s = \int_\Omega fv\,\mathrm{d}x\,.$$

The function spaces for u and v are the same as in the problem with $\kappa = 1$, implying that the boundary integral vanishes since $v = 0$ on $\partial\Omega$ where we have Dirichlet conditions. The variational forms a and L in the variational problem $a(u,v) = L(v)$ then become

$$a(u,v) = \int_\Omega \kappa\nabla u\cdot\nabla v\,\mathrm{d}x, \quad L(v) = \int_\Omega fv\,\mathrm{d}x\,. \tag{5.5}$$

We must thus replace

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

by

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

Moreover, the definitions of `k` and `f` in the test problem read

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

No additional modifications are necessary. The file `ft11_poisson_bcs.py` (Poisson problem, variable coefficients) is a copy of `ft14_poisson_iterative.py` with the mentioned changes incorporated. Observe that $\kappa = 1$ recovers the original problem in `ft14_poisson_iterative.py`.

You can execute the file and confirm that it recovers the exact solution u at the nodes.

5.3.2 Flux computations

It is often of interest to compute the flux $Q = -\kappa\nabla u$. Since $u = \sum_{j=1}^{N} U_j\phi_j$, it follows that

$$Q = -\kappa \sum_{j=1}^{N} U_j \nabla\phi_j \,.$$

However, the gradient of a piecewise continuous finite element scalar field is a discontinuous vector field since the basis functions $\{\phi_j\}$ have discontinuous derivatives at the boundaries of the cells. For example, using Lagrange elements of degree 1, u is linear over each cell, and the gradient 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*.

Projection is a common operation in finite element analysis and FEniCS has a function for easily performing the projection: `project(expression, W)`, which returns the projection of some expression into the space `W`.

In our case, the flux $Q = -\kappa\nabla u$ is vector-valued and we need to pick `W` as the vector-valued function space of the same degree as the space `V` where `u` resides:

```
V = u.function_space()
```

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

grad_u = project(grad(u), W)
flux_u = project(-k*grad(u), W)
```

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.

Plotting the flux vector field is naturally as easy as plotting anything else:

```
plot(flux_u, title='flux field')

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

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

```
flux_x_nodal_values = flux_x.vector().dofs()
flux_y_nodal_values = flux_y.vector().dofs()
```

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

```
flux_u_nodal_values = flux_u.vector().array()
```

However, this is a flat `numpy` array containing the degrees of freedom for both the x and y components of the flux and the ordering of the components may be mixed up by FEniCS in order to improve computational efficiency.

The function `demo_test_flux` in the program `ft11_poisson_bcs.py` demonstrates the computations described above.

Manual projection.

Although you will always use `project` to project a finite element function, it can be instructive to look at how to formulate the projection mathematically and implement its steps manually in FEniCS.

Let's say we have an expression $g = g(u)$ that we want to project into some space W. The mathematical formulation of the (L^2) projection $w = P_W g$ into W is the variational problem

$$\int_\Omega wv\,\mathrm{d}x = \int_\Omega gv\,\mathrm{d}x \tag{5.6}$$

for all test functions $v \in W$. In other words, we have a standard variational problem $a(w,v) = L(v)$ where now

$$a(w,v) = \int_\Omega wv\,\mathrm{d}x, \tag{5.7}$$

$$L(v) = \int_\Omega gv\,\mathrm{d}x\,. \tag{5.8}$$

Note that when the functions in W are vector-valued, as is the case when we project the gradient $g(u) = \nabla u$, we must replace the products above by $w \cdot v$ and $g \cdot v$.

The variational problem is easy to define in FEniCS.

```
w = TrialFunction(W)
v = TestFunction(W)

a = w*v*dx # or dot(w, v)*dx when w is vector-valued
L = g*v*dx # or dot(g, v)*dx when g is vector-valued
w = Function(W)
solve(a == L, w)
```

The boundary condition argument to `solve` is dropped since there are no essential boundary conditions in this problem.

5.3.3 Computing functionals

After the solution u of a PDE is computed, we occasionally want to compute functionals of u, for example,

$$\frac{1}{2}||\nabla u||^2 = \frac{1}{2}\int_\Omega \nabla u \cdot \nabla u\,\mathrm{d}x, \tag{5.9}$$

which often reflects some energy quantity. Another frequently occurring functional is the error

$$||u_\mathrm{e} - u|| = \left(\int_\Omega (u_\mathrm{e} - u)^2\,\mathrm{d}x\right)^{1/2}, \tag{5.10}$$

where u_e is the exact solution. The error is of particular interest when studying convergence properties of finite element methods. Other times, we may instead be interested in computing the flux out through a part Γ of the boundary $\partial\Omega$,

$$F = -\int_\Gamma \kappa\nabla u \cdot n\,\mathrm{d}s, \tag{5.11}$$

where n is an outward unit normal at Γ and κ is a coefficient (see the problem in Section 5.3 for a specific example).

All these functionals are easy to compute with FEniCS, as we shall see in the examples below.

Energy functional. The integrand of the energy functional (5.9) 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 functional `energy` is evaluated by calling the `assemble` function that we have previously used to assemble matrices and vectors. FEniCS will recognize that the form has "rank 0" (since it contains no trial and test functions) and return the result as a scalar value.

Error functional. Computing the functional (5.10) can be done as follows: by

```
error = (u_e - u)**2*dx
E = sqrt(abs(assemble(error)))
```

The exact solution u_{e} is here in a `Function` or `Expression` object `u_e`, while `u` is the finite element approximation (and thus a `Function`). 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 demonstrated in Section 5.3.4, the integration of `(u_e - u)**2*dx` can result in too optimistic convergence rates unless one is careful how `u_e` is transferred onto a mesh. The general recommendation for reliable error computation is to use the `errornorm` function (see `help(errornorm)` and Section 5.3.4 for more information):

```
E = errornorm(u_e, u)
```

Flux Functional. To compute flux integrals like $F = -\int_\Gamma \kappa \nabla u \cdot n \,\mathrm{d}s$, we need to define the 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 = -k*dot(grad(u), n)*ds
total_flux = assemble(flux)
```

Although `grad(u)` and `nabla_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 `nabla_grad(u)` we must in that case write `dot(n, nabla_grad(u))`.

It is possible to restrict the integration to a part of the boundary by using a mesh function to mark the relevant part, as explained in Section 4.4. Assuming that the part corresponds to subdomain number `i`, the relevant syntax for the variational formulation of the flux is `-k*dot(grad(u), n)*ds(i)`.

5.3.4 Computing convergence rates

A central question for any numerical method is its *convergence rate*: how fast does the error approach zero when the resolution is increased? For finite element methods, this typically corresponds to proving, theoretically or empirically, that the error $e = u_{\mathrm{e}} - u$ is bounded by the mesh size h to some power r; that is, $\|e\| \leq Ch^r$ for some constant C. The number r is called the *convergence rate* of the method. Note that different norms, like the L^2-norm $\|e\|$ or H_0^1-norm $\|\nabla e\|$ typically have different convergence rates.

To illustrate how to compute errors and convergence rates in FEniCS, we have included the function `convergence_rate` in `ft11_poisson_bcs.py`. This is a tool that is very handy when verifying finite element codes and will therefore be explained in detail here.

Computing error norms. As we have already seen, the L^2-norm of the error $\boldsymbol{u}_e - u$ can be implemented in FEniCS by

```
error = (u_e - u)**2*dx
E = sqrt(abs(assemble(error)))
```

As above, we have used `abs` in the expression for `E` above to ensure a positive value for the `sqrt` function.

It is important to understand how FEniCS computes the error from the above code, since we may otherwise run into subtle issues when using the value for computing convergence rates. The first subtle issue is that if `u_e` is not already a finite element function (an object created using `Function(V)`), which is the case if `u_e` is defined as an `Expression`, FEniCS must interpolate `u_e` into some local finite element space on each element of the mesh. The degree used for the interpolation is determined by the mandatory keyword argument to the `Expression` class, for example:

```
u_e = Expression('sin(x[0])', degree=1)
```

This means that the error computed will not be equal to the actual error $\|u_{\mathrm{e}} - u\|$ but rather the difference between the finite element solution u and the piecewise linear interpolant of u_{e}. This may yield a too optimistic (too small) value for the error. A better value may be achieved by interpolating the exact solution into a higher-order function space, which can be done by simply increasing the degree:

```
u_e = Expression('sin(x[0])', degree=3)
```

The second subtle issue is that when FEniCS evaluates the expression `(u_e - u)**2`, this will be expanded into `u_e**2 + u**2 - 2*u_e*u`. If the error is small (and the solution itself is of moderate size), this calculation will correspond to the subtraction of two positive numbers (`u_e**2 + u**2` ~ 1 and `2*u_e*u` ~ 1) yielding a small number. Such a computation is very prone to round-off errors, which may again lead to an unreliable value for the error. To make this situation worse, FEniCS may expand this computation into a large number of terms, in particular for higher order elements, making the computation very unstable.

To help with these issues, FEniCS provides the built-in function `errornorm` which computes the error norm in a more intelligent way. First, both `u_e` and `u` are interpolated into a higher-order function space. Then, the degrees of freedom of `u_e` and `u` are subtracted to produce a new function in the higher-order function space. Finally, FEniCS integrates the square of the difference function to get the value of the error norm. Using the `errornorm` function is simple:

```
E = errornorm(u_e, u, normtype='L2')
```

It is illustrative to look at a short implementation of `errornorm`:

```
def errornorm(u_e, u):
    V = u.function_space()
    mesh = V.mesh()
    degree = V.ufl_element().degree()
    W = FunctionSpace(mesh, 'P', degree + 3)
    u_e_W = interpolate(u_e, W)
    u_W = interpolate(u, W)
    e_W = Function(W)
    e_W.vector()[:] = u_e_W.vector().array() - u_W.vector().array()
    error = e_W**2*dx
    return sqrt(abs(assemble(error)))
```

Sometimes it is of interest to compute the error of the gradient field: $||\nabla(u_{\mathrm{e}} - u)||$, often referred to as the H_0^1 or H^1 seminorm of the error. This can either be expressed as above, replacing the expression for `error` by `error = dot(grad(e_W), grad(e_W))*dx`, or by calling `errornorm` in FEniCS:

```
E = errornorm(u_e, u, norm_type='H10')
```

Type `help(errornorm)` in Python for more information about available norm types.

The function `compute_errors` in `ft11_poisson_bcs.py` illustrates the computation of various error norms in FEniCS.

Computing convergence rates. Let's examine how to compute convergence rates in FEniCS. The `solver` function in `ft11_poisson_bcs.py` allows us to easily compute solutions for finer and finer meshes and enables us to study the convergence rate. Define the element size $h = 1/n$, where n is the

number of cell divisions in the x and y directions (`n=Nx=Ny` in the code). We perform experiments with $h_0 > h_1 > h_2 > \cdots$ and compute the corresponding errors E_0, E_1, E_2 and so forth. Assuming $E_i = Ch_i^r$ for unknown constants C and r, we can compare two consecutive experiments, $E_{i-1} = Ch_{i-1}^r$ and $E_i = Ch_i^r$, 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 (typically the polynomial degree + 1 for the L^2-error) as i increases.

The procedure above can easily be turned into Python code. Here we run through a list of element degrees (P_1, P_2, P_3, and P_4), 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, u_D, kappa):
    """
    Compute convergence rates for various error norms for a
    sequence of meshes and elements.
    """

    h = {}  # discretization parameter: h[degree][level]
    E = {}  # error measure(s): E[degree][level][error_type]
    degrees = 1, 2, 3, 4
    num_levels = 5

    # Iterate over degrees and mesh refinement levels
    for degree in degrees:
        n = 4  # coarsest mesh division
        h[degree] = []
        E[degree] = []
        for i in range(num_levels):
            n *= 2
            h[degree].append(1.0 / n)
            u = solver(kappa, f, u_D, n, n, degree,
                       linear_solver='direct')
            errors = compute_errors(u_exact, u)
            E[degree].append(errors)
            print('2 x (%d x %d) P%d mesh, %d unknowns, E1=%g' %
                  (n, n, degree, u.function_space().dim(),
                   errors['u - u_exact']))

    # Compute 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 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
```

Test problem. To demonstrate the computation of convergence rates, we will pick an exact solution u_{e} given by

$$u_{\mathrm{e}}(x,y) = \sin(\omega\pi x)\sin(\omega\pi y)$$

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 the boundary value is given by $u_{\mathrm{D}} = 0$.

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), 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. An implementation of the computation of the convergence rate can be found in the function `convergence_rate_sin()` in the demo program `ft11_poisson_bcs.py`. We achieve some interesting results. Using the error measure `E5` based on the infinity norm of the difference of the degrees of freedom, we obtain the following table.

element	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
P_1	1.99	1.97	1.99	2.00	2.00
P_2	3.99	3.96	3.99	4.00	3.99
P_3	3.96	3.89	3.96	3.99	4.00
P_4	3.75	4.99	5.00	5.00	

An entry like 3.96 for $n=32$ and P_3 means that we estimate the rate 3.96 by comparing two meshes, with resolutions $n=32$ and $n=16$, using P_3 elements. The coarsest mesh has $n=4$. The best estimates of the rates appear in the right-most column, since these rates are based on the finest resolutions and are hence deepest into the asymptotic regime.

The computations with P_4 elements on a $2\times(128\times128)$ mesh with a direct solver (UMFPACK) on a small laptop broke down so these results have been left out of the table. Otherwise, we achieve expected results: the error goes like h^{d+1} for elements of degree d. Also the L^2-norm errors computed using

the FEniCS `errornorm` function show the expected h^{d+1} rate for u and h^d for ∇u.

However, using `(u_e - u)**2` for the error computation, with the same degree for the interpolation of `u_e` as for `u`, gives strange results:

element	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
P_1	1.98	1.94	1.98	2.0	2.0
P_2	3.98	3.95	3.99	3.99	3.99
P_3	3.69	4.03	4.01	3.95	2.77

This is an example where it is important to interpolate `u_e` 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 5.2.6 and many other places in this tutorial).

5.3.5 Taking advantage of structured mesh data

Many readers have extensive experience with visualization and data analysis of 1D, 2D, and 3D scalar and vector fields on *uniform, structured meshes*, while FEniCS solvers exclusively work with *unstructured* meshes. Since it can many times be practical to work with structured data, we discuss in this section how to extract structured data for finite element solutions computed with FEniCS.

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 book, we have included the Python module `BoxField` that provides utilities for working with structured mesh data in FEniCS. 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
```

AL 1: Comment below needs to be modified if interpolation to P1 is included in `BoxField`.

Note that we can only turn functions on meshes with P_1 elements into `BoxField` objects, so if `u` is based on another element type, we first interpolate the scalar field onto a mesh with P_1 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])`

AL 2: Is something missing in the last line above? The `i` and `j` indices?

Iterating over points and values. Let us go back to the `solver` function in the `ft11_poisson_bcs.py` code from Section 5.3, 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, u_b, nx, ny, 1, linear_solver='direct')
u_box = structured_mesh(u, (nx, ny))
u_ = u_box.values       # numpy array

print('u_ is defined on a structured mesh with %s points' %
      str(u_.shape))

# Iterate over 2D mesh points (i,j)
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]))
```

Computing finite difference approximations. Using the multidimensional array `u_ = u_box.values`, we can easily express finite difference approximations 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
```

Making surface plots. The ability to access a finite element field as structured data is handy in many occasions, e.g., for visualization and data analysis. Using Matplotlib, we can create a surface plot, as shown in Figure 5.1 (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_`.

Making contour plots. 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 5.1 (upper right).

Making curve plots through the domain. A handy feature of `BoxField` objects is the ability to give a starting point in the domain and a direction, and then extract the field and corresponding coordinates along the nearest line of *mesh points*. We have already seen how to interpolate the solution along a line in the mesh, but with `BoxField` you can pick out the computational points (vertices) for examination of these points. Numerical methods often show improved behavior at such points so this is of interest. For 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`, can be extracted by

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

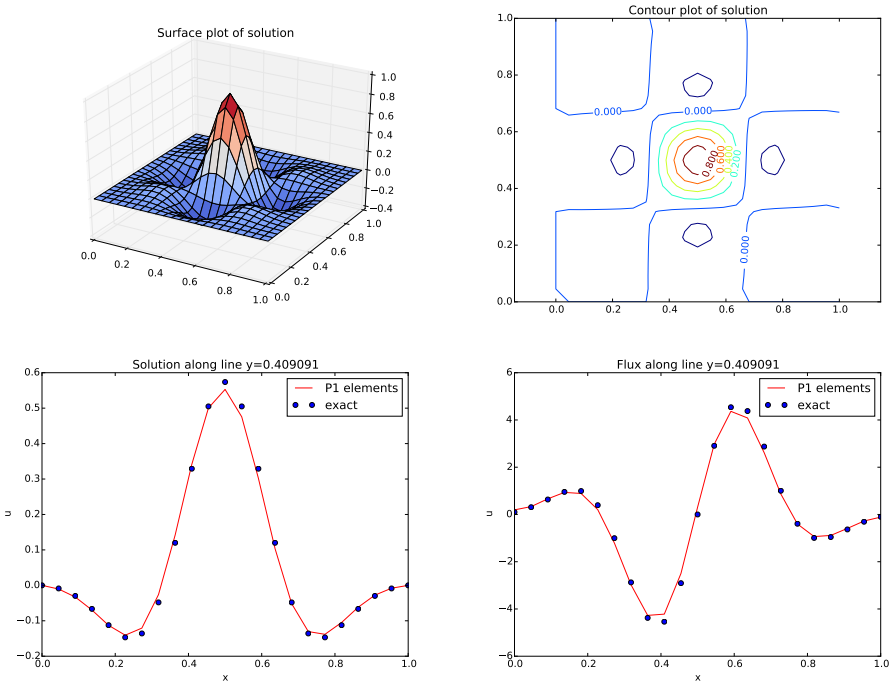


Fig. 5.1 Various plots of the solution on a structured mesh.

The variable `snapped` is true if the line is snapped onto to nearst gridline and in that case `y_fixed` holds the snapped (altered) y value. (A keyword argument `snap` is by default `True` to avoid interpolation and force snapping.)

A comparison of the numerical and exact solution along the line $y \approx 0.41$ (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 = [u_b((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 5.1 (lower left) for the resulting curve plot.

Making curve plots of the flux. Let us also compare the numerical and exact flux $-\kappa \partial u/\partial x$ 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
if flux_u_x.ufl_element().degree() == 1:
   flux2_x = flux_u_x
else:
   V1 = FunctionSpace(u.function_space().mesh(), 'P', 1)
   flux2_x = interpolate(flux_x, V)
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 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 package one can access Matplotlib, Gnuplot, MATLAB, OpenDX, VisIt, and other plotting engines through the same API.

Test problem. The graphics referred to in Figure 5.1 correspond to a test problem with prescribed solution $u_{\mathrm{e}} = H(x)H(y)$, where

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

The corresponding right-hand side f is obtained by inserting the exact solution into the PDE and differentiating as before. 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 3.2.3.

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)
```

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')
u_b = Expression(u_c)
```

Thereafter, we can progress with the computation of $f = -\nabla \cdot (\kappa \nabla u)$:

```
kappa = 1
f = sym.diff(-kappa*sym.diff(u, x), x) + \
    sym.diff(-kappa*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 $-\kappa \partial u/\partial x$:

```
flux_u_x_exact = sym.lambdify([x, y], -kappa*sym.diff(u, x),
                              modules='numpy')
```

It remains to define `kappa = Constant(1)` and set `nx` and `ny` before calling `solver` to compute the finite element solution of this problem.

References

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