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

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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* [20]. This tutorial is a further development of the opening chapter in [20].

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 [20]. We are particularly thankful to Professor Douglas Arnold for very valuable feedback on early versions of the text. ÅYstein SÅyrensen pointed out a lot of typos and contributed with many helpful comments. Many errors and typos were also reported by Mauricio Angeles, Ida DrÅysdal, Miroslav Kuchta, Hans Ekkehard Plessner, Marie Rognes, and Hans Joachim Scroll. Ekkehard Ellmann as well as two anonymous reviewers provided a series of suggestions and improvements.

Oslo, May 2016

Hans Petter Langtangen, Anders Logg

Watch out for shortcomings!

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

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Chapter 1

Preliminaries

1.1 The FEniCS Project

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

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

1.2 What you will learn

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

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

1.3 Working with this tutorial

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

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

1.4 Obtaining the software

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

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

FEniCS download and installation

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

1.4.1 Installation using Docker containers

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

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

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

²<https://www.docker.com>

Terminal

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

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

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

Terminal

```
Terminal> fenicsproject run
```

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

Sharing files with FEniCS containers

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

1.4.2 Installation using Ubuntu packages

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

Terminal

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

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

Watch out for old packages!

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

1.4.3 Testing your installation

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

Terminal

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

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

1.5 Obtaining the tutorial examples

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

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

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

1.6 Background knowledge

1.6.1 Programming in Python

While you can likely pick up basic Python programming by working through the examples in this tutorial, you may want to have some additional material on the language. A natural starting point for beginners is the classical *Python Tutorial* [10], or a tutorial geared towards scientific computing [18]. In the latter, you will also find lots of pointers to other tutorials for scientific computing in Python. Among ordinary books we recommend the general introduction *Dive into Python* [23] as well as texts that focus on scientific computing with Python [13–17].

Python versions

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

```
from __future__ import print_function
```

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

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

1.6.2 The finite element method

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

AL 1: Missing link to fem-book in PDF.

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

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

Readers with a background in the engineering “structural analysis” version of the finite element method may find Bickford [3] as an attractive bridge over to the abstract mathematical formulation that FEniCS builds upon. Those who have a weak background in differential equations in general should consult a more fundamental book, and Eriksson *et al.* [8] is a very good choice. On the other hand, FEniCS users with a strong background in mathematics and interest in the mathematical properties of the finite element method, will appreciate the texts by Brenner and Scott [5], Braess [4], Ern and Guermond [9], Quarteroni and Valli [24], or Ciarlet [6].

AL 2: Add reference to new book by Mats Larson?

Chapter 2

Fundamentals

The goal of this chapter is to show how a range of important PDEs from science and engineering can be quickly solved with a few lines of FEniCS code. We introduce the most fundamental FEniCS objects such as `Mesh`, `Function`, `FunctionSpace`, `TrialFunction`, and `TestFunction`, and learn how to set up the variational formulation of the PDE problem in a way that closely resembles the mathematics.

The code is made as simple as possible, we solve all linear systems by (sparse) Gaussian elimination, we don't use any problem-dependent optimizations of algorithms and code, and we only treat examples taking place in homogeneous media. Subsequent chapters will extend the examples here with more general, efficient, and sophisticated implementations.

2.1 The Poisson equation

2.1.1 Mathematical problem formulation

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

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

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

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

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

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

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

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

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

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

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

2.1.2 Finite element variational formulation

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

The basic recipe for turning a PDE into a variational problem is to multiply the PDE by a function v , integrate the resulting equation over the domain Ω , and perform integration by parts of terms with second-order derivatives. The function v which multiplies the PDE is called a *test function*. The unknown function u to be approximated is referred to as a *trial function*. The terms

test and trial function are used in FEniCS programs too. Suitable function spaces must be specified for the test and trial functions. For standard PDEs arising in physics and mechanics such spaces are well known.

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

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

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

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

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

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

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

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

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

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

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

In short, $H^1(\Omega)$ is the mathematically well-known Sobolev space containing functions v such that v^2 and $|\nabla v|^2$ have finite integrals over Ω (essentially meaning that the functions are continuous). The solution of the underlying PDE must lie in a function space where also the derivatives are continuous, but the Sobolev space $H^1(\Omega)$ allows functions with discontinuous derivatives. This weaker continuity requirement of u in the variational statement (2.7), as

a result of the integration by parts, has great practical consequences when it comes to constructing finite element function spaces. In particular, it allows the use of piecewise polynomial function spaces; i.e., function spaces constructed by stitching together polynomial functions on simple domains such as intervals, triangles, or tetrahedrons.

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

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

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

What we mean by the notation u and V

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

2.1.3 Abstract finite element variational formulation

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

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

For the Poisson equation, we have:

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

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

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

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

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

2.1.4 Choosing a test problem

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

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

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

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

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

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

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

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

A common approach to testing the implementation of a numerical method is to compare the numerical solution with an exact analytical solution of the test problem and conclude that the program works if the error is “small enough”. Unfortunately, it is impossible to tell if an error of size 10^{-5} on a 20×20 mesh of linear elements is the expected (in)accuracy of the numerical approximation or if the error also contains the effect of a bug in the code. All we usually know about the numerical error is its *asymptotic properties*, for instance that it is proportional to h^2 if h is the size of a cell in the mesh. Then we can compare the error on meshes with different h values to see if the asymptotic behavior is correct. This is a very powerful verification technique and is explained in detail in Section 3.3.2. However, if we have a test problem for which we know that there should be no approximation errors, we know that the analytical solution of the PDE problem should be reproduced to machine precision by the program. That is why we emphasize this kind of test problems throughout this tutorial. Typically, elements of degree r can reproduce polynomials of degree r exactly, so this is the starting point for constructing a solution without numerical approximation errors.

2.1.5 FEniCS implementation

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

```
from fenics import *

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

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

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

```

bc = DirichletBC(V, u0, u0_boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Constant(-6.0)
a = dot(grad(u), grad(v))*dx
L = f*v*dx

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

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

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

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

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

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

# Hold plot
interactive()

```

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

2.1.6 Running the program

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

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

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

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

```
Terminal> python ft01_poisson_flat.py
```

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

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

AL 3: Add text here discussing what to expect in terms of plotting. Perhaps we have seamless notebook plotting working soon...

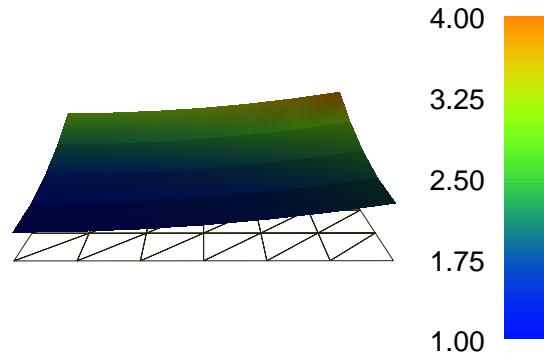


Fig. 2.1 Plot of the solution in the first FEniCS example.

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

Jupyter notebooks. Notebooks make it possible to mix text and executable code in the same document, but you can also just use it to run programs in a web browser. Start `jupyter notebook` from a terminal window, find the **New** pulldown menu in the upper right part of the GUI, choose a new notebook in Python 2 or 3, write `%load ft01_poisson_flat.py` in the blank cell of this notebook, then write Shift+Enter to execute the cell. The file `ft01_poisson_flat.py` will be loaded into the notebook. Re-execute the cell (Shift+Enter) to run the program. You may divide the entire program into several cells to examine intermediate results: place the cursor where you want to split the cell and choose **Edit - Split Cell**.

hpl 4: Need to describe this with more care. The first program seems to have some problems with printing the error to the notebook unless we drop the plot commands. Anyway, there should be in-browser plot commands.

2.1.7 Dissection of the program

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

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

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

```
from fenics import *
```

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

Generating simple meshes. The statement

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

¹<http://docs.python.org/tutorial/>

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.

hpl 5: Note that plot was made by the old partitioning 6×4 . Probably no issue.

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

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

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

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

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

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

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

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

where `u0` is an expression defining the solution values on the boundary, and `u0_boundary` is a function (or object) defining which points belong to the boundary.

²<http://femtable.org>

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

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

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

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

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

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

String expressions must have valid C++ syntax!

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

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

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

is implemented as

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

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

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

At any time, parameters can be updated:

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

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

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

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

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

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

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

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

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

or with the `near` command in FEniCS:

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

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

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

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

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

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

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

In essence, these two lines specify the PDE to be solved. Note the very close correspondence between the Python syntax and the mathematical formulas $\nabla u \cdot \nabla v dx$ and $f v dx$. This is a key strength of FEniCS: the formulas in the variational formulation translate directly to very similar Python code, a feature that makes it easy to specify and solve complicated PDE problems. The language used to express weak forms is called UFL (Unified Form Language) [1, 20] and is an integral part of FEniCS.

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

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

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

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

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

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

Figure 2.1 displays the resulting u function.

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

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

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

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

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

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 `u0`, which in this example happens to be the same as the `Expression` used to set the boundary conditions. We compute the error in two different ways. First, we compute the L^2 norm of the error, defined by

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

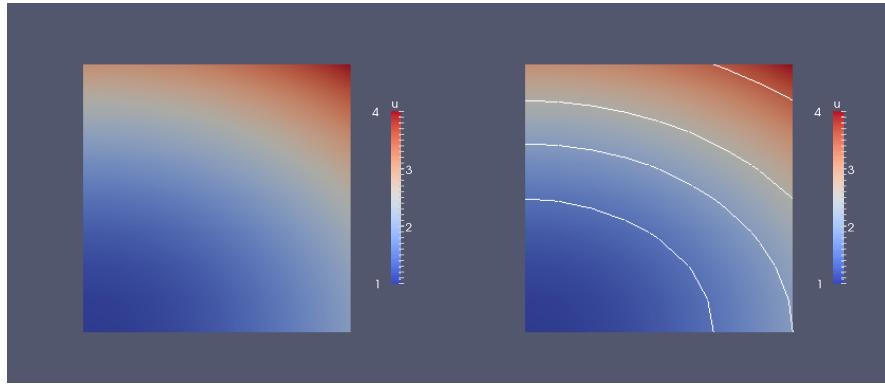


Fig. 2.2 Visualization of test problem in ParaView, with contour lines added in the right plot.

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

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

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

We also compute the maximum value of the error at all the vertices of the finite element mesh. As mentioned above, we expect this error to be zero to within machine precision for this particular example. To compute the error at the vertices, we first ask FEniCS to compute the value of both `u0` and `u` at all vertices, and then subtract the results:

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

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

How to check that the error vanishes?

With inexact arithmetics, as we always have on a computer, the maximum error at the vertices is not zero, but should be a small number. The machine precision is about 10^{-16} , but in finite element calculations, rounding errors of this size may accumulate, to produce an error larger than 10^{-16} . Experiments show that increasing the number of elements

and increasing the degree of the finite element polynomials increases the error. For a mesh with $2 \times (20 \times 20)$ cubic Lagrange elements (degree 3) the error is about $2 \cdot 10^{-12}$, while for 81 linear elements the error is about $2 \cdot 10^{-15}$.

2.1.8 Degrees of freedom and vertex values

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

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

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

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

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

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

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

With `numpy` arrays we can write MATLAB-like code to analyze the data. Indexing is done with square brackets: `u_array[j]`, where the index j always starts at 0. If the solution is computed with piecewise linear Lagrange elements (P_1), then the size of the array `u_array` is equal to the number of vertices, and each `u[j]` is the value at some vertex in the mesh. However, the degrees of freedom are not necessarily numbered in the same way as the vertices of the mesh, see Section 3.2.3 for details. If we therefore want to know the values at the vertices, we need to call the function `u.compute_vertex_values()`. This function returns the values at all the

vertices of the mesh as a `numpy` array with the same numbering as for the vertices of the mesh, for example:

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

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

2.2 Deflection of a membrane

AL 6: I AM HERE

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

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

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

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

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

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

2.2.1 Scaling

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

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

where

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

With an appropriate scaling, \bar{w} and its derivatives are of size unity, so the left-hand side of the scaled PDE is about unity in size, while the right-hand side has α as its characteristic size. This suggest choosing α to be unity, or around unit. We shall in particular choose $\alpha = 4$. With this value, the solution is $w(\bar{x}, \bar{y}) = 1 - \bar{x}^2 - \bar{y}^2$. (One can also find the analytical solution in scaled coordinates and show that the maximum deflection $D(0,0)$ is D_c if we choose $\alpha = 4$ to determine D_c .) With $D_c = AR^2/(8\pi\sigma T)$ and dropping the bars we get the scaled problem

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

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

Given a computed w , the physical deflection is given by

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

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

2.2.2 Defining the mesh

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

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

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

2.2.3 Defining the load

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

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

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

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

2.2.4 Variational form

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

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

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

2.2.5 Visualization

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

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

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

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

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

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

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

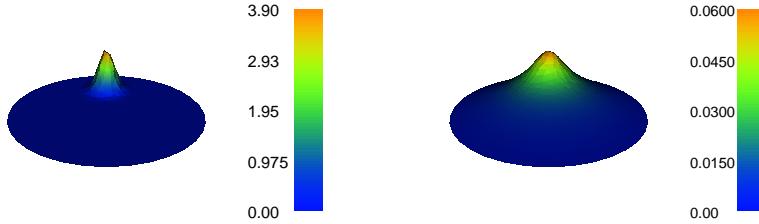


Fig. 2.3 Load (left) and resulting deflection (right) of a circular membrane.

2.2.6 Curve plots through the domain

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

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

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

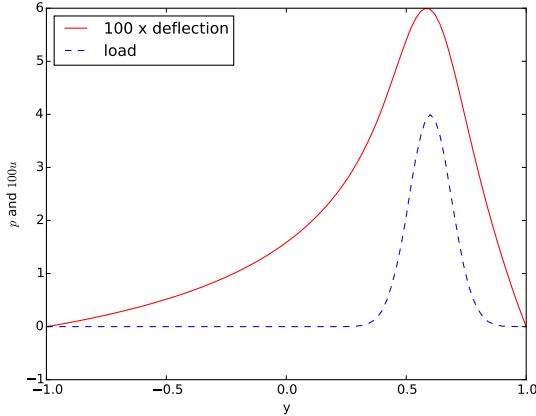


Fig. 2.4 Comparison of membrane load and deflection.

2.2.7 Running ParaView

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

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

1. Start the ParaView application.
2. Open a file with **File - Open....** You will see a list of `.pvd` and `.vtu` files. More specifically you see `membrane_deflection.pvd`. Choose this file.
3. Click on **Apply** to the left (*Properties* pane) in the GUI, and ParaView will visualize the contents of the file, here as a color image.
4. To get rid of the axis in the lower left corner of the plot area and axis cross in the middle of the circle, find the *Show Orientation Axis* and *Show Center* buttons to the right in the second row of buttons at the top of the GUI. Click on these buttons to toggle axis information on/off.

³<http://www.paraview.org>

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

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 [25] (free PDF available) and to the ParaView tutorial⁴ as well as an instruction video⁵.

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

⁵<https://vimeo.com/34037236>

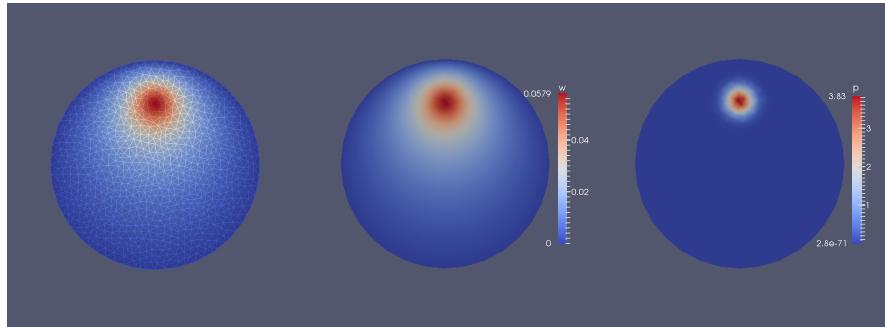


Fig. 2.5 Default visualizations in ParaView: deflection (left, middle) and pressure load (right).

2.2.8 Using the built-in visualization tool

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

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

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

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

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

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

```
plot(f, hardcopy_prefix='pressure').
```

Plots stored in PDF format need to be rotated 90 degrees before inclusion in documents. This can be done by the `convert -rotate 90` command (from the ImageMagick utility), but the resulting file has then no more high-

resolution PDF vector graphics. A better solution is therefore to use `pdftk` to preserve the vector graphics:

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

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

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

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

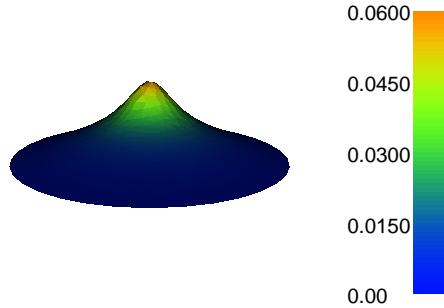


Fig. 2.6 Plot of the deflection of a membrane.

2.3 The time-dependent diffusion equation

The examples in Section 2.1.5 illustrate that solving linear, stationary PDE problems with the aid of FEniCS is easy and requires little programming. FEniCS clearly automates the spatial discretization by the finite element method. One can use a separate, one-dimensional finite element method in the domain as well, but very often, it is easier to just use a finite difference

method, or to formulate the problem as an ODE system and leave the time-stepping to an ODE solver.

hpl 7: Should exemplify all three approaches? With emphasis on simple finite differences?

2.3.1 Variational formulation

Our model problem for time-dependent PDEs reads

$$\frac{\partial u}{\partial t} = \nabla^2 u + f \text{ in } \Omega, \quad (2.17)$$

$$u = u_0 \text{ on } \partial\Omega, \quad (2.18)$$

$$u = I \text{ at } t = 0. \quad (2.19)$$

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

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

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

$$\frac{\partial}{\partial t} u^k = \nabla^2 u^k + f^k. \quad (2.20)$$

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

$$\frac{\partial}{\partial t} u^k \approx \frac{u^k - u^{k-1}}{\Delta t}, \quad (2.21)$$

where Δt is the time discretization parameter. Inserting (2.21) in (2.20) yields

$$\frac{u^k - u^{k-1}}{\Delta t} = \nabla^2 u^k + f^k. \quad (2.22)$$

This is our time-discrete version of the diffusion PDE (2.17).

We may reorder (2.22) so that the left-hand side contains the terms with the unknown u^k and the right-hand side contains computed terms only. The

result is a recursive set of spatial (stationary) problems for u^k (assuming u^{k-1} is known from computations at the previous time level):

$$u^0 = I, \quad (2.23)$$

$$u^k - \Delta t \nabla^2 u^k = u^{k-1} + \Delta t f^k, \quad k = 1, 2, \dots \quad (2.24)$$

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

An alternative to (2.24), which can be convenient in implementations, is to collect all terms on one side of the equality sign:

$$F(u; v) = u^k - \Delta t \nabla^2 u^k - u^{k-1} - \Delta t f^k = 0, \quad k = 1, 2, \dots \quad (2.25)$$

We use a finite element method to solve (2.23) and either of the equations (2.24) or (2.25). This requires turning the equations into weak forms. As usual, we multiply by a test function $v \in \hat{V}$ and integrate second-derivatives by parts. Introducing the symbol u for u^k (which is natural in the program), the resulting weak form arising from formulation (2.24) can be conveniently written in the standard notation:

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

where

$$a(u, v) = \int_{\Omega} (uv + \Delta t \nabla u \cdot \nabla v) \, dx, \quad (2.26)$$

$$L(v) = \int_{\Omega} (u^{k-1} + \Delta t f^k) v \, dx. \quad (2.27)$$

The alternative form (2.25) has an abstract formulation

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

where

$$F = \int_{\Omega} \left(uv + \Delta t \nabla u \cdot \nabla v - (u^{k-1} - \Delta t f^k) v \right) \, dx. \quad (2.28)$$

The initial condition (2.23) can also be turned into a weak form,

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

with

$$a_0(u, v) = \int_{\Omega} uv \, dx, \quad (2.29)$$

$$L_0(v) = \int_{\Omega} Iv \, dx. \quad (2.30)$$

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

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

Approximate solutions in space are found by restricting the functional spaces V and \hat{V} to finite-dimensional spaces, exactly as we have done in the Poisson problems. We shall use the symbol u for the finite element approximation at time t_k . In case we need to distinguish this space-time discrete approximation from the exact solution of the continuous diffusion problem, we use u_e for the latter. By u^{k-1} we mean the finite element approximation of the solution at time t_{k-1} .

Instead of solving (2.23) by a finite element method, i.e., projecting I onto V via the problem $a_0(u, v) = L_0(v)$, we could simply interpolate u^0 from I . That is, if $u^0 = \sum_{j=1}^N U_j^0 \phi_j$, we simply set $U_j = I(x_j, y_j)$, where (x_j, y_j) are the coordinates of node number j . We refer to these two strategies as computing the initial condition by either projecting I or interpolating I . Both operations are easy to compute through one statement, using either the `project` or `interpolate` function.

2.3.2 A simple implementation

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

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

$$u = 1 + x^2 + \alpha y^2 + \beta t, \quad (2.31)$$

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 (2.31) in the PDE problem (2.17), it follows that u_0 must be given as (2.31) and that $f(x, y, t) = \beta - 2 - 2\alpha$ and $I(x, y) = 1 + x^2 + \alpha y^2$.

The code. A new programming issue is how to deal with functions that vary in space *and time*, such as the boundary condition u_0 given by (2.31). A natural solution is to apply an `Expression` object with time t as a parameter, in addition to the parameters α and β :

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

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

```
u0.t = t
```

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

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

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

We shall use `u` for the unknown u at the new time level and `u_1` for u at the previous time level. The initial value of `u_1`, implied by the initial condition on u , can be computed by either projecting or interpolating I . The $I(x,y)$ function is available in the program through `u0`, as long as `u0.t` is zero. We can then do

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

Projecting versus interpolating the initial condition

To actually recover the exact solution (2.31) to machine precision, it is important not to compute the discrete initial condition by projecting I , but by interpolating I so that the degrees of freedom have exact values at $t = 0$ (projection results in approximative values at the nodes).

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

```
dt = 0.3      # time step

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

```
f = Constant(beta - 2 - 2*alpha)

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

Finally, we perform the time stepping in a loop:

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

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

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

Remember to update expression objects with the current time!

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

The time loop above does not contain any comparison of the numerical and the exact solution, which we must include in order to verify the implementation. As in the Poisson equation example in Section 2.1.7, we compute the difference between the array of nodal values of `u` and the array of the interpolated exact solution. The following code is to be included inside the loop, after `u` is found:

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

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

```
from fenics import *
import numpy as np

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

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

```

        alpha=alpha, beta=beta, t=0)

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, boundary)

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

dt = 0.3      # time step

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

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

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

    # Verify
    u_e = interpolate(u0, V)
    error = np.abs(u_e.vector().array() -
                   u.vector().array()).max()
    print('error, t=% .2f: %-.3g' % (t, error))

    t += dt
    u_1.assign(u)

```

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

2.3.3 Diffusion of a Gaussian function

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

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

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

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

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

The complete program appears below.

```
from fenics import *
import time

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

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

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

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

dt = 0.01      # time step

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

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

# Compute solution
u = Function(V)          # the unknown at a new time level
```

```

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

    t += dt
    u_1.assign(u)

```

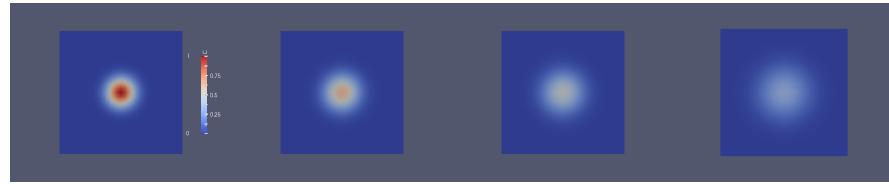
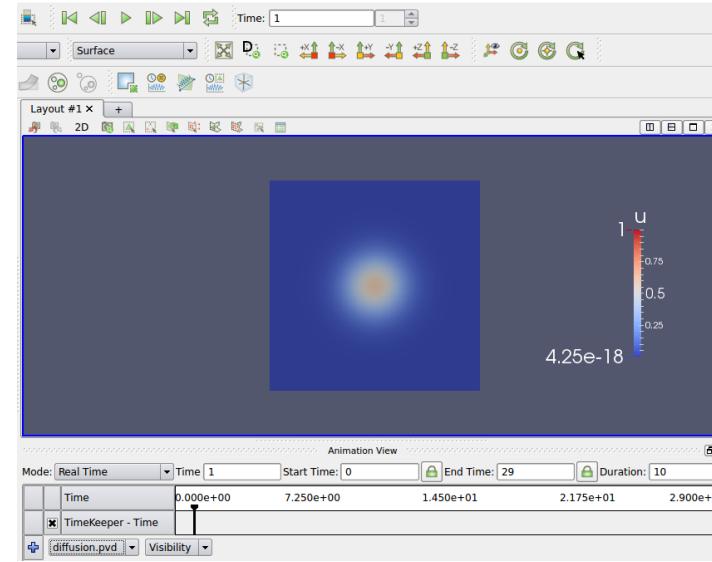
Visualization in ParaView. Start ParaView, choose **File - Open**, open the file `diffusion.pvd`, click the green **Apply** button on the left to see the initial condition being plotting. Choose **View - Animation View**. Click on the play button or (better) the next frame button in the row of buttons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



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



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



2.4 A nonlinear Poisson equation

2.4.1 Variational formulation

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

$$-\nabla \cdot (q(u) \nabla u) = f, \quad (2.32)$$

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

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

$$F(u; v) = 0 \quad \forall v \in \hat{V}, \quad (2.33)$$

where

$$F(u;v) = \int_{\Omega} (q(u)\nabla u \cdot \nabla v + fv) dx, \quad (2.34)$$

and

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

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

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

$$F(u;v) = 0 \quad \forall v \in \hat{V}, \quad (2.35)$$

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

2.4.2 A simple implementation

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

```
from fenics import *

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

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

def u0_boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, u0_boundary)

# Define variational problem
u = Function(V)
```

```

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

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

```

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

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

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

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

```

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

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

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

```

Define symbolic coordinates as required in Expression objects

Note that we would normally write `x, y = sym.symbols('x y')`, but if we want the resulting expressions to be valid syntax for `Expression` objects, and then x reads `x[0]` and y must be `x[1]`. This is easily ac-

complished with `sympy` by defining the names of `x` and `y` as `x[0]` and `x[1]: x, y = sym.symbols('x[0] x[1]').`

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

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

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

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

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

```
u0 = Expression(u_code)
```

Similarly, we define the right-hand side function as

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

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

Name clash between `fenics` and program variables

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

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

The current example shows how easy it is to solve a nonlinear problem in FEniCS. However, experts on numerical solution of nonlinear PDEs know very well that automated procedures may fail in nonlinear problems, and that

it is often necessary to have much more manual control of the solution process than what we have in the current case. Therefore, we return to this problem in Chapter 5 and show how we can implement our own solution algorithms for nonlinear equations and also how we can steer the parameters in the automated Newton method used above. You will then realize how easy it is to implement tailored solution strategies for nonlinear problems in FEniCS.

2.5 The equations of linear elasticity

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

2.5.1 Variational formulation

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

$$\nabla \cdot \sigma = \varrho f \text{ in } \Omega, \quad (2.36)$$

$$\sigma = \lambda \operatorname{tr} \varepsilon I + 2\mu \varepsilon, \quad (2.37)$$

$$\varepsilon = \frac{1}{2} (\nabla u + (\nabla u)^T), \quad (2.38)$$

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

We shall combine (2.37) and (2.38) to

$$\sigma = \lambda \nabla \cdot u I + \mu (\nabla u + (\nabla u)^T). \quad (2.39)$$

Note that (2.36)-(2.38) can easily be transformed to a vector PDE for u , which is the governing PDE for the unknown u . In the derivation of the variational formulation, however, the splitting of the equations as done above is convenient.

The variational formulation of (2.36)-(2.38) consists of forming the inner product of (2.36) and a *vector* test function $v \in \hat{V}$, where \hat{V} is a test vector function space, and integrating over the domain Ω :

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

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

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

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

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

Inserting (2.39) for σ gives the variational form with u as unknown.

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

$$a(u, v) = L(v) \quad \forall v \in \hat{V}, \quad (2.40)$$

where

$$a(u, v) = \int_{\Omega} \sigma(u) : \nabla v \, dx, \quad (2.41)$$

$$\sigma(u) = \lambda \nabla \cdot u I + \mu (\nabla u + (\nabla u)^T), \quad (2.42)$$

$$L(v) = - \int_{\Omega} \varrho f \cdot v \, dx + \int_{\partial\Omega_T} T \cdot v \, ds. \quad (2.43)$$

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

$$a(u, v) = \int_{\Omega} \sigma(u) : \varepsilon(v) \, dx, \quad (2.44)$$

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

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

2.5.2 A simple implementation

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

Let us scale the problem. **hpl 8:** This was meant to simplify the problem so we don't need values for λ , μ , ϱ , etc for a specific material, but the scaling requires some care. In the equation for u , arising from inserting (2.37) and (2.38) in (2.36),

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

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

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

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

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

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

Code. hpl 9: Must explain the code. New concepts here, though not many.

```
from fenics import *

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

```

mu = beta
g = gamma

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

# Define boundary conditions
tol = 1E-14

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

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

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

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

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

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

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

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

```

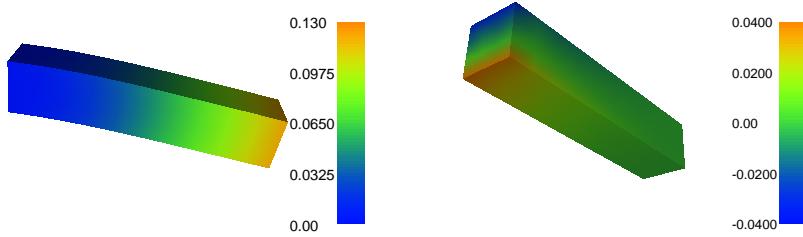


Fig. 2.7 Gravity-induced deformation of a clamped beam: deflection (left) and stress intensity (right).

2.6 The Navier–Stokes equations

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

2.6.1 Variational formulation

2.6.2 A simple implementation

Chapter 3

The Poisson solver revisited

hpl 10: I don't like this title, but have no other good alternative...

3.1 Refactored implementation

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

3.1.1 A general solver function

We consider the flat program developed in Section 2.1.5. Some of the code in this program is needed to solve any Poisson problem $-\nabla^2 u = f$ on $[0, 1] \times [0, 1]$ with $u = u_0$ on the boundary, while other statements arise from our simple test problem. Let us collect the general, reusable code in a function `solver`. Our special test problem will then just be an application of `solver` with some additional statements. We limit the `solver` function to just *compute the numerical solution*. Plotting and comparing the solution with the exact solution are considered to be problem-specific activities to be performed elsewhere.

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

```
from fenics import *

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

    def u0_boundary(x, on_boundary):
        return on_boundary

    bc = DirichletBC(V, u0, u0_boundary)

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

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

    return u
```

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

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

Make a module! The refactored code is put in a file `ft04_poisson_func.py`. We should make sure that such a file can be imported (and hence reused)

in other programs. Then all statements in the main program should appear with a test `if __name__ == '__main__':`. This test is true if the file is executed as a program, but false if the file is imported. If we want to run this file in the same way as we can run `ft04_poisson_func.py`, the main program is simply a call to `application_test()` followed by a call `interactive()` to hold the plot:

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

3.1.2 Verification and unit tests

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

Mathematically, our unit test is that the finite element solution of our problem when $f = -6$ equals the exact solution $u = u_0 = 1 + x^2 + 2y^2$. We have already created code that finds the maximum error in the numerical solution. Because of rounding errors, we cannot demand this maximum error to be zero, but we have to use a tolerance, which depends to the number of elements and the degrees of the polynomials in the finite element basis functions. In Section 2.1.7 we reported some experiments with the size of the maximum error. If we want to test that `solver` works for meshes up to $2(20 \times 20)$ elements and cubic Lagrange elements, 10^{-11} is an appropriate tolerance for testing that the maximum error vanishes.

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

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

Regarding the last point, `success` is a boolean expression that is `False` if the test fails, and in that case the string `msg` is written to the screen. When the

test fails, `assert` raises an `AssertionError` exception in Python, otherwise the statement runs silently. The `msg` string is optional, so `assert success` is the minimal test. In our case, we will do `assert max_error < tol`, where `tol` is the tolerance (10^{-11}) mentioned above.

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

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

We can at any time run

Terminal

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

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

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

Tip: Print messages in test functions

The `assert` statement runs silently when the test passes so users may become uncertain if all the statements in a test function are really executed. A psychological help is to print out something before `assert` (as we do in the example above) such that it is clear that the test really

takes place. (Note that `py.test` needs the `-s` option to show printout from the test functions.)

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

3.2 Useful extensions

hpl 11: Need a little intro.

3.2.1 Controlling the solution process

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

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

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

```
solver_parameters=dict(linear_solver='gmres',
                      preconditioner='ilu'))
```

Section 6.4.4 lists the most popular choices of Krylov solvers and preconditioners available in FEniCS.

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

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

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

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

```
list_linear_algebra_backends()
```

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

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

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

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

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

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

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

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

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

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

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

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

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

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

```
from fenics import *

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

    def u0_boundary(x, on_boundary):
        return on_boundary

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

```

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

# Compute solution
u = Function(V)

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

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

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

    def u0_boundary(x, on_boundary):
        return on_boundary

    bc = DirichletBC(V, u0, u0_boundary)

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

    # Compute solution
    u = Function(V)

```

```

problem = LinearVariationalProblem(a, L, u, bc)
solver = LinearVariationalSolver(problem)

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

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

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

3.2.2 Linear variational problem and solver objects

The `solve(a == L, u, bc)` call is just a compact syntax alternative to a slightly more comprehensive specification of the variational equation and the solution of the associated linear system. This alternative syntax is used in a

lot of FEniCS applications and will also be used later in this tutorial, so we show it already now:

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

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

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

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

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

3.2.3 Writing out the discrete solution

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

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

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

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

```
>>> from fenics import *
>>>
```

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

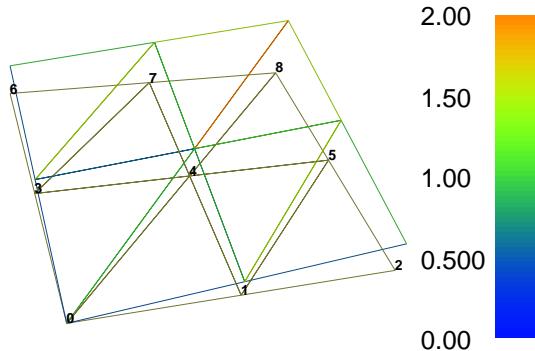
We see from this output that vertices are first numbered along $y = 0$ with increasing x coordinate, then along $y = 0.5$, and so on.

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

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

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

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



Already in Section 2.1.7 we explained that the vertex values of a `Function` object can be extracted `u.compute_vertex_values()`, which returns an array where element `i` is the value of `u` at vertex `i`:

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

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

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

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

For Lagrange elements of degree larger than 1, there are degrees of freedom (nodes) that do not correspond to vertices. **hpl 12:** Anders, is the following true? There is no simple way of getting the coordinates associated with the non-vertex degrees of freedom, so if we want to write out the values of a finite element solution, the following code snippet does the task at the vertices, and this will work for all kinds of Lagrange elements.

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

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

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

Cheap vs expensive function evaluation

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

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

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

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

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

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

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

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

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

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

That is, we manipulate `u_array` as desired, and then we insert this array into `u`'s `Vector` object. The `/=` operator implies an in-place modification of the object on the left-hand side: all elements of the `u_array` are divided by

the value `max_u`. Alternatively, one could write `u_array = u_array/max_u`, which implies creating a new array on the right-hand side and assigning this array to the name `u_array`.

Be careful when manipulating degrees of freedom

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

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

3.2.4 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_flat.py` or `ft04_poisson_func.py` and change the mesh construction from `UnitSquareMesh(6, 4)` to `UnitCubeMesh(6, 4, 5)`. Now the domain is the unit cube partitioned into $6 \times 4 \times 5$ boxes, and each box is divided into six tetrahedra-shaped finite elements for computations. Run the program and observe that we can solve a 3D problem without any other modifications (!). The visualization allows you to rotate the cube and observe the function values as colors on the boundary.

Generating a hypercube. The syntax for generating a unit interval, square, or box is different, so we need to encapsulate this part of the code. Given a list or tuple with the divisions into cells in the various spatial direction, the following function returns the mesh in a d -dimensional problem:

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

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

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

is equivalent to

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

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

3.2.5 Computing derivatives

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

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

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

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

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

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

Figure 3.1 shows example of how such a smoothed `gradu(u)` vector field is visualized.

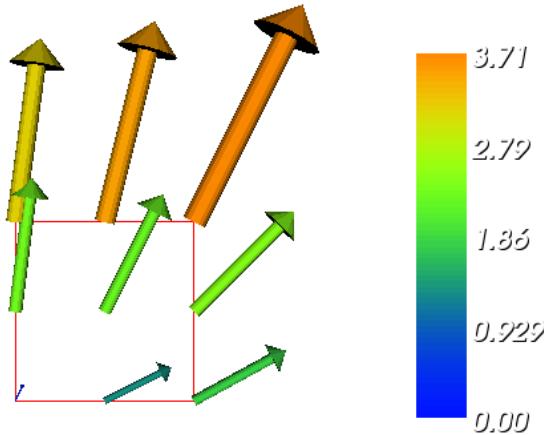


Fig. 3.1 Example of visualizing the vector field ∇u by arrows at the nodes.

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

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

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

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

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

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

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

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

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

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

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

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

Detour: Manual projection.

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

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

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

$$a(w, v) = L(v) \quad \forall v \in V^{(\hat{g})}, \quad (3.1)$$

where

$$a(w, v) = \int_{\Omega} w \cdot v \, dx, \quad (3.2)$$

$$L(v) = \int_{\Omega} \nabla u \cdot v \, dx. \quad (3.3)$$

The function spaces $V^{(g)}$ and $V^{(\hat{g})}$ (with the superscript g denoting “gradient”) are vector versions of the function space for u , with bound-

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

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

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

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

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

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

3.2.6 A variable-coefficient Poisson problem

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

$$\begin{aligned} -\nabla \cdot [p(x, y) \nabla u(x, y)] &= f(x, y) \quad \text{in } \Omega, \\ u(x, y) &= u_0(x, y) \quad \text{on } \partial\Omega. \end{aligned} \tag{3.4}$$

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

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

Modifications of the PDE solver. What are the modifications we need to do in the previously shown codes to incorporate the variable coefficient p ? from Section 3.2.3?

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

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

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

The function spaces for u and v are the same as in Section 2.1.2, implying that the boundary integral vanishes since $v = 0$ on $\partial\Omega$ where we have Dirichlet conditions. The weak form $a(u, v) = L(v)$ then has

$$a(u, v) = \int_{\Omega} p \nabla u \cdot \nabla v \, dx, \quad (3.5)$$

$$L(v) = \int_{\Omega} f v \, dx. \quad (3.6)$$

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

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

by

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

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

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

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

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

Modifications of the flux computations. The flux $-p \nabla u$ may be of particular interest in variable-coefficient Poisson problems as it often has an interesting physical significance. As explained in Section 3.2.5, we normally want the piecewise discontinuous flux or gradient to be approximated by a continuous vector field, using the same elements as used for the numerical solution u . The approximation now consists of solving $w = -p \nabla u$ by a finite element method: find $w \in V^{(g)}$ such that

$$a(w, v) = L(v) \quad \forall v \in V^{\hat{g}}, \quad (3.7)$$

where

$$a(w, v) = \int_{\Omega} w \cdot v \, dx, \quad (3.8)$$

$$L(v) = \int_{\Omega} (-p \nabla u) \cdot v \, dx. \quad (3.9)$$

This problem is identical to the one in Section 3.2.5, except that p enters the integral in L .

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

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

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

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

def application_test_flux(Nx=6, Ny=4):
    u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
    p = Expression('x[0] + x[1]')
    f = Expression('-8*x[0] - 10*x[1]')
    u = solver(p, f, u0, Nx, Ny, 1, linear_solver='direct')
    u.rename('u', 'solution')
    flux_u = flux(u, p)
    # Grab each component as a scalar field
    flux_u_x, flux_u_y = flux_u.split(deepcopy=True)
    flux_u_x.rename('flux(u)_x', 'x-component of flux(u)')
    flux_u_y.rename('flux(u)_y', 'y-component of flux(u)')
    plot(u, title=u.label())
    plot(flux_u, title=flux_u.label())
    plot(flux_u_x, title=flux_u_x.label())
    plot(flux_u_y, title=flux_u_y.label())

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

    coor = u.function_space().mesh().coordinates()
    if len(coor) < 50:
        # Quite large errors for coarse meshes, but the error
        # decreases with increasing resolution
```

```

for i, value in enumerate(flux_u_x.compute_vertex_values()):
    print('vertex %d, %s, -p*u_x=%g, error=%g' %
          (i, tuple(coor[i]), value,
           flux_x_exact(*coor[i]) - value))
for i, value in enumerate(flux_u_y.compute_vertex_values()):
    print('vertex %d, %s, -p*u_y=%g, error=%g' %
          (i, tuple(coor[i]), value,
           flux_y_exact(*coor[i]) - value))
else:
    # Compute integrated L2 error of the flux components
    # (Will this work for unstructured mesh? Need to think about that)
    xv = coor.T[0]
    yv = coor.T[1]

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

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

    V = u.function_space()

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

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

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

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

```

```

        error = e_Ve**2*dx(Ve.mesh())
        return sqrt(abs(assemble(error))), e_Ve
E4, e_Ve = errornorm(u_exact, u, Ve)

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

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

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

return errors

def convergence_rate(u_exact, f, u0, p, degrees,
                     n=[2**(k+3) for k in range(5)]):
    """
    Compute convergence rates for various error norms for a
    sequence of meshes with Nx=Ny=b and P1, P2, ...,
    Pdegrees elements. Return rates for two consecutive meshes:
    rates[degree][error_type] = r0, r1, r2, ...
    """
    h = {} # Discretization parameter, h[degree][experiment]
    E = {} # Error measure(s), E[degree][experiment][error_type]
    P_degrees = 1,2,3,4
    num_meshes = 5

    # Perform experiments with meshes and element types
    for degree in P_degrees:
        n = 4 # Coarsest mesh division
        h[degree] = []
        E[degree] = []
        for i in range(num_meshes):
            n *= 2
            h[degree].append(1.0/n)
            u = solver(p, f, u0, n, n, degree,
                       linear_solver='direct')
            errors = compute_errors(u, u_exact)
            E[degree].append(errors)
            print('2*(%dx%d) P%d mesh, %d unknowns, E1=%g, %'
                  (n, n, degree, u.function_space().dim(),
                   errors['u - u_exact']))
    # Convergence rates
    from math import log as ln # log is a fenics name too
    error_types = list(E[1][0].keys())

```

```

rates = {}
for degree in P_degrees:
    rates[degree] = {}
    for error_type in sorted(error_types):
        rates[degree][error_type] = []
        for i in range(num_meshes):
            Ei = E[degree][i][error_type]
            Eim1 = E[degree][i-1][error_type]
            r = ln(Ei/Eim1)/ln(h[degree][i]/h[degree][i-1])
            rates[degree][error_type].append(round(r,2))
return rates

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

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

def application_structured_mesh(model_problem=1):
    if model_problem == 1:
        # Numerical solution is exact
        u0 = Expression('1 + x[0]*x[0] + 2*x[1]*x[1]')
        p = Expression('x[0] + x[1]')
        f = Expression('-8*x[0] - 10*x[1]')
        flux_u_x_exact = lambda x, y: -(x + y)*2*x
        nx = 6; ny = 4
    elif model_problem == 2:
        # Mexican hat solution
        from sympy import exp, sin, pi  # for use in math formulas
        import sympy as sym

```

```

H = lambda x: exp(-16*(x-0.5)**2)*sin(3*pi*x)
x, y = sym.symbols('x[0], x[1]')
u = H(x)*H(y)
u_c = sym.printing.ccode(u)
# '-exp(-16*pow(x - 0.5, 2) - 16*pow(y - 0.5, 2))',
# 'sin(3*M_PI*x)*sin(3*M_PI*y)'
u_c = u_c.replace('M_PI', 'DOLFIN_PI')
print('u in C:', u_c)
u0 = Expression(u_c)

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

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

# Iterate over 2D mesh points (i,j)
print('u_ is defined on a structured mesh with %s points' %
      str(u_.shape))
if u.function_space().dim() < 100:
    for j in range(u_.shape[1]):
        for i in range(u_.shape[0]):
            print('u[%d,%d]=u(%g,%g)=%g' %
                  (i, j,
                   u_box.grid.coor[X][i], u_box.grid.coor[Y][j],
                   u_[i,j]))

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

# Make contour plot
fig = plt.figure()
ax = fig.gca()

```

```

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

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

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

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

# Plot the numerical and exact flux along the same line
flux2_x = flux_u_x if flux_u_x.ufl_element().degree() == 1 \
    else interpolate(flux_x,
                     FunctionSpace(u.function_space().mesh(),
                                   'P', 1))
flux_u_x_box = structured_mesh(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='best')
plt.title('Flux along line y=%g' % y_fixed)
plt.xlabel('x'); plt.ylabel('u')
plt.savefig('tmp3.png'); plt.savefig('tmp3.pdf')

plt.show()

def solver_linalg(
    p, f, u0, Nx, Ny, degree=1,
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,            # Relative tolerance in Krylov solver
    max_iter=1000,           # Max no of iterations in Krylov solver
    log_level=PROGRESS,      # Amount of solver output
    dump_parameters=False,    # Write out parameter database?
    assembly='variational',  # or 'matvec' or 'system'
    start_vector='zero',     # or 'random'
):
    """
"""

```

```

Solve -div(p*grad(u))=f on [0,1]x[0,1] with 2*Nx*Ny Lagrange
elements of specified degree and u=u0 (Expression) on
the boundary.
"""

# Create mesh and define function space
mesh = UnitSquareMesh(Nx, Ny)
V = FunctionSpace(mesh, 'P', degree)

def u0_boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, u0, u0_boundary)

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

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

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

    solve(a == L, u, bc, solver_parameters=solver_parameters)
    A = None # Cannot return coefficient matrix
else:
    if assembly == 'matvec':
        A = assemble(a)
        b = assemble(L)
        bc.apply(A, b)
        if linear_solver == 'direct':
            solve(A, U, b)
        else:
            solver = KrylovSolver('gmres', 'ilu')

```

```

        prm = solver.parameters
        prm['absolute_tolerance'] = abs_tol
        prm['relative_tolerance'] = rel_tol
        prm['maximum_iterations'] = max_iter
        prm['nonzero_initial_guess'] = True
        solver.solve(A, U, b)
    elif assembly == 'system':
        A, b = assemble_system(a, L, [bc])
        if linear_solver == 'direct':
            solve(A, U, b)
        else:
            solver = KrylovSolver('cg', 'ilu')
            prm = solver.parameters
            prm['absolute_tolerance'] = abs_tol
            prm['relative_tolerance'] = rel_tol
            prm['maximum_iterations'] = max_iter
            prm['nonzero_initial_guess'] = True
            solver.solve(A, U, b)
    return u, A

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

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

```

```

are also allowed.
"""
# Create mesh and define function space
mesh = UnitSquareMesh(Nx, Ny)
V = FunctionSpace(mesh, 'P', degree)

tol = 1E-14

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

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

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

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

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

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

# Mark boundaries
boundary_parts = FacetFunction('size_t', mesh)
boundary_parts.set_all(9999)

```

```

bx0 = BoundaryX0()
bx1 = BoundaryX1()
by0 = BoundaryY0()
by1 = BoundaryY1()
bx0.mark(boundary_parts, 0)
bx1.mark(boundary_parts, 1)
by0.mark(boundary_parts, 2)
by1.mark(boundary_parts, 3)
# boundary_parts.array() is a numpy array

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

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


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

if debug:
    # Print the vertices that are on the boundaries
    coor = mesh.coordinates()
    for x in coor:
        if bx0.inside(x, True): print('%s is on x=0' % x)
        if bx1.inside(x, True): print('%s is on x=1' % x)
        if by0.inside(x, True): print('%s is on y=0' % x)
        if by1.inside(x, True): print('%s is on y=1' % x)

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

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

    Neumann_integrals = []
    for n in boundary_conditions:
        if 'Neumann' in boundary_conditions[n]:
            if boundary_conditions[n]['Neumann'] != 0:

```

```

g = boundary_conditions[n]['Neumann']
Neumann_integrals.append(g*v*ds(n))

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

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

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

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

# Compute solution
u = Function(V)

if linear_solver == 'Krylov':
    prm = parameters['krylov_solver'] # short form
    prm['absolute_tolerance'] = abs_tol
    prm['relative_tolerance'] = rel_tol
    prm['maximum_iterations'] = max_iter
    print(parameters['linear_algebra_backend'])
    set_log_level(log_level)
    if dump_parameters:
        info(parameters, True)
        solver_parameters = {'linear_solver': 'gmres',
                             'preconditioner': 'ilu'}
    else:
        solver_parameters = {'linear_solver': 'lu'}
solve(a == L, u, bcs, solver_parameters=solver_parameters)
return u, p # Note: p may be modified (Function on V0)

def application_bc_test():
    # Define manufactured solution in sympy and derive f, g, etc.
    import sympy as sym
    x, y = sym.symbols('x[0] x[1]') # UFL needs x[0] for x etc.
    u = 1 + x**2 + 2*y**2

```

```

f = -sym.diff(u, x, 2) - sym.diff(u, y, 2) # -Laplace(u)
f = sym.simplify(f)
u_00 = u.subs(x, 0) # x=0 boundary
u_01 = u.subs(x, 1) # x=1 boundary
g = -sym.diff(u, y).subs(y, 1) # x=1 boundary, du/dn=-du/dy
r = 1000 # any function can go here
s = u

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

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

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

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

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

# Print numerical and exact solution at the vertices
if u.function_space().dim() < 50: # (small problems only)
    u_e_at_vertices = u_e.compute_vertex_values()
    u_at_vertices = u.compute_vertex_values()
    coor = u.function_space().mesh().coordinates()

```

```

        for i, x in enumerate(coor):
            print('vertex %2d (%9g,%9g): error=%g %g vs %g'
                  % (i, x[0], x[1],
                      u_e_at_vertices[i] - u_at_vertices[i],
                      u_e_at_vertices[i], u_at_vertices[i]))

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

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

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

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

    for Nx, Ny in [(3,3), (3,5), (5,3), (20,20)]:
        for degree in 1, 2, 3:
            for linear_solver in ['direct']:
                print('solving on 2(%dx%dx) mesh with P%d elements'
                      % (Nx, Ny, degree)),
                print(' %s solver, %s function' %

```

```

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

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

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

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

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

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

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

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

```

```

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

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

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

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

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

    subdomains = [Omega0(), Omega1()]
    p_values = [2.0, 13.0]
    boundary_conditions = {
        0: {'Neumann': 0},
        1: {'Neumann': 0},
        2: {'Dirichlet': Constant(0)}, # y=0
        3: {'Dirichlet': Constant(1)}, # y=1
    }

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

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

    # Compute max error in infinity norm
    u_e = interpolate(u_exact, u.function_space())
    import numpy as np

```

```

max_error = np.abs(u_e.vector().array() -
                   u.vector().array()).max()
assert max_error < tol, 'max error: %g' % max_error

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

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

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

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

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

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

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

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

```

Plotting the flux vector field is naturally as easy as plotting the gradient (see Section 3.2.5):

```

plot(flux, title='flux field')

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

```

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

```

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

```

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

3.2.7 Creating the linear system explicitly

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

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

which is nothing but a linear system,

$$AU = b,$$

where the entries in A and b are given by

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

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

```

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

```

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

The matrix A and vector b are first assembled without incorporating essential (Dirichlet) boundary conditions. Thereafter, the call `bc.apply(A, b)` performs the necessary modifications of the linear system such that `u` is guaranteed to equal the prescribed boundary values. When we have multiple Dirichlet conditions stored in a list `bcs`, as explained in Section 3.4.2, we must apply each condition in `bcs` to the system:

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

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

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

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

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

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

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

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

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

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

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

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

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

Appropriate names of solvers and preconditioners are found in Section 6.4.4.

To control tolerances in the stopping criterion and the maximum number of iterations, one can explicitly form a `KrylovSolver` object and set items in its `parameters` attribute (see also Section 3.2.2):

```
solver = KrylovSolver('cg', 'ilu')
prm = solver.parameters
prm['absolute_tolerance'] = 1E-7
prm['relative_tolerance'] = 1E-4
prm['maximum_iterations'] = 1000
u = Function(V)
U = u.vector()
set_log_level(DEBUG)
solver.solve(A, U, b)
```

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

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

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

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

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

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

3.2.8 Taking advantage of structured mesh data

When finite element computations are done on a structured rectangular mesh, maybe with uniform partitioning, VTK-based tools for completely unstructured 2D/3D meshes are not required. Instead we can use visualization and data analysis tools for *structured data*. Such data typically appear in finite difference simulations and image analysis. Analysis and visualization of structured data are faster and easier than doing the same with data on unstructured meshes, and the collection of tools to choose among is much larger. We shall demonstrate the potential of such tools and how they allow for tailored and flexible visualization and data analysis.

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

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

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

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

The `u_box` object contains several useful data structures:

- `u_box.grid`: object for the structured mesh
- `u_box.grid.coor[X]`: grid coordinates in X=0 direction
- `u_box.grid.coor[Y]`: grid coordinates in Y=1 direction
- `u_box.grid.coor[Z]`: grid coordinates in Z=2 direction
- `u_box.grid.coorv[X]`: vectorized version of `u_box.grid.coor[X]` (for vectorized computations or surface plotting)
- `u_box.grid.coorv[Y]`: vectorized version of `u_box.grid.coor[Y]`
- `u_box.grid.coorv[Z]`: vectorized version of `u_box.grid.coor[Z]`
- `u_box.values`: numpy array holding the `u` values; `u_box.values[i,j]` holds `u` at the mesh point with coordinates
 $(u_box.grid.coor[X], u_box.grid.coor[Y])$

Iterating over points and values. Let us go back to the `solver` function in the `ft06_poisson_vc.py` code from Section 3.2.6, compute `u`, map it onto a `BoxField` object for a structured mesh representation, and write out the coordinates and function values at all mesh points:

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

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

Finite difference approximations. Note that with \mathbf{u}_- , we can easily express finite difference approximation of derivatives:

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

Surface plot. The ability to access a finite element field in the way one can access a finite difference-type of field is handy in many occasions, including visualization and data analysis. With Matplotlib we can create a surface plot, see Figure 3.2 (upper left):

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

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

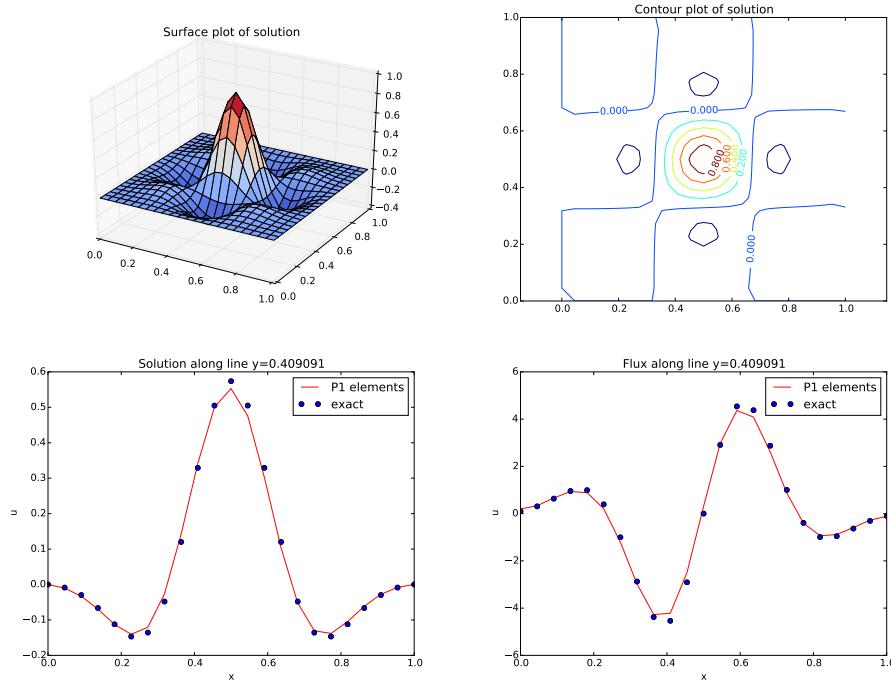


Fig. 3.2 Various plots of the solution on a structured mesh.

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

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

The result appears in Figure 3.2 (upper right).

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

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

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

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

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

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

See Figure 3.2 (lower left) for the resulting curve plot.

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

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

# Plot the numerical and exact flux along the same line
flux2_x = flux_u_x if flux_u_x.ufl_element().degree() == 1 \
    else interpolate(flux_x,
                     FunctionSpace(u.function_space().mesh(),
                                   'P', 1))
flux_u_x_box = structured_mesh(flux2_x, (nx, ny))
```

```

x, flux_u_val, y_fixed, snapped = \
    flux_u_x_box.gridline(start, direction=X)
y = y_fixed

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

```

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

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

Test problem. The graphics referred to in Figure 3.2 correspond to a test problem with prescribed solution $u_e = H(x)H(y)$, where

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

We just fit a function $f(x,y)$ in the PDE (can choose $p=1$), and notice that $u=0$ along the boundary of the unit square. Although it is easy to carry out the differentiation of f by hand and hardcode the resulting expressions in an `Expression` object, a more reliable habit is to use Python's symbolic computing engine, SymPy, to perform mathematics and automatically turn formulas into C++ syntax for `Expression` objects. A short introduction was given in Section 2.4.2.

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

```

from sympy import exp, sin, pi # for use in math formulas
import sympy as sym
H = lambda x: exp(-16*(x-0.5)**2)*sin(3*pi*x)
x, y = sym.symbols('x[0], x[1]')
u = H(x)*H(y)

```

Define symbolic coordinates as required in Expression objects

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

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

¹<https://github.com/hplgit/scitools>

```
u_c = sym.printing.ccode(u)
```

Printing out `u_c` gives (the output is here manually broken into two lines):

```
-exp(-16*pow(x[0] - 0.5, 2) - 16*pow(x[1] - 0.5, 2))*  
sin(3*M_PI*x[0])*sin(3*M_PI*x[1])
```

The necessary syntax adjustment is replacing the symbol `M_PI` for π in C/C++ by `pi` (or `DOLFIN_PI`):

```
u_c = u_c.replace('M_PI', 'pi')  
u0 = Expression(u_c)
```

Thereafter, we can progress with the computation of $f = -\nabla \cdot (p\nabla u)$:

```
p = 1  
f = sym.diff(-p*sym.diff(u, x), x) + sym.diff(-p*sym.diff(u, y), y)  
f = sym.simplify(f)  
f_c = sym.printing.ccode(f)  
f_c = f_c.replace('M_PI', 'pi')  
f = Expression(f_c)
```

We also need a Python function for the exact flux $-p\partial u/\partial x$:

```
flux_u_x_exact = sym.lambdify([x, y], -p*sym.diff(u, x),  
modules='numpy')
```

It remains to define `p = Constant(1)` and set `nx` and `ny` before calling `solver` to compute the finite element solution of this problem.

3.3 Postprocessing computations

hpl 11: Need a little intro.

3.3.1 Computing functionals

After the solution u of a PDE is computed, we occasionally want to compute functionals of u , for example,

$$\frac{1}{2} \|\nabla u\|^2 \equiv \frac{1}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx, \quad (3.10)$$

which often reflects some energy quantity. Another frequently occurring functional is the error

$$\|u_e - u\| = \left(\int_{\Omega} (u_e - u)^2 \, dx \right)^{1/2}, \quad (3.11)$$

where u_e is the exact solution. The error is of particular interest when studying convergence properties. Sometimes the interest concerns the flux out of a part Γ of the boundary $\partial\Omega$,

$$F = - \int_{\Gamma} p \nabla u \cdot \mathbf{n} \, ds, \quad (3.12)$$

where \mathbf{n} is an outward unit normal at Γ and p is a coefficient (see the problem in Section 3.2.6 for a specific example). All these functionals are easy to compute with FEniCS, and this section describes how it can be done.

Energy functional. The integrand of the energy functional (3.10) is described in the UFL language in the same manner as we describe weak forms:

```
energy = 0.5*dot(grad(u), grad(u))*dx
E = assemble(energy)
```

The `assemble` call performs the integration. It is possible to restrict the integration to subdomains, or parts of the boundary, by using a mesh function to mark the subdomains as explained in Section 3.4.4.

Error functional. Computation of (3.11) is typically done by

```
error = (u - u_exact)**2*dx
E = sqrt(abs(assemble(error)))
```

The exact solution u_e is here in a `Function` or `Expression` object `u_exact`, while `u` is the finite element approximation. (Sometimes, for very small error values, the result of `assemble(error)` can be a (very small) negative number, so we have used `abs` in the expression for `E` above to ensure a positive value for the `sqrt` function.)

As will be explained and demonstrate in Section 3.3.2, the integration of `(u - u_exact)**2*dx` can result in too optimistic convergence rates unless one is careful how `u_exact` is transferred onto a mesh. The general recommendation for reliable error computation is to use the `errornorm` function (see `pydoc fenics.errornorm` and Section 3.3.2 for more information):

```
E = errornorm(u_exact, u)
```

Flux Functionals. To compute flux integrals like $F = - \int_{\Gamma} p \nabla u \cdot \mathbf{n} \, ds$ we need to define the \mathbf{n} vector, referred to as *facet normal* in FEniCS. If the surface domain Γ in the flux integral is the complete boundary we can perform the flux computation by

```
n = FacetNormal(mesh)
flux = -p*dot(grad(u), n)*ds
total_flux = assemble(flux)
```

Although `grad(u)` and `grad(u)` are interchangeable in the above expression when `u` is a scalar function, we have chosen to write `grad(u)` because this is the right expression if we generalize the underlying equation to a vector

Laplace/Poisson PDE. With `grad(u)` we must in that case write `dot(n, grad(u))`.

It is possible to restrict the integration to a part of the boundary using a mesh function to mark the relevant part, as explained in Section 3.4.4. Assuming that the part corresponds to subdomain number `i`, the relevant syntax for the variational formulation of the flux is `-p*dot(grad(u), n)*ds(i)`.

3.3.2 Computing convergence rates

hpl 15: Newer FEniCS examples have `dx(degree)`. Should explain that syntax. Also `Expression(string, degree)`.

To illustrate error computations and convergence of finite element solutions, we have included a function `convergence_rate` in the `ft06_poisson_vc.py` program. This is a tool that is very handy when verifying finite element codes and will therefore be explained in detail here.

The L^2 norm of the error in a finite element approximation u , u_e being the exact solution, is given by

Various ways of computing the error.

$$E = \left(\int_{\Omega} (u_e - u)^2 dx \right)^{1/2},$$

and implemented in FEniCS by

```
error = (u - u_e)**2*dx
E = sqrt(abs(assemble(error)))
```

Sometimes, for very small error values, the result of `assemble(error)` can be a (very small) negative number, so we have used `abs` in the expression for `E` above to ensure a positive value for the `sqrt` function.

We remark that `u_e` will, in the expression above, be interpolated onto the function space `V` before `assemble` can perform the integration over the domain. This implies that the exact solution used in the integral will vary linearly over the cells, and not as a sine function, if `V` corresponds to linear Lagrange elements. This situation may yield a smaller error `u - u_e` than what is actually true. More accurate representation of the exact solution is easily achieved by interpolating the formula onto a space defined by higher-order elements, say of third degree:

```
Ve = FunctionSpace(mesh, 'P', degree=3)
u_e_Ve = interpolate(u_e, Ve)
error = (u - u_e_Ve)**2*dx
E = sqrt(assemble(error))
```

To achieve complete mathematical control of which function space the computations are carried out in, we can explicitly interpolate `u` to the same space:

```
u_Ve = interpolate(u, Ve)
error = (u_Ve - u_e_Ve)**2*dx
```

The square in the expression for `error` will be expanded and lead to a lot of terms that almost cancel when the error is small, with the potential of introducing significant rounding errors. The function `errornorm` is available for avoiding this effect by first interpolating `u` and `u_exact` to a space with higher-order elements, then subtracting the degrees of freedom, and then performing the integration of the error field. The usage is simple:

```
E = errornorm(u_exact, u, normtype='L2', degree=3)
```

It is illustrative to look at the short implementation of `errornorm`:

```
def errornorm(u_exact, u, Ve):
    u_Ve = interpolate(u, Ve)
    u_e_Ve = interpolate(u_exact, Ve)
    e_Ve = Function(Ve)
    # Subtract degrees of freedom for the error field
    e_Ve.vector()[:] = u_e_Ve.vector().array() - \
        u_Ve.vector().array()
    error = e_Ve**2*dx
    return sqrt(assemble(error))
```

The `errornorm` procedure turns out to be identical to computing the expression $(u_e - u)^{2*dx}$ directly in the present test case.

Sometimes it is of interest to compute the error of the gradient field: $\|\nabla(u - u_e)\|$ (often referred to as the H^1 seminorm of the error). Given the error field `e_Ve` above, we simply write

```
H1seminorm = sqrt(assemble(dot(grad(e_Ve), grad(e_Ve))*dx))
```

All the various types of error computations here are placed in a function `compute_errors` in `ft06_poisson_vc.py`: **hpl 16**: Necessary to repeat code? New info is essentiall the return dict. **hpl 17**: Anders, I (in 2010...) ran into problems with `fenics.errornorm`, see comments in the code below, and made the version below. We should check out these problems again and adjust `fenics.errornorm` if necessary.

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

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

    V = u.function_space()

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

    # Explicit interpolation of u_e onto the same space as u:
```

```

u_e = interpolate(u_exact, V)
error = (u - u_e)**2*dx
E2 = sqrt(abs(assemble(error)))

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

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

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

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

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

return errors

```

Computing convergence rates empirically. Calling the `solver` function for finer and finer meshes enables us to study the convergence rate. Define the element size $h = 1/n$, where n is the number of cell divisions in x and y direction ($n=Nx=Ny$ in the code). We perform experiments with $h_0 > h_1 > h_2 \dots$ and compute the corresponding errors E_0, E_1, E_3 and so forth. Assuming

$E_i = Ch_i^r$ for unknown constants C and r , we can compare two consecutive experiments, $E_i = Ch_i^r$ and $E_{i-1} = Ch_{i-1}^r$, and solve for r :

$$r = \frac{\ln(E_i/E_{i-1})}{\ln(h_i/h_{i-1})}.$$

The r values should approach the expected convergence rate `degree+1` as i increases.

The procedure above can easily be turned into Python code. Here we run through a different types of elements (P1, P2, P3, and P4), perform experiments over a series of refined meshes, and for each experiment report the six error types as returned by `compute_errors`:

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

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

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

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

```

        r = ln(Ei/Eim1)/ln(h[degree][i]/h[degree][i-1])
        rates[degree][error_type].append(round(r,2))
    return rates

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

```

Note how we make a complete general function `convergence_rate`, aimed at any 2D Poisson problem in the class we now can solve, and then call this general function in `convergence_rate_sin` for a special test case.

Test problem. Section 3.2.5 specifies a more complicated solution,

$$u(x, y) = \sin(\omega\pi x)\sin(\omega\pi y)$$

on the unit square. This choice implies $f(x, y) = 2\omega^2\pi^2u(x, y)$. With ω restricted to an integer it follows that $u_0 = 0$.

We need to define the appropriate boundary conditions, the exact solution, and the f function in the code:

```

def boundary(x, on_boundary):
    return on_boundary

bc = DirichletBC(V, Constant(0.0), boundary)

omega = 1.0
u_e = Expression('sin(omega*pi*x[0])*sin(omega*pi*x[1])',
                 omega=omega)

f = 2*pi**2*omega**2*u_e

```

Experiments. Calling `convergence_rate_sin()` gives some interesting results. Using the error measure E5 based on the infinity norm of the difference of the degrees of freedom, we have

	element	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
P1		1.99	1.97	1.99	2.0	2.0
P2		3.99	3.96	3.99	4.0	3.99
P3		3.96	3.89	3.96	3.99	4.0
P4		3.75	4.99	5.0	5.0	

The computations with P4 elements on a 128×128 with a direct solver (UMFPACK) on a small laptop broke down. Otherwise we achieve expected results: the error goes like h^{d+1} for elements of degree d . Also L^2 norms based on the `errornorm` gives the expected h^{d+1} rate for u and h^d for ∇u .

However, using `(u - u_exact)**2` for the error computation, which implies interpolating `u_exact` onto the same space as `u`, results in h^4 convergence for P2 elements.

	element	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
P1		1.98	1.94	1.98	2.0	2.0
P2		3.98	3.95	3.99	3.99	3.99
P3		3.69	4.03	4.01	3.95	2.77

This is an example where it is important to interpolate `u_exact` to a higher-order space (polynomials of degree 3 are sufficient here) to avoid computing a too optimistic convergence rate.

Checking convergence rates is the next best method for verifying PDE codes (the best being a numerical solution without approximation errors as in Section 3.2.3 and many other places in this tutorial).

3.4 Multiple domains and boundaries

hpl 11: Need a little intro.

3.4.1 Combining Dirichlet and Neumann conditions

Let us make a slight extension of our two-dimensional Poisson problem from Section 2.1.1 and add a Neumann boundary condition. The domain is still the unit square, but now we set the Dirichlet condition $u = u_0$ at the left and right sides, $x = 0$ and $x = 1$, while the Neumann condition

$$-\frac{\partial u}{\partial n} = g$$

is applied to the remaining sides $y = 0$ and $y = 1$. The Neumann condition is also known as a *natural boundary condition* (in contrast to an essential boundary condition).

PDE problem. Let Γ_D and Γ_N denote the parts of $\partial\Omega$ where the Dirichlet and Neumann conditions apply, respectively. The complete boundary-value problem can be written as

$$-\nabla^2 u = f \text{ in } \Omega, \quad (3.13)$$

$$u = u_0 \text{ on } \Gamma_D, \quad (3.14)$$

$$-\frac{\partial u}{\partial n} = g \text{ on } \Gamma_N. \quad (3.15)$$

Again we choose $u = 1 + x^2 + 2y^2$ as the exact solution and adjust f , g , and u_0 accordingly:

$$\begin{aligned} f &= -6, \\ g &= \begin{cases} -4, & y = 1 \\ 0, & y = 0 \end{cases} \\ u_0 &= 1 + x^2 + 2y^2. \end{aligned}$$

For ease of programming we may introduce a g function defined over the whole of Ω such that g takes on the right values at $y = 0$ and $y = 1$. One possible extension is

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

Variational formulation. The first task is to derive the variational problem. This time we cannot omit the boundary term arising from the integration by parts, because v is only zero on Γ_D . We have

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

and since $v = 0$ on Γ_D ,

$$-\int_{\partial\Omega} \frac{\partial u}{\partial n} v \, ds = -\int_{\Gamma_N} \frac{\partial u}{\partial n} v \, ds = \int_{\Gamma_N} g v \, ds,$$

by applying the boundary condition on Γ_N . The resulting weak form reads

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx + \int_{\Gamma_N} g v \, ds = \int_{\Omega} f v \, dx. \quad (3.16)$$

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

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (3.17)$$

$$L(v) = \int_{\Omega} fv \, dx - \int_{\Gamma_N} gv \, ds. \quad (3.18)$$

Implementation. How does the Neumann condition impact the implementation? Let us go back to the very simplest file, `ft01_poisson_flat.py`, from Section 2.1.5, we realize that the statements remain almost the same. Only two adjustments are necessary:

- The function describing the boundary where Dirichlet conditions apply must be modified.
- The new boundary term must be added to the expression in L.

The first adjustment can be coded as

```
def Dirichlet_boundary(x, on_boundary):
    if on_boundary:
        if x[0] == 0 or x[0] == 1:
            return True
        else:
            return False
    else:
        return False
```

A more compact implementation reads

```
def Dirichlet_boundary(x, on_boundary):
    return on_boundary and (x[0] == 0 or x[0] == 1)
```

Never use `==` for comparing real numbers!

A list like `x[0] == 1` should never be used if `x[0]` is a real number, because rounding errors in `x[0]` may make the test fail even when it is mathematically correct. Consider

```
>>> 0.1 + 0.2 == 0.3
False
>>> 0.1 + 0.2
0.30000000000000004
```

Comparison of real numbers need to use tolerances! The values of the tolerances depend on the size of the numbers involved in arithmetic operations:

```
>>> abs(0.1+0.2 - 0.3)
5.551115123125783e-17
>>> abs(1.1+1.2 - 2.3)
```

```

0.0
>>> abs(10.1+10.2 - 20.3)
3.552713678800501e-15
>>> abs(100.1+100.2 - 200.3)
0.0
>>> abs(1000.1+1000.2 - 2000.3)
2.2737367544323206e-13
>>> abs(10000.1+10000.2 - 20000.3)
3.637978807091713e-12

```

For numbers around unity, tolerances as low as $3 \cdot 10^{-16}$ can be used (in fact, this tolerance is known as the constant `DOLFIN_EPS` in FEniCS), otherwise an appropriate tolerance must be found.

Testing for `x[0] == 1` should therefore be implemented as

```

tol = 1E-14
if abs(x[0] - 1) < tol:
    ...

```

Here is a new boundary function using tolerances in the test:

```

def Dirichlet_boundary(x, on_boundary):
    tol = 1E-14    # tolerance for coordinate comparisons
    return on_boundary and \
        (abs(x[0]) < tol or abs(x[0] - 1) < tol)

```

The second adjustment of our program concerns the definition of `L`, where we have to add a boundary integral and a definition of the `g` function to be integrated:

```

g = Expression('-4*x[1]')
L = f*v*dx - g*v*ds

```

The `ds` variable implies a boundary integral, while `dx` implies an integral over the domain Ω . No more modifications are necessary.

3.4.2 Multiple Dirichlet conditions

The PDE problem from the previous section applies a function $u_0(x, y)$ for setting Dirichlet conditions at two parts of the boundary. Having a single function to set multiple Dirichlet conditions is seldom possible. The more general case is to have m functions for setting Dirichlet conditions on m parts of the boundary. The purpose of this section is to explain how such multiple conditions are treated in FEniCS programs.

Let us return to the case from Section 3.4.1 and define two separate functions for the two Dirichlet conditions:

$$\begin{aligned} -\nabla^2 u &= -6 \text{ in } \Omega, \\ u &= u_L \text{ on } \Gamma_0, \\ u &= u_R \text{ on } \Gamma_1, \\ -\frac{\partial u}{\partial n} &= g \text{ on } \Gamma_N. \end{aligned}$$

Here, Γ_0 is the boundary $x = 0$, while Γ_1 corresponds to the boundary $x = 1$. We have that $u_L = 1 + 2y^2$, $u_R = 2 + 2y^2$, and $g = -4y$.

Functions for marking Dirichlet boundaries. For the left boundary Γ_0 we define the usual triple of a function for the boundary value, a function for defining the boundary of interest, and a `DirichletBC` object:

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

def left_boundary(x, on_boundary):
    tol = 1E-14    # tolerance for coordinate comparisons
    return on_boundary and abs(x[0]) < tol

Gamma_0 = DirichletBC(V, u_L, left_boundary)
```

For the boundary $x = 1$ we write a similar code snippet:

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

def right_boundary(x, on_boundary):
    tol = 1E-14    # tolerance for coordinate comparisons
    return on_boundary and abs(x[0] - 1) < tol

Gamma_1 = DirichletBC(V, u_R, right_boundary)
```

The various essential conditions are then collected in a list and used in the solution process:

```
bcs = [Gamma_0, Gamma_1]
...
solve(a == L, u, bcs)
# or
problem = LinearVariationalProblem(a, L, u, bcs)
solver = LinearVariationalSolver(problem)
solver.solve()
```

In other problems, where the u values are constant at a part of the boundary, we may use a simple `Constant` object instead of an `Expression` object.

3.4.3 Working with subdomains

Solving PDEs in domains made up of different materials is a frequently encountered task. In FEniCS, these kind of problems are handled by defining

subdomains inside the domain. The subdomains may represent the various materials. We can thereafter define material properties through functions, known in FEniCS as *mesh functions*, that are piecewise constant in each subdomain. A simple example with two materials (subdomains) in 2D will demonstrate the basic steps in the process.

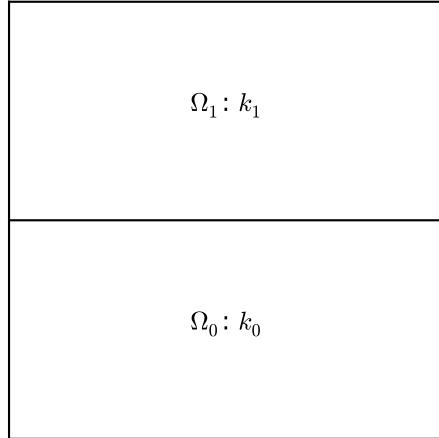


Fig. 3.3 Medium with discontinuous material properties.

Suppose we want to solve

$$\nabla \cdot [k(x,y)\nabla u(x,y)] = 0, \quad (3.19)$$

in a domain Ω consisting of two subdomains where k takes on a different value in each subdomain. For simplicity, yet without loss of generality, we choose for the current implementation the domain $\Omega = [0, 1] \times [0, 1]$ and divide it into two equal subdomains, as depicted in Figure 3.3,

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

We define $k(x,y) = k_0$ in Ω_0 and $k(x,y) = k_1$ in Ω_1 , where $k_0 > 0$ and $k_1 > 0$ are given constants.

Physically, the present problem may correspond to heat conduction, where the heat conduction in Ω_1 is more efficient than in Ω_0 . An alternative interpretation is flow in porous media with two geological layers, where the layers' ability to transport the fluid differ.

Expression objects with if test. The simplest way of implementing a variable k is to define an `Expression` object where we return the appropriate k value depending on the position in space. Since we need some testing on the coordinates, the most straightforward approach is to define a subclass of `Expression`, where we can use a full Python method instead of just a C++

string formula for specifying a function. The method that defines the function is called `eval`:

```
class K(Expression):
    def set_k_values(self, k0, k1):
        self.k0, self.k1 = k0, k1

    def eval(self, value, x):
        """x: spatial point, value[0]: function value."""
        # Fill in-place value[0] for scalar function,
        # value[:] for vector function (no return)

        tol = 1E-14 # Tolerance for coordinate comparisons
        if x[1] <= 0.5+tol:
            value[0] = self.k0
        else:
            value[0] = self.k1

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

The `eval` method gives great flexibility in defining functions, but a downside is that C++ calls up `eval` in Python for each point `x`, which is a slow process, and the number of calls is proportional to the number of numerical integration points in the mesh (about the number of degrees of freedom). Function expressions in terms of strings are compiled to efficient C++ functions, being called from C++, so we should try to express functions as string expressions if possible. (The `eval` method can also be defined through C++ code, but this is much more complicated and not covered here.) The idea is to use inline if tests in C++:

```
tol = 1E-14
k0 = 1.0
k1 = 0.01
k = Expression('x[1] <= 0.5+tol? k0 : k1',
               tol=tol, k0=k0, k1=k1)
```

The method with if tests on the location is feasible when the subdomains have very simple shapes. A completely general method, utilizing *mesh functions*, is described next.

Mesh functions. We now address how to specify the subdomains Ω_0 and Ω_1 so that the method also works for subdomains of any shape. For this purpose we need to use subclasses of class `SubDomain`, not only plain functions as we have used so far for specifying boundaries. Consider the boundary function

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

for defining the boundary $x = 0$. Instead of using such a stand-alone function, we can create an instance (or object) of a subclass of `SubDomain`, which implements the `inside` method as an alternative to the `boundary` function:

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

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

A word about computer science terminology may be used here: The term *instance* means a Python object of a particular type (such as `SubDomain`, `Function`, `FunctionSpace`, etc.). Many use *instance* and *object* as interchangeable terms. In other computer programming languages one may also use the term *variable* for the same thing. We mostly use the well-known term *object* in this text.

A subclass of `SubDomain` with an `inside` method offers functionality for marking parts of the domain or the boundary. Now we need to define one class for the subdomain Ω_0 where $y \leq 1/2$ and another for the subdomain Ω_1 where $y \geq 1/2$:

```
tol = 1E-14 # Tolerance for coordinate comparisons

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

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

Notice the use of `<=` and `>=` in both tests. For a cell to belong to, e.g., Ω_1 , the `inside` method must return `True` for all the vertices `x` of the cell. So to make the cells at the internal boundary $y = 1/2$ belong to Ω_1 , we need the test `x[1] >= 0.5`. However, because of potential rounding errors in the coordinates `x[1]`, we use a tolerance in the comparisons: `x[1] >= 0.5-tol`.

The next task is to use a *mesh function* to mark all cells in Ω_0 with the subdomain number 0 and all cells in Ω_1 with the subdomain number 1. Our convention is to number subdomains as 0, 1, 2,

A `MeshFunction` object is a discrete function that can be evaluated at a set of so-called *mesh entities*. Examples of mesh entities are cells, facets, and vertices. A `MeshFunction` over cells is suitable to represent subdomains (materials), while a `MeshFunction` over facets is used to represent pieces of external or internal boundaries. Mesh functions over vertices can be used to describe continuous fields. The specialized classes `CellFunction` and `FacetFunction` are used to construct mesh functions of cells and facets, respectively.

Since we need to define subdomains of Ω in the present example, we make use of a `CellFunction`. The constructor is fed with two arguments: 1) the

type of value: 'int' for integers, 'uint' for positive (unsigned) integers, 'double' for real numbers, and 'bool' for logical values; 2) a `Mesh` object. Alternatively, the constructor can take just a filename and initialize the `CellFunction` from data in a file.

We start with creating a `CellFunction` whose values are non-negative integers ('`uint`') for numbering the subdomains. The appropriate code for two subdomains then reads

```
materials = CellFunction('size_t', mesh)
# Mark subdomains with numbers 0 and 1
subdomain0 = Omega0()
subdomain0.mark(materials, 0)
subdomain1 = Omega1()
subdomain1.mark(materials, 1)

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

Calling `materials.array()` returns a `numpy` array of the subdomain values. That is, `materials.array()[i]` is the subdomain value of cell number i . This array is used to look up the subdomain or material number of a specific element.

We need a function `k` that is constant in each subdomain Ω_0 and Ω_1 . Since we want `k` to be a finite element function, it is natural to choose a space of functions that is constant over each element. The family of discontinuous Galerkin methods, in FEniCS denoted by '`DG`', is suitable for this purpose. Since we want functions that are piecewise constant, the value of the degree parameter is zero:

```
V0 = FunctionSpace(mesh, 'DG', 0)
k = Function(V0)
```

To fill `k` with the right values in each element, we loop over all cells (i.e., indices in `materials.array()`), extract the corresponding subdomain number of a cell, and assign the corresponding k value to the `k.vector()` array:

```
k_values = [1.5, 50] # values of k in the two subdomains
for cell_no in range(len(materials.array())):
    material_no = materials.array()[cell_no]
    k.vector()[cell_no] = k_values[material_no]
```

Long loops in Python are known to be slow, so for large meshes it is preferable to avoid such loops and instead use *vectorized code*. Normally this implies that the loop must be replaced by calls to functions from the `numpy` library that operate on complete arrays (in efficient C code). The functionality we want in the present case is to compute an array of the same size as `materials.array()`, but where the value i of an entry in `materials.array()` is replaced by `k_values[i]`. Such an operation is carried out by the `numpy` function `choose`:

```
help = numpy.asarray(materials.array(), dtype=numpy.int32)
k.vector()[:] = numpy.choose(help, k_values)
```

The `help` array is required since `choose` cannot work with `materials.array()` because this array has elements of type `uint32`. We must therefore transform this array to an array `help` with standard `int32` integers.

The next section exemplifies a complete solver with a piecewise constant coefficient, like k , defined through `SubDomain` objects, combined with different types of boundary conditions.

C++ strings for subdomain definitions. The `SubDomain` class in Python is convenient, but leads to lots of function calls from C++ to Python, which are slow. In large problems, the subdomains should be defined through C++ code. This is easy to achieve using the `CompiledSubDomain` object. Consider the definition of classes `Omega0` and `Omega1` above in Python. The key strings that define these subdomain can be expressed in C++ syntax and fed to `CompiledSubDomain` as follows:

```
tol = 1E-14 # Tolerance for coordinate comparisons

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

As seen, one can have parameters in the strings and specify their values by keyword arguments. The resulting objects, `subdomain0` and `subdomain1`, can be used as ordinary `SubDomain` objects.

Compiled subdomain strings can be applied for specifying boundaries as well, e.g.,

```
y_R = CompiledSubDomain('on_boundary && near(x[1], R, eps=tol)',
                        tol=1E-14, R=2) # y=2
```

It is possible to feed the C++ string (without parameters) directly as the third argument to `DirichletBC` without explicitly constructing a `CompiledSubDomain` object:

```
bc1 = DirichletBC(V, value, 'on_boundary && near(x[1], 2, 1E-14)')
```

3.4.4 Multiple Neumann, Robin, and Dirichlet condition

Consider the model problem from Section 3.4.2 where we had both Dirichlet and Neumann conditions. The term `v*g*ds` in the expression for `L` implies a boundary integral over the complete boundary, or in FEniCS terms, an integral over all exterior facets. However, the contributions from the parts of the boundary where we have Dirichlet conditions are erased when the linear system is modified by the Dirichlet conditions. We would like, from an efficiency

point of view, to integrate `v*g*ds` only over the parts of the boundary where we actually have Neumann conditions. And more importantly, in other problems one may have different Neumann conditions or other conditions like the Robin type condition. With the mesh function concept we can mark different parts of the boundary and integrate over specific parts. The same concept can also be used to treat multiple Dirichlet conditions. The forthcoming text illustrates how this is done.

Three types of boundary conditions. We extend our repertoire of boundary conditions to three types: Dirichlet, Neumann, and Robin. Dirichlet conditions apply to some parts $\Gamma_{D,0}, \Gamma_{D,1}, \dots$, of the boundary:

$$u_{0,0} \text{ on } \Gamma_{D,0}, \quad u_{0,1} \text{ on } \Gamma_{D,1}, \dots$$

where $u_{0,i}$ are prescribed functions, $i = 0, 1, \dots$. On other parts, $\Gamma_{N,0}, \Gamma_{N,1}, \dots$, we have Neumann conditions

$$-p \frac{\partial u}{\partial n} = g_0 \text{ on } \Gamma_{N,0}, \quad -p \frac{\partial u}{\partial n} = g_1 \text{ on } \Gamma_{N,1}, \quad \dots$$

Finally, we have *Robin conditions*

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

where r and s are specified functions. The Robin condition is most often used to model heat transfer to the surroundings and arise naturally from Newton's cooling law. In that case, r is a heat transfer coefficient, and s is the temperature of the surroundings. Both can be space and time-dependent. The Robin conditions apply at some parts $\Gamma_{R,0}, \Gamma_{R,1}, \dots$

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

A general model problem. With the notation above, the model problem to be solved with multiple Dirichlet, Neumann, and Robin conditions can formally be defined as

$$-\nabla \cdot (p \nabla u) = -f, \text{ in } \Omega, \tag{3.20}$$

$$u = u_{0,i} \text{ on } \Gamma_{D,i}, \quad i = 0, 1, \dots \tag{3.21}$$

$$-p \frac{\partial u}{\partial n} = g_i \text{ on } \Gamma_{N,i}, \quad i = 0, 1, \dots \tag{3.22}$$

$$-p \frac{\partial u}{\partial n} = r_i(u - s_i) \text{ on } \Gamma_{R,i}, \quad i = 0, 1, \dots \tag{3.23}$$

Variational formulation. Integration by parts of $-\int_{\Omega} v \nabla \cdot (p \nabla u) dx$ becomes as usual

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

The boundary integral does not apply to the parts of the boundary where we have Dirichlet conditions ($\Gamma_{D,i}$). Moreover, on the remaining parts, we must split the boundary integral into the parts where we have Neumann and Robin conditions such that we insert the right conditions as integrands. Specifically, we have

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

The variational formulation then becomes

$$F = \int_{\Omega} p \nabla u \cdot \nabla v dx + \sum_i \int_{\Gamma_{N,i}} g_i v ds + \sum_i \int_{\Gamma_{R,i}} r_i(u - s_i) v ds - \int_{\Omega} f v dx = 0. \quad (3.24)$$

We have been used to writing this variational formulation in the standard notation $a(u, v) = L(v)$, which requires that we identify all integrals with *both* u and v , and collect these in $a(u, v)$, while the remaining integrals with v and not u go into $L(v)$. The integral from the Robin condition must of this reason be split in two parts:

$$\int_{\Gamma_{R,i}} r_i(u - s_i) v ds = \int_{\Gamma_{R,i}} r_i u v ds - \int_{\Gamma_{R,i}} r_i s_i v ds.$$

We then have

$$a(u, v) = \int_{\Omega} p \nabla u \cdot \nabla v dx + \sum_i \int_{\Gamma_{R,i}} r_i u v ds, \quad (3.25)$$

$$L(v) = \int_{\Omega} f v dx - \sum_i \int_{\Gamma_{N,i}} g_i v ds + \sum_i \int_{\Gamma_{R,i}} r_i s_i v ds. \quad (3.26)$$

Implementation of boundary conditions. Looking at our previous `solver` functions for solving the 2D Poisson equation, the following new aspects must be taken care of:

1. definition of a mesh function over the boundary,
2. marking each side as a subdomain, using the mesh function,
3. splitting a boundary integral into parts.

A general approach to the first task is to mark each of the desired boundaries with markers 0, 1, 2, and so forth. Here we aim at the four sides of the unit square, marked with 0 ($x = 0$), 1 ($x = 1$), 2 ($y = 0$), and 3 ($y = 1$). The marking of boundaries makes use of a mesh function object, but contrary to Section 3.4.3, this is not a function over cells, but a function over cell facets. We apply the `FacetFunction` for this purpose:

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

As in Section 3.4.3 we use a subclass of `SubDomain` to identify the various parts of the mesh function. Problems with domains of more complicated geometries may set the mesh function for marking boundaries as part of the mesh generation. In our case, the $x = 0$ boundary can be marked by

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

bx0 = BoundaryX0()
bx0.mark(boundary_parts, 0)
```

Similarly, we make the classes `BoundaryX1` for the $x = 1$ boundary, `BoundaryY0` for the $y = 0$ boundary, and `BoundaryY1` for the $y = 1$ boundary, and mark these as subdomains 1, 2, and 3, respectively.

For generality of the implementation, we let the user specify what kind of boundary condition that applies to each of the four boundaries. We set up a Python dictionary for this purpose, with the key as subdomain number and the value as a dictionary specifying the kind of condition as key and a function as its value. For example,

```
boundary_conditions = {
    0: {'Dirichlet': u0},
    1: {'Robin': (r, s)},
    2: {'Neumann': g},
    3: {'Neumann', 0}}
```

specifies

- a Dirichlet condition, with values implemented by an `Expression` or `Constant` object `u0`, on subdomain 0, i.e., the $x = 1$ boundary;
- a Robin condition (3.4.4) on subdomain 1, $x = 1$, with `Expression` or `Constant` objects `r` and `s` specifying r and s ;
- a Neumann condition $\partial u / \partial n = g$ on subdomain 2, $y = 0$, where an `Expression` or `Constant` object `g` implements the value `g`;
- a homogeneous Neumann condition $\partial u / \partial n = 0$ on subdomain 3, $y = 1$.

As explained in Section 3.4.2, multiple Dirichlet conditions must be collected in a list of `DirichletBC` objects. Based on the `boundary_conditions` data structure above, we can construct this list by the following snippet:

```
bcs = [] # List of Dirichlet conditions
```

```

for n in boundary_conditions:
    if 'Dirichlet' in boundary_conditions[n]:
        bcs.append(
            DirichletBC(V, boundary_conditions[n]['Dirichlet'],
                        boundary_parts, n))

```

The new aspect of the variational problem is the two distinct boundary integrals over $\Gamma_{N,i}$ and $\Gamma_{R,i}$. Having a mesh function over exterior cell facets (our `boundary_parts` object), where subdomains (boundary parts) are numbered as $0, 1, 2, \dots$, the special symbol `ds(0)` implies integration over subdomain (part) 0, `ds(1)` denotes integration over subdomain (part) 1, and so on. The idea of multiple `ds`-type objects generalizes to volume integrals too: `dx(0)`, `dx(1)`, etc., are used to integrate over subdomain 0, 1, etc., inside Ω .

Before we have `ds(n)` for integers n defined, we must do

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

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

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

where `domains` is a `CellFunction` defining subdomains in Ω .

Suppose we have a Robin condition with values r and s on subdomain R , a Neumann condition with value g on subdomain N , the variational form can be written

```

a = dot(grad(u), grad(v))*dx + r*u*v*ds(R)
L = f*v*dx - g*v*ds(N) + r*s*v*ds(R)

```

In our case things get a bit more complicated since the information about integrals in Neumann and Robin conditions are in the `boundary_conditions` data structure. We can collect all Neumann conditions by the code

```

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

```

Applying `sum(Neumann_integrals)` will apply the `+` operator to the variational forms in the `Neumann_integrals` list and result in the integrals we need for the right-hand side L of the variational form.

The integrals in the Robin condition can similarly be collected in lists:

```

Robin_a_integrals = []
Robin_L_integrals = []
for n in boundary_conditions:
    if 'Robin' in boundary_conditions[n]:
        r, s = boundary_conditions[n]['Robin']

```

```
Robin_a_integrals.append(r*u*v*ds(n))
Robin_L_integrals.append(r*s*v*ds(n))
```

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

```
a = dot(p*grad(u), grad(v))*dx + \
        sum(Robin_a_integrals)
L = f*v*dx - sum(Neumann_integrals) + sum(Robin_L_integrals)
```

Simplified handling of the variational formulation. We carefully ordered the terms in the variational formulation above into the a and L parts. This requires a splitting of the Robin condition and makes the a and L expressions less readable (still we think understanding this splitting is key for any finite element programmer!). Fortunately, UFL allow us to specify the complete variational form (3.24) as *one expression* and offer tools to extract what goes into the bilinear form $a(u, v)$ and the linear form $L(v)$:

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

This time we can more naturally define the integrals from the Robin condition as $r*(u-s)*v*ds(n)$:

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

The complete code is in the `solver_bc` function in the `ft06_poisson_vc.py` file.

Test problem. Let us continue to use $u_e = 1 + x^2 + 2y^2$ as the exact solution, and set $p = 1$ and $f = -6$ in the PDE. Our domain is the unit square, and we assign Dirichlet conditions at $x = 0$ and $x = 1$, a Neumann condition at $y = 1$, and a Robin condition at $y = 0$. With the given u_e , we realize that the Neumann condition is $-4y$ (which means -4 at $y = 1$), while the Robin condition can be selected in many ways. Since $\partial u / \partial n = -\partial u / \partial y = 0$ at $y = 0$, we can select $s = u$ and have r arbitrary in the Robin condition.

The boundary parts are $\Gamma_{D,0}$: $x = 0$, $\Gamma_{D,1}$: $x = 1$, $\Gamma_{R,0}$: $y = 0$, and $\Gamma_{N,0}$: $y = 1$.

When implementing this test problem (and especially other test problems with more complicated expressions), it is advantageous to use symbolic computing. Below we define u_e as a `sympy` expression and derive other functions from their mathematical definitions. Then we turn these expressions into C/C++ code, which can be fed into `Expression` objects.

```
def application_bc_test():
    # Define manufactured solution in sympy and derive f, g, etc.
```

```

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

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

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

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

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

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

# Print numerical and exact solution at the vertices
if u.function_space().dim() < 50: # (small problems only)

```

```

u_e_at_vertices = u_e.compute_vertex_values()
u_at_vertices = u.compute_vertex_values()
coor = u.function_space().mesh().coordinates()
for i, x in enumerate(coor):
    print('vertex %2d (%9g,%9g): error=%g %g vs %g'
        % (i, x[0], x[1],
           u_e_at_vertices[i] - u_at_vertices[i],
           u_e_at_vertices[i], u_at_vertices[i]))

```

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

Debugging the setting of boundary conditions. It is easy to make mistakes when implementing a problem with many different types of boundary conditions, as in the present case. Some helpful debugging output is to run through all vertex coordinates and check if the `SubDomain.inside` method marks the vertex as on the boundary. Another useful printout is to list which degrees of freedom that are subject to Dirichlet conditions, and for first-order Lagrange elements, add the corresponding vertex coordinate to the output.

```

if debug:
    # Print the vertices that are on the boundaries
    coor = mesh.coordinates()
    for x in coor:
        if bx0.inside(x, True): print('%s is on x=0' % x)
        if bx1.inside(x, True): print('%s is on x=1' % x)
        if by0.inside(x, True): print('%s is on y=0' % x)
        if by1.inside(x, True): print('%s is on y=1' % x)
    # Print the Dirichlet conditions
    print('No of Dirichlet conditions:', len(bcs))
    d2v = dof_to_vertex_map(V)
    for bc in bcs:
        bc_dict = bc.get_boundary_values()
        for dof in bc_dict:
            print('dof %2d: u=%g' % (dof, bc_dict[dof]))
            if V.ufl_element().degree() == 1:
                print(' at point %s' %
                    (str(tuple(coor[d2v[dof]].tolist())))))

```

In addition, it is helpful to print the exact and the numerical solution at all the vertices as shown in Section 3.2.3.

Implementation of multiple subdomains. Section 3.4.3 explains how to deal with multiple subdomains of Ω and a piecewise constant coefficient function p that takes on different constant values in the different subdomains. We can easily add this type of p coefficient to the `solver_bc` function. The signature of the function is

```

def solver_bc(
    p, f,                      # Coefficients in the PDE
    boundary_conditions,       # Dict of boundary conditions
    Nx, Ny,                   # Cell division of the domain
    degree=1,                  # Polynomial degree

```

```

    subdomains=[],          # List of SubDomain objects in domain
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol=1E-5,           # Absolute tolerance in Krylov solver
    rel_tol=1E-3,           # Relative tolerance in Krylov solver
    max_iter=1000,          # Max no of iterations in Krylov solver
    log_level=PROGRESS,     # Amount of solver output
    dump_parameters=False,   # Write out parameter database?
    debug=False,
):
...
    return u, p  # p may be modified

```

If `subdomain` is an empty list, we assume there are no subdomains, and `p` is an `Expression` or `Constant` object specifying a formula for `p`. If not, `subdomain` is a list of `SubDomain` objects, defining different parts of the domain. The first element is a dummy object, defining “the rest” of the domain. The next elements define specific geometries in the `inside` methods. We start by marking all elements with subdomain number 0, this will then be “the rest” after marking subdomains 1, 2, and so on. The next step is to define `p` as a piecewise constant function over cells and fill it with values. We assume that the user-argument `p` is an array (or list) holding the values of `p` in the different parts corresponding to `subdomains`. The returned `p` is needed for flux computations. If there are no subdomains, the returned `p` is just the original `p` argument.

The appropriate code for computing `p` becomes

```

import numpy as np
if subdomains:
    # subdomains is list of SubDomain objects,
    # p is array of corresponding constant values of p
    # in each subdomain
    materials = CellFunction('size_t', mesh)
    materials.set_all(0) # "the rest"
    for m, subdomain in enumerate(subdomains[1:], 1):
        subdomain.mark(materials, m)

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

```

We define $p(x, y) = p_0$ in Ω_0 and $k(x, y) = p_1$ in Ω_1 , where $p_0 > 0$ and $p_1 > 0$ are given constants. As boundary conditions, we choose $u = 0$ at $y = 0$, $u = 1$ at $y = 1$, and $\partial u / \partial n = 0$ at $x = 0$ and $x = 1$. One can show that the exact solution is now given by

$$u(x, y) = \begin{cases} \frac{2yp_1}{p_0+p_1}, & y \leq 1/2 \\ \frac{(2y-1)p_0+p_1}{p_0+p_1}, & y \geq 1/2 \end{cases} \quad (3.27)$$

As long as the element boundaries coincide with the internal boundary $y = 1/2$, this piecewise linear solution should be exactly recovered by Lagrange elements of any degree. We can use this property to verify the implementation and make a unit test for a series of function spaces:

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

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

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

    subdomains = [Omega0(), Omega1()]
    p_values = [2.0, 13.0]
    boundary_conditions = {
        0: {'Neumann': 0},
        1: {'Neumann': 0},
        2: {'Dirichlet': Constant(0)}, # y=0
        3: {'Dirichlet': Constant(1)}, # y=1
    }

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

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

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

3.4.5 Refactoring of a solver function into solver and problem classes

A FEniCS solver for a PDE can be implemented in a general way, but the problem-dependent data, like boundary conditions, must be specified in each case by the user. The implementation in the previous section required the user to supply a `boundary_conditions` dictionary with specifications of the boundary condition on each of the four sides of the unit square. If we, e.g., want two Dirichlet conditions at one side, as our mathematical formulation of the problem in the previous section in fact supports, this is not possible without extending the `solver_bc` function.

A different software design is to introduce a problem class and methods, supplied by the user from case to case, where boundary conditions and other input data are defined. Such a design is used in a lot of more advanced FEniCS application codes, and it is time to exemplify it here. As a counterpart to the solver function, we introduce a solver class, but all the arguments for various input data are instead method calls to an instance of a *problem class*. This puts a somewhat greater burden on the programmer, but it allows for more flexibility, and the code for, e.g., boundary conditions can be more tailored to the problem at hand than the code we introduced in the `solver_bc` function in the previous section.

The solver class will need problem information and for this purpose call up the methods in a problem class. For example, the solver gets the `f` and `p` functions in the PDE problem by calling `problem.f_rhs()` and `problem.p_coeff()`. The mesh object and the polynomial degree of the elements are supposed to be returned from `problem.mesh_degree()`. Furthermore, the problem class defines the boundary conditions in the problem as lists of minimal information from which the solver can build proper data structures.

The solver class is a wrapping of the previous `solver_bc` and `flux` functions as methods in a class, but some of the code for handling boundary conditions in `solver_bc` is now delegated to the user in the problem class.

```
from fenics import *
import numpy as np

class Solver(object):
    def __init__(self, problem, debug=False):
        self.mesh, degree = problem.mesh_degree()
        self.V = V = FunctionSpace(self.mesh, 'P', degree)
        Dirichlet_cond = problem.Dirichlet_conditions()
        if isinstance(Dirichlet_cond, (Expression)):
            # Just one Expression for Dirichlet conditions on
            # the entire boundary
            self.bcs = [DirichletBC(
                V, Dirichlet_cond,
                lambda x, on_boundary: on_boundary)]
```

```

else:
    # Boundary SubDomain markers
    self.bcs = [
        DirichletBC(V, value, boundaries, index)
        for value, boundaries, index
        in Dirichlet_cond]

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

u = TrialFunction(V)
v = TestFunction(V)
p = problem.p_coeff()
self.p = p # store for flux computations
f = problem.f_rhs()
F = dot(p*grad(u), grad(v))*dx
F -= f*v*dx
F -= sum([g*v*ds_
          for g, ds_ in problem.Neumann_conditions()])
F += sum([r*(u-s)*ds_
          for r, s, ds_ in problem.Robin_conditions()])
self.a, self.L = lhs(F), rhs(F)

if debug and V.dim() < 50:
    A = assemble(self.a)
    print('A:\n', A.array())
    b = assemble(self.L)
    print('b:\n', b.array())

def solve(self, linear_solver='direct'):
    # Compute solution
    self.u = Function(self.V)

    if linear_solver == 'Krylov':
        solver_parameters = {'linear_solver': 'gmres',
                             'preconditioner': 'ilu'}
    else:
        solver_parameters = {'linear_solver': 'lu'}

    solve(self.a == self.L, self.u, self.bcs,
          solver_parameters=solver_parameters)
    return self.u

def flux(self):

```

```
"""Compute and return flux -p*grad(u)."""
mesh = self.u.function_space().mesh()
degree = self.u.ufl_element().degree()
V_g = VectorFunctionSpace(mesh, 'P', degree)
self.flux_u = project(-self.p*grad(self.u), V_g)
self.flux_u.rename('flux(u)', 'continuous flux field')
return self.flux_u
```

Note that this is a general Poisson problem solver that works in any number of space dimensions and with any mesh and composition of boundary conditions.

Tip: Be careful with the `mesh` variable!

In classes, one often stores the mesh in `self.mesh`. When you need the mesh, it is easy to write just `mesh`, but this gives rise to peculiar error messages, since `mesh` is a Python module imported by `from fenics import *` and already available as a name in your file. When encountering strange error messages in statements containing a variable `mesh`, make sure you use `self.mesh`.

Below is the specific problem class for solving a scaled 2D Poisson problem. We have a two-material domain where a rectangle $[0.3, 0.7] \times [0.3, 0.7]$ is embedded in the unit square and where p has a constant value inside the rectangle and another value outside. On $x = 0$ and $x = 1$ we have homogeneous Neumann conditions, and on $y = 0$ and $y = 1$ we have the Dirichlet conditions $u = 1$ and $u = 0$, respectively.

```
class Problem1(Problem):
    """
    -div(p*grad(u))=f on the unit square.
    General Dirichlet, Neumann, or Robin condition along each
    side. Can have multiple subdomains with p constant in
    each subdomain.
    """
    def __init__(self, Nx, Ny):
        """Initialize mesh, boundary parts, and p."""
        self.mesh = UnitSquareMesh(Nx, Ny)

        tol = 1E-14

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

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

        class BoundaryY0(SubDomain):
            def inside(self, x, on_boundary):
```

```

        return on_boundary and abs(x[1]) < tol

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

        # Mark boundaries
        #self.boundary_parts = FacetFunction('size_t', mesh)
        self.boundary_parts = FacetFunction('uint', self.mesh)
        self.boundary_parts.set_all(9999)
        self.bx0 = BoundaryX0()
        self.bx1 = BoundaryX1()
        self.by0 = BoundaryY0()
        self.by1 = BoundaryY1()
        self.bx0.mark(self.boundary_parts, 0)
        self.bx1.mark(self.boundary_parts, 1)
        self.by0.mark(self.boundary_parts, 2)
        self.by1.mark(self.boundary_parts, 3)
        self.ds = Measure(
            'ds', domain=self.mesh,
            subdomain_data=self.boundary_parts)

    # The domain is the unit square with an embedded rectangle
    class Rectangle(SubDomain):
        def inside(self, x, on_boundary):
            return 0.3 <= x[0] <= 0.7 and 0.3 <= x[1] <= 0.7

            self.materials = CellFunction('size_t', self.mesh)
            self.materials.set_all(0) # "the rest"
            subdomain = Rectangle()
            subdomain.mark(self.materials, 1)
            self.V0 = FunctionSpace(self.mesh, 'DG', 0)
            self.p = Function(self.V0)
            help = np.asarray(self.materials.array(), dtype=np.int32)
            p_values = [1, 1E-3]
            self.p.vector()[:] = np.choose(help, p_values)

        def mesh_degree(self):
            return self.mesh, 2

        def p_coeff(self):
            return self.p

        def f_rhs(self):
            return Constant(0)

        def Dirichlet_conditions(self):
            """Return list of (value,boundary) pairs."""
            return [(1.0, self.boundary_parts, 2),
                    (0.0, self.boundary_parts, 3)]

        def Neumann_conditions(self):
            """Return list of g*ds(n) values."""
            return [(0, self.ds(0)), (0, self.ds(1))]
```

A specific problem can be solved by

```
def demo():
    problem = Problem1(Nx=20, Ny=20)
    problem.solve(linear_solver='direct')
    u = problem.solution()
    u.rename('u', 'potential') # name 'u' is used in plot
    plot(u)
    flux_u = problem.solver.flux()
    plot(flux_u)
    vtkfile = File('poisson.pvd')
    vtkfile << u
    interactive()
```

The complete code is found in the file `ft08_poisson_class.py`.

Pros and cons of solver/problem classes vs solver function

What are the advantages of class `Solver` and `Problem` over the function implementation in Section 3.4.4? The primary advantage is that the class version works for any mesh and any composition of boundary conditions, while the solver function is tied to a mesh over the unit square, only one type of boundary condition on each side, and a piecewise constant p function. The programmer has to supply more code in the class version, but gets greater flexibility. The disadvantage of the class version is that it applies the class concept so one needs experience with Python class programming.

Chapter 4

The diffusion solver revisited

This chapter is devoted to solving diffusion problems of the form

$$-\nabla \cdot (p \nabla u) = f,$$

with initial condition $u = I$ and various types of Dirichlet, Neumann, and Robin conditions. A very simple FEniCS program for a diffusion equation was introduced in Section 2.3, but here we shall discuss important algorithmic optimization strategies, how to store and animate time-dependent data, and how to construct more advanced solvers in terms of classes.

4.1 Optimization of algorithms and implementations

4.1.1 Avoiding some assembly

The time-dependent diffusion equation gives rise to a linear system $AU = b$ at each time level, where the coefficient matrix A is constant, but b depends on u at the previous time level. To increase the computational efficiency, we can therefore assemble A once and for all before the time loop. To be able to do this, we need to explicitly create matrices and vectors as demonstrated in Section 3.2.7.

Let us express the solution procedure in algorithmic form, writing u for the unknown spatial function at the new time level (u^k) and u_1 for the spatial solution at one earlier time level (u^{k-1}):

- define Dirichlet boundary condition (u_0 , Dirichlet boundary, etc.)
- let u_1 interpolate I or be the projection of I
- define a and L
- assemble matrix A from a

- set some stopping time T
- $t = \Delta t$
- while $t \leq T$
 - assemble vector b from L
 - apply essential boundary conditions
 - solve $AU = b$ for U and store in u
 - $t \leftarrow t + \Delta t$
 - $u_1 \leftarrow u$ (be ready for next step)

The code features the following changes from the `ft02_diffusion_flat1.py` program. We may define a and L from F as before, or do it explicitly:

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

Prior to the time loop we assemble the coefficient matrix A once and for all:

```
A = assemble(a) # assemble only once, before the time stepping
```

At each time level we can do a similar `b = assemble(L)`. With this construction, a new vector for `b` is allocated in memory in every pass of the time loop. It would be much more memory friendly to reuse the storage of the `b` we already have. This is easily accomplished by

```
b = assemble(L, tensor=b)
```

That is, we send in our previous `b`, which is then filled with new values and returned from `assemble`. Now there will be only a single memory allocation of the right-hand side vector. Before the time loop we set `b = None` such that `b` is defined in the first call to `assemble`.

The necessary changes inside the time loop go as follows:

```
while t <= T:
    b = assemble(L, tensor=b)
    u0.t = t
    bc.apply(A, b)
    solve(A, u.vector(), b)
```

The update `u0.t = t` is of key importance as `bc.apply(A, b)` will look up the `u0` object to find the proper values in the Dirichlet condition, and these change with time in our test problem!

The complete program is found in the file `ft09_diffusion_flat2.py`.

4.1.2 Avoiding all assembly

The purpose of this section is to present a technique for speeding up FEniCS simulators for time-dependent problems where it is possible to perform all

assembly operations prior to the time loop. There are two costly operations in the time loop: assembly of the right-hand side b and solution of the linear system via the `solve` call. The assembly process involves work proportional to the number of degrees of freedom N , while the solve operation has a work estimate of $\mathcal{O}(N^\alpha)$, for some $\alpha \geq 1$. Typically, $\alpha \in [1, 2]$. As $N \rightarrow \infty$, the solve operation will dominate for $\alpha > 1$, but for the values of N typically used on smaller computers, the assembly step may still represent a considerable part of the total work at each time level. Avoiding repeated assembly can therefore contribute to a significant speed-up of a finite element code in time-dependent problems.

Deriving recursive linear systems. To see how repeated assembly can be avoided, we look at the $L(v)$ form in (2.27), which in general varies with time through u^{k-1} , f^k , and possibly also with Δt if the time step is adjusted during the simulation. The technique for avoiding repeated assembly consists in expanding the finite element functions in sums over the basis functions ϕ_i , as explained in Section 3.2.7, to identify matrix-vector products that build up the complete system. We have $u^{k-1} = \sum_{j=1}^N U_j^{k-1} \phi_j$, and we can expand f^k as $f^k = \sum_{j=1}^N F_j^k \phi_j$. Inserting these expressions in $L(v)$ and using $v = \hat{\phi}_i$ result in

$$\begin{aligned} \int_\Omega (u^{k-1} + \Delta t f^k) v \, dx &= \int_\Omega \left(\sum_{j=1}^N U_j^{k-1} \phi_j + \Delta t \sum_{j=1}^N F_j^k \phi_j \right) \hat{\phi}_i \, dx, \\ &= \sum_{j=1}^N \left(\int_\Omega \hat{\phi}_i \phi_j \, dx \right) U_j^{k-1} + \Delta t \sum_{j=1}^N \left(\int_\Omega \hat{\phi}_i \phi_j \, dx \right) F_j^k. \end{aligned}$$

Introducing $M_{ij} = \int_\Omega \hat{\phi}_i \phi_j \, dx$, we see that the last expression can be written

$$\sum_{j=1}^N M_{ij} U_j^{k-1} + \Delta t \sum_{j=1}^N M_{ij} F_j^k,$$

which is nothing but two matrix-vector products,

$$MU^{k-1} + \Delta t MF^k,$$

if M is the matrix with entries M_{ij} ,

$$U^{k-1} = (U_1^{k-1}, \dots, U_N^{k-1})^T,$$

and

$$F^k = (F_1^k, \dots, F_N^k)^T.$$

We have immediate access to U^{k-1} in the program since that is the vector in the `u_1` function. The F^k vector can easily be computed by interpolating the prescribed f function (at each time level if f varies with time). Given M , U^{k-1} , and F^k , the right-hand side b can be calculated as

$$b = MU^{k-1} + \Delta t MF^k.$$

That is, no assembly is necessary to compute b .

The coefficient matrix A can also be split into two terms. We insert $v = \hat{\phi}_i$ and $u^k = \sum_{j=1}^N U_j^k \phi_j$ in the expression (2.26) to get

$$\sum_{j=1}^N \left(\int_{\Omega} \hat{\phi}_i \phi_j \, dx \right) U_j^k + \Delta t \sum_{j=1}^N \left(\int_{\Omega} \nabla \hat{\phi}_i \cdot \nabla \phi_j \, dx \right) U_j^k,$$

which can be written as a sum of matrix-vector products,

$$MU^k + \Delta t K U^k = (M + \Delta t K) U^k,$$

if we identify the matrix M with entries M_{ij} as above and the matrix K with entries

$$K_{ij} = \int_{\Omega} \nabla \hat{\phi}_i \cdot \nabla \phi_j \, dx. \quad (4.1)$$

The matrix M is often called the “mass matrix” while “stiffness matrix” is a common nickname for K . The associated bilinear forms for these matrices, as we need them for the assembly process in a FEniCS program, become

$$a_K(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (4.2)$$

$$a_M(u, v) = \int_{\Omega} uv \, dx. \quad (4.3)$$

The linear system at each time level, written as $AU^k = b$, can now be computed by first computing M and K , and then forming $A = M + \Delta t K$ at $t = 0$, while b is computed as $b = MU^{k-1} + \Delta t MF^k$ at each time level.

Implementation. The following modifications are needed in the `ft10_diffusion_func.py` program from the previous section in order to implement the new strategy of avoiding assembly at each time level:

1. Define separate forms a_M and a_K
2. Assemble a_M to M and a_K to K
3. Compute $A = M + \Delta t, K$
4. Define f as an `Expression`
5. Interpolate the formula for f to a finite element function F^k
6. Compute $b = MU^{k-1} + \Delta t MF^k$

The relevant code segments become

```
# 1.
a_K = dot(grad(u), grad(v))*dx
a_M = u*v*dx
# No need for L

# 2. and 3.
M = assemble(a_M)
K = assemble(a_K)
A = M + dt*K

# 4.
f = Expression('beta - 2 - 2*alpha', beta=beta, alpha=alpha)

# 5. and 6.
while t <= T:
    f_k = interpolate(f, V)
    F_k = f_k.vector()
    b = M*u_1.vector() + dt*M*F_k
```

hpl 19: I wonder if the refactoring should have a function first and then a class or if we jump right to the class. From now on we could use classes as the packaging of FEniCS programs.

We implement these modification in a refactored version of the program `ft09_diffusion_flat2.py`, where the solver is a function as explained in Section 3.1 rather than a flat program. The new `solver_minimize_assembly` function resides in `ft10_diffusion_func.py`.

```
def solver_minimize_assembly(
    alpha, f, u0, I, dt, T, Nx, Ny, degree=1,
    user_action=None, I_project=False):
    # Create mesh and define function space
    mesh = UnitSquareMesh(Nx, Ny)
    V = FunctionSpace(mesh, 'P', degree)

    class Boundary(SubDomain): # define the Dirichlet boundary
        def inside(self, x, on_boundary):
            return on_boundary

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

    # Initial condition
    u_1 = project(I, V) if I_project else interpolate(I, V)
    if user_action is not None:
        user_action(0, u_1, 0)

    # Define variational problem
    u = TrialFunction(V)
    v = TestFunction(V)
    a_M = u*v*dx
    a_K = alpha*dot(grad(u), grad(v))*dx
```

```

M = assemble(a_M)
K = assemble(a_K)
A = M + dt*K
# Compute solution
u = Function(V)    # the unknown at a new time level
b_assemble = 0      # CPU time for assembling all the b vectors
timestep = 1
t = dt
while t <= T:
    t0 = time.clock()
    f_k = interpolate(f, V)
    F_k = f_k.vector()
    b = M*u_1.vector() + dt*M*F_k
    b_assemble += time.clock() - t0
    try:
        u0.t = t
        f.t = t
    except AttributeError:
        pass    # ok if no t attribute in u0
    bc.apply(A, b)
    solve(A, u.vector(), b)

    if user_action is not None:
        user_action(t, u, timestep)
    t += dt
    timestep += 1
    u_1.assign(u)
    info('total time for assembly of right-hand side: %.2f' % b_assemble)

def application_animate(model_problem):
    import numpy as np, time

    if model_problem == 1:
        # Test problem with exact solution at the nodes also for P1 elements
        alpha = 3; beta = 1.2
        u0 = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                        alpha=alpha, beta=beta, t=0)
        f = Constant(beta - 2 - 2*alpha)
        I = u0
        dt = 0.05; T = 2
        Nx = Ny = 20
        u_range = [1, 1+1+alpha*1+beta*T]
    elif model_problem == 2:
        # Diffusion of a sin^8 spike
        I = Expression('pow(sin(pi*x[0])*sin(pi*x[1]), 8)')
        f = Constant(0)
        u0 = Constant(0)
        dt = 0.0005; T = 20*dt
        Nx = Ny = 60
        u_range = [0, 1]

    vtkfile = File('diffusion.pvd')

```

```

def animate(t, u, timestep):
    global p
    if t == 0:
        p = plot(u, title='u',
                  range_min=float(u_range[0]), # must be float
                  range_max=float(u_range[1])) # must be float
    else:
        p.plot(u)
    print('t=%g' % t)
    time.sleep(0.5)
    vtkfile << (u, float(t)) # store time-dep Function

    solver_minimize_assembly(
        1.0, f, u0, I, dt, T, Nx, Ny, degree=2,
        user_action=animate, I_project=False)

```

A special feature in this program is the `user_action` callback function: at every time level, the solution is sent to `user_action`, which is some function provided by the user where the solution can be processed, e.g., stored, analyzed, or visualized. In a unit test for the test example without numerical approximation errors, we can write a call to the solver function,

```

def test_solver():
    import numpy as np
    alpha = 3; beta = 1.2
    u0 = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
                    alpha=alpha, beta=beta, t=0)
    f = Constant(beta - 2 - 2*alpha)
    dt = 0.3; T = 1.9
    u0.t = 0

    # Define assert_error callback function
    ...

    solver_minimize_assembly(
        f, u0, u0, dt, T, Nx, Ny, degree,
        user_action=assert_error, I_project=False)

```

The `user_action` function `assert_error` asserts equality of the exact and numerical solution at every time level:

```

def assert_error(t, u, timestep):
    u_e = interpolate(u0, u.function_space())
    error = np.abs(u_e.vector().array() -
                   u.vector().array()).max()
    tol = 2E-12
    assert error < tol, 'error: %g' % error

```

One can also use the user action callback function to visualize the solution:

```

def assert_error(t, u, timestep):
    global p
    if t == 0:
        p = plot(u, title='u',

```

```

# Fix the color scale
range_min=float(u_range[0]), # must be float
range_max=float(u_range[1])) # must be float
else:
    p.plot(u)
print('t=%g' % t)
time.sleep(0.5)

```

It is key to fix the color scale to get a meaningful animation.

A complete function calling up `solver_minimize_assembly` for animating the solution in two test problems is found in the function `application_animate` in `ft10_diffusion_func.py`.

Note that `p`, which must survive between subsequent calls to the callback function, has to be declared as a global variable. This is necessary when the user action function is a *closure* (function inside function, “remembering” variables in the parent function) and `p` is changed inside the closure. Some programmers find it more convenient to let the user action be class instead, where `p` can be an attribute. Later examples employ the class design.

hpl 20: The function `solver_vs_solver_minimize_assembly` measures the impact of this optimization. It is not big: a factor of 1-2 for P1 elements but hardly anything for P2 elements. Tested up to 10^5 unknowns. However, the technique is important and it gave a significant speed-up when used in the Oasis CFD code by Mikael and co-workers (that code is open source).

hpl 21: I AM HERE!

4.2 A welding example with post processing and animation

The focus so far in this tutorial has been on producing the solution of PDE problems. For scientific investigations, the primary work is often with post processing results: computing quantities derived from the solution and inspecting these with visualization or data analysis tools. This is the focus of the present section. To ease the programming, we shall make use of a convenient tool, `cbcpost`, for post processing, saving data to file(s), and animating solutions. We recommend to use `cbcpost` in all time-dependent FEniCS solvers, but it also has a lot to offer in stationary problems too.

To explain the usage of `cbcpost` for storage and plotting, we address a real physical application: welding of a plate, where a moving heat source gives rise to a moving temperature field.

4.2.1 Post processing data and saving to file

Installation. The `cbcpost` package is not a part of the `fenics` package so you will need to install it. The simplest installation method is to use `pip`. We recommend to install a companion package `fenicstools` as well. Just run

```
sudo pip install git+https://bitbucket.org/simula_cbc/cbcpost.git
sudo pip install git+https://github.com/mikaem/fenicstools.git
```

in a terminal window (skip `sudo` on Windows machines). Alternatively, you can grab the source code and run `setup.py` the usual way Python packages are installed from source:

Terminal

```
Terminal> git clone https://bitbucket.org/simula_cbc/cbcpost.git
Terminal> cd cbcpost
Terminal> python setup.py install
Terminal> cd ..
Terminal> git clone https://github.com/mikaem/fenicstools.git
Terminal> cd fenicstools
Terminal> python setup.py install
```

Basic commands. We must create a *post processor* and then specify what kind of results we want to be stored on file and (optionally) get visualized. Suppose we have a field with logical name `Temperature` that we want to save in XDMF/HDF5 format in files in a fresh subdirectory `Results`:

```
import cbcpost as post
# Create post processor
pp = post.PostProcessor(dict(casedir='Results', clean_casedir=True))
# Specify storage of a "Temperature" field
pp.add_field(post.SolutionField(
    'Temperature',
    dict(save=True,
        save_as=['hdf5', 'xdmf'],
        plot=True,
        plot_args=dict(range_min=0.0, range_max=1.2))))
```

The `plot=True` automatically launches `fenics.plot` commands of this scalar field during the simulation. The ranges of the color scale must be given (as `float` variables) so that the color scale stays fixed during the animation on the screen.

Inside the time loop, we have to feed a new solution to the post processor to get it saved:

```
pp.update_all({'Temperature': lambda: T}, t, timestep)
```

Here, `T` is the `Function` object that we have solved for, `t` is current time, and `timestep` is the corresponding time step number.

One can specify many fields to be saved (and plotted), but even more important: `cbcpost` can calculate a lot of derived quantities from the solution, such as

- time derivatives and integrals of vector/scalar fields
- extraction of fields over subdomains
- slicing of fields in 3D geometries
- averaging of fields in space or time
- norms and point values of fields as function of time
- user-defined post processing of fields

Tip: Use `cbcpost` to visualize time-dependent data

Instead of issuing your own `plot` commands in time-dependent problems, it is safer and more convenient to specify `plot=True` and fix the range of the color scale, when you add fields to the post processor. Multiple fields will be synchronized during the animation.

4.2.2 Heat transfer due to a moving welding source

Let us solve a real diffusion problem taken from welding. A moving welding equipment acts as a moving heat source at the top of a thin metal plate. The question is how the heat from the equipment spreads out in the material that is being welded. We use the standard heat equation, treat the material as two dimensional, and do not take phase transitions into account. The governing PDE is then

$$\varrho c \frac{\partial u}{\partial t} = k \nabla^2 u + f,$$

where u is temperature, ϱ is the density of the material, c is the heat capacity at constant volume, k is the heat conduction coefficient, and f models the heat source from the welding equipment. The domain is $\Omega = [0, L] \times [0, L]$. An additional major simplification is that we set $u = U_s$ at the boundary, where U_s is the temperature of the surroundings (a Robin condition, modeling cooling at the boundary would be more accurate, but then we should also consider cooling in the third dimension as well). The initial condition reads $u = U_s$.

A welding source is moving and very localized in space. The localization can be modeled by a peak-shaped Gaussian function. The movement is taken to be a circle with radius R about a point (x_0, y_0) . An appropriate f is

$$f(x, y, t) = A \exp \left(-\frac{1}{2\sigma^2} (x - (x_0 + R \cos \omega t))^2 - \frac{1}{2} (y - (y_0 + R \sin \omega t))^2 \right).$$

The parameter A is the strength of the heat source, and σ is the “standard deviation” (i.e., a measure of the width) of the Gaussian function.

4.2.3 Scaling of the welding problem

There are 10 physical parameters in the problem: L , ϱ , c , k , A , x_0 , y_0 , R , ω , σ . Scaling can dramatically reduce the number of parameters and also introduce new parameters that are much easier to assign numerical values. We therefore scale the problem. As length scale, we choose L so the scaled domain becomes the unit square. As time scale and characteristic size of u , we just introduce t_c and u_c . This means that we introduce scaled variables

$$\bar{x} = \frac{x}{L}, \quad \bar{y} = \frac{y}{L}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{u} = \frac{u - U_s}{u_c}.$$

The scaled form of f is naturally $\bar{f} = f/A$, since this makes $\bar{f} \in (0, 1]$. The arguments in the exponential function in f can also be scaled:

$$\begin{aligned} \bar{f} &= \exp\left(-\frac{1}{2\sigma^2} (\bar{x}L - (L\bar{x}_0 + L\bar{R}\cos\omega t_c \bar{t}))^2 - \frac{1}{2\sigma^2} (L\bar{y} - (L\bar{y}_0 + L\bar{R}\sin\omega t_c \bar{t}))^2\right) \\ &= \exp\left(-\frac{1}{2} \frac{L^2}{\sigma^2} (x - (\bar{x}_0 + \bar{R}\cos\omega t_c \bar{t}))^2 - \frac{1}{2} (\bar{y} - (\bar{y}_0 + \bar{R}\sin\omega t_c \bar{t}))^2\right) \\ &= \exp\left(-\frac{1}{2} \beta \left(x - \left(\frac{1}{2} + \bar{R}\cos\bar{t}\right)\right)^2 - \frac{1}{2} \left(\bar{y} - \left(\frac{1}{2} + \bar{R}\sin\bar{t}\right)\right)^2\right), \end{aligned}$$

where β is a dimensionless parameter,

$$\beta = \frac{L}{\sigma},$$

reflecting the ratio of the domain size and the width of the heat source. Moreover, we have restricted the rotation point to be the center point of the domain:

$$(\bar{x}_0, \bar{y}_0) = \left(\frac{1}{2}, \frac{1}{2}\right).$$

The time scale in diffusion problems is usually related to the “speed of the diffusion”, but in this problem it is more natural to base the time scale on the movement of the heat source, which suggests setting $t_c = 1/\omega$.

Inserting the new scaled variables in the PDE leads to

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{k}{\omega \varrho c L^2} \bar{\nabla}^2 \bar{u} + \frac{A}{\omega u_c \varrho c} \bar{f}(\bar{x}, \bar{y}, \bar{t}).$$

The first coefficient is a dimensionless number,

$$\gamma = \frac{k}{\omega \varrho c L^2},$$

while the second coefficient can be used to determine u_c by demanding the source term to balance the time derivative term,

$$u_c = \frac{A}{\omega \varrho c}.$$

Our aim is to have $\bar{u} \in [0, 1]$, but this u_c do not capture the precise magnitude of u . However, we believe that the characteristic size of u is

$$u_c = \delta^{-1} \frac{A}{\omega \varrho c},$$

for a scaling factor δ . Using this u_c gives the PDE

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \gamma \bar{\nabla}^2 \bar{u} + \delta \bar{f}(\bar{x}, \bar{y}, \bar{t}),$$

with two dimensionless variables, but δ is tuned from experiments to give \bar{u} a typically size of unity.

Looking at γ , we see that it can be written

$$\gamma = \frac{1/\omega}{\varrho c L^2/k},$$

which is the ratio of the time scale for the heat source and the time scale for diffusion. Multiplying by R/R gives another interpretation: γ is the ratio of the speed of diffusion and the speed of the heat source.

The benefits of scaling

The physics of our problem depends now on β , \bar{R} , and γ , just three ratios of physical effects instead of 10 independent parameters. Setting $\bar{R} = 0.2$ is an appropriate choice. For a quite localized heat source in space, $\beta = 10$ is a suitable value. Then we are actually left with only one interesting parameter to adjust: γ . It is so much easier to assign this parameter a value (speed of diffusion versus speed of heat source) than to set ϱ , c , and k for some chosen material, and then determine relevant values for A , L , etc. There are no approximations in the scaling procedure; it just dramatically simplifies numerical simulations. The book [19] gives a comprehensive treatment of scaling.

4.2.4 A function-based solver

We can use the `solver_minimize_assembly` function to solve the welding problem. The application code just declares the problem-dependent parameters and calls the solver function. From a trial run we find that $\delta = 700$ gives \bar{u} of unit size for moderate γ values.

```
def application_welding(gamma=1, delta=1, beta=10, num_rotations=2):
    """Circular moving heat source for simulating welding."""
    from math import pi, sin, cos
    u0 = Constant(0)
    I = Constant(0)
    R = 0.2
    f = Expression(
        'delta*exp(-0.5*pow(beta,2)*(pow(x[0]-(0.5+R*cos(t)),2) + '
        'pow(x[1]-(0.5+R*sin(t)),2)))',
        delta=delta, beta=beta, R=R, t=0)
    # Simulate to rotations with the equipment
    omega = 1.0      # Scaled angular velocity
    P = 2*pi/omega  # One period of rotation
    T = 2*P          # Total simulation time
    dt = P/40         # 40 steps per rotation
    Nx = Ny = 60
    solver_minimize_assembly(
        gamma, f, u0, I, dt, T, Nx, Ny, degree=1,
        user_action=ProcessResults(), I_project=False)
```

The remaining task is to write the user action callback function to process the solution at each time step. We want to make use of `cbcpost` for storage and plotting. Since we need the post processor variable, called `pp` in Section 4.2.1, needs to survive between calls to the user action function, we find it most convenient to implement this function in terms of a class with `pp` as attribute and `__call__` as the user action function. We want to make comparisons between the heat source and the temperature response, so we register both fields for storage and plotting:

```
import cbcpost as post
class ProcessResults(object):
    def __init__(self):
        self.pp = post.PostProcessor(
            dict(casedir='Results', clean_casedir=True))
        self.pp.add_field(
            post.SolutionField(
                'Temperature',
                dict(save=True,
                    save_as=['hdf5', 'xdmf'], # format
                    plot=True,
                    plot_args=
                        dict(range_min=0.0, range_max=1.1)
                )))
        self.pp.add_field(
            post.SolutionField(
```

```

    "Heat_source",
    dict(save=True,
        save_as=["hdf5", "xdmf"], # format
        plot=True,
        plot_args=
            dict(range_min=0.0, range_max=float(delta))
        )))
# Save separately to VTK files as well
self.vtkfile_T = File('temperature.pvd')
self.vtkfile_f = File('source.pvd')
def __call__(self, t, T, timestep):
    # Store temperature and heat source to cbcpost file
    # and to VTK file
    T.rename('T', 'solution')
    f_Function = interpolate(f, T.function_space())
    f_Function.rename('f', 'welding equipment')
    self.pp.update_all(
        {'Temperature': lambda: T,
         'Heat_source': lambda: f_Function},
        t, timestep)
    self.vtkfile_T << (T, float(t))
    self.vtkfile_f << (f_Function, float(t))

```

We took the opportunity in the callback function (`__call__`) to also store the `u` and `f` functions to VTK files, although this is really not necessary since ParaView or VisIt can read XDMF files.

Note that the use of `cbcpost` is usually very dependent on the problem at hand, so it does not make sense to include `cbcpost` code in a general PDE solver, only in problem-specific code such as the user action function.

Getting an animation on the screen with the built-in plotting tool is a matter of running the welding example:

```

>>> from diffusion_func import application_welding as a
>>> a(gamma=10, delta=700)

```

(We introduced the synonym `a` to save some typing.) Or you can run this as a command in the terminal:

Terminal> python -c '\nfrom diffusion_func import application_welding as a;\na(gamma=10, delta=700)'
Terminal

Since we have fixed the color scale of the temperature to have values in $[0, 1.1]$, we must adjust δ appropriately to γ . For example, running $\gamma = 40$ reveals, from the output in the terminal, that the maximum temperature is about 0.25, and consequently we do not see much. For any given γ , run the problem with $\delta = 1$ (and say `num_rotations=0.2` to make a quick simulation), and rerun with δ as one over the maximum temperature. Here we get an approximate $\delta = 66.7\gamma$ for $\gamma \leq 0.1$. Try running $\gamma = 0.01$ and $\delta = 1$ to observe some more significant heat transfer away from the welding equipment.

With $\gamma = 0.001$ there is significant heat build-up, but for so small γ we should re-scale the problem and use the diffusion time scale as time scale.

In ParaView, load `Results/Temperature/Temperature.xdmf` as file, click **Apply**, then the play button for animation. If the animation is not correct, repeat the procedure. Thereafter, split the layout in two, choose **3D View**, load `Results/Heat source/Heat_source.xmdf`, click **Apply**, and run the animation. The two plots are synchronized in time.

Movie 1: Welding example with $\gamma = 1$. https://github.com/hplgit/fenics-tutorial/tree/brief/doc/pub/mov/welding_gamma1.ogg

4.3 Refactored implementation

The flat program for the diffusion solver in `ft02_diffusion_flat1.py` and `ft09_diffusion_flat2.py` was refactored in `ft10_diffusion_func.py` in terms of a `solver` function with the general code for solving the PDE problem, a callback function for processing the solution at each time step, and an application function defining the callback function and calling the solver to solve a specific problem. However, for time-dependent problems a solver function that gets all its input through a set of arguments is less flexible than a solver *class*, which can demand its input both through arguments and through functions (in subclasses) provided by the user. The following text requires you to be familiar with class programming in Python (tailored learning material is Chapter 7, 9, and Appendix E in [17]).

When we work with a PDE project, we often want to explore a range or similar problems where the PDE model basically stays the same, but coefficients in the PDE, boundary and initial conditions, as well as domains change. This means that some of our code related to solving the PDE is always the same, while some of our code is strongly dependent upon a particular application. To avoid copying code (which is considered evil in computer programming), we need to collect the common code for all problems of this type in one place and then create an API (application programming interface) to the code that will be different from application to application. To this end, we introduce a *solver class* that applies FEniCS to solve the PDE. It requires access to a *problem class* where all the application-specific details are defined. This problem class defines an API that the solver class applies for communication.

The solver class will usually have only a constructor to set up data structures (typically the variational formulation), a `step` function to advance the solution one time step, and a `solve` function to run the time loop. Every time the solver class needs problem-specific information, it needs to get that from the problem class, either in terms of attributes (variables) in the class or in terms of method (function) calls. The forthcoming examples are tied

to the diffusion equation, but should be sufficiently general to be reused for most time-dependent FEniCS applications.

4.3.1 A class-based solver for a general diffusion problem

The simplest part is the solver class. It contains the data structures and actions from previous programs, but needs to ask the problem class about the mesh, boundary conditions, the time step, and so forth. We therefore need to define the API of the problem class first so we know how the solver class can ask for the mesh, for instance.

Here is an abstract problem class:

```
class Problem(object):
    """Abstract base class for specific diffusion applications."""

    def solve(self, solver_class=Solver, linear_solver='direct',
              abs_tol=1E-6, rel_tol=1E-5, max_iter=1000):
        """Solve the PDE problem for the primary unknown."""
        self.solver = solver_class(self)
        iterative_solver = KrylovSolver('gmres', 'ilu')
        prm = iterative_solver.parameters
        prm['absolute_tolerance'] = abs_tol
        prm['relative_tolerance'] = rel_tol
        prm['maximum_iterations'] = max_iter
        prm['nonzero_initial_guess'] = True # Use u (last sol.)
        return self.solver.solve()

    def flux(self):
        """Compute and return flux -p*grad(u)."""
        mesh = self.mesh()
        degree = self.solution().ufl_element().degree()
        V_g = VectorFunctionSpace(mesh, 'P', degree)
        self.flux_u = project(-self.p*grad(self.u), V_g)
        self.flux_u.rename('flux(u)', 'continuous flux field')
        return self.flux_u

    def mesh_degree(self):
        """Return mesh, degree."""
        raise NotImplementedError('Must implement mesh')

    def I(self):
        """Return initial condition."""
        return Constant(0.0)

    def p_coeff(self):
        return Constant(1.0)

    def f_rhs(self):
```

```

        return Constant(0.0)

    def time_step(self, t):
        raise NotImplentedError('Must implement time_step')

    def end_step(self):
        raise NotImplentedError('Must implement end_time')

    def solution(self):
        return self.solver.u

    def user_action(self, t, u):
        """Post process solution u at time t."""
        pass

    def update_boundary_conditions(self, t):
        """Update t parameter in Expression objects in BCs."""
        pass

    def Dirichlet_conditions(self):
        """Return either an Expression (for the entire boundary) or
        a list of (value,boundary_parts,index) triplets."""
        return []

    def Neumann_conditions(self):
        """Return list of (g,ds(n)) pairs."""
        return []

    def Robin_conditions(self):
        """Return list of (r,s,ds(n)) triplets."""
        return []

```

The meaning of the different methods in this class will be evident as we present specific examples on implementations.

The idea now is that different problems are implemented as different subclasses of `Problem`. The `solve` and `flux` methods are general and can be inherited, while the rest of the methods must be implemented in the subclass.

As a simple example, consider the test problem where we have a manufactured solution $u = 1 + x^2 + \alpha y^2 + \beta t$ on a uniform mesh over the unit square and Dirichlet conditions on the entire boundary. Suppose we have $\Delta t = 0.3$ and want to simulate for $t \in [0, 0.9]$. A problem class is then

```

class TestProblemExact(Problem):
    def __init__(self, Nx, Ny):
        self.mesh = UnitSquareMesh(Nx, Ny)
        alpha = 3; beta = 1.2
        self.u0 = Expression(
            '1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t',
            alpha=alpha, beta=beta, t=0)
        self.f = Constant(beta - 2 - 2*alpha)
    def time_step(self, t):
        return 0.3

```

```

def end_time(self):
    return 0.9
def mesh_degree(self):
    return self.mesh, 1
def I(self):
    """Return initial condition."""
    return self.u0
def f_rhs(self):
    return self.f
def Dirichlet_conditions(self):
    return self.u0
def update_boundary_conditions(self, t):
    """Update t parameter in Expression objects in BCs."""
    self.u0.t = t
def user_action(self, t, u):
    """Post process solution u at time t."""
    u_e = interpolate(self.u0, u.function_space())
    error = np.abs(u_e.vector().array() -
                   u.vector().array()).max()
    print('error at %g: %g' % (t, error))
    assert error < 2E-15, 'max_error: %g' % error

```

The problem is now solved by

```

problem = TestProblemExact(Nx=2, Ny=2)
problem.solve(linear_solver='direct')
u = problem.solution()

```

The solver class will call the `user_action` function at every time level, and this function will assert that we recover the solution to machine precision (note that if we change the degree of the elements, or increase the mesh size, we need a less restrict tolerance!).

The solver class, here based on the algorithm in Section 4.1.2, can be coded as follows:

```

class Solver(object):
    def __init__(self, problem):
        self.problem = problem
        self.mesh, degree = problem.mesh_degree()
        self.V = V = FunctionSpace(self.mesh, 'P', degree)

        # Initial condition
        if hasattr(problem, 'I_project'):
            I_project = getattr(problem, 'I_project')
        else:
            I_project = False
        self.u_1 = project(problem.I(), V) if I_project \
                  else interpolate(problem.I(), V)
        self.u_1.rename('u', 'initial condition')
        problem.user_action(0, self.u_1)

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

```

```

    p = problem.p_coeff()
    self.p = p # store for flux computations
    a_M = u*v*dx
    a_K = dot(p*grad(u), grad(v))*dx
    a_K += sum([r*u*v*ds_
        for r, s, ds_ in problem.Robin_conditions()])
    self.M = assemble(a_M)
    self.K = assemble(a_K)

    self.f = problem.f_rhs() # used in step()
    L = Constant(0)*v*dx # Must initialize L if next line has empty lists
    # f is handled in the time loop by interpolation and M matrix
    L -= sum([g*v*ds_
        for g, ds_ in problem.Neumann_conditions()])
    L -= sum([r*s*v*ds_
        for r, s, ds_ in problem.Robin_conditions()])
    # Note: updating of Expression objects (t attribute)
    # does not change these a_* and L expressions.
    self.b_surface_int = assemble(L)
    self.u = Function(V) # the unknown at a new time level
    self.u.rename('u', 'solution')
    self.T = problem.end_time()

def step(self, t, linear_solver='direct',
        abs_tol=1E-6, rel_tol=1E-5, max_iter=1000):
    """Advance solution one time step."""
    # Find new Dirichlet conditions at this time step
    Dirichlet_cond = self.problem.Dirichlet_conditions()
    if isinstance(Dirichlet_cond, Expression):
        # Just one Expression for Dirichlet conditions on
        # the entire boundary
        self.bcs = [DirichletBC(
            self.V, Dirichlet_cond,
            lambda x, on_boundary: on_boundary)]
    else:
        # Boundary SubDomain markers
        self.bcs = [
            DirichletBC(self.V, value, boundaries, index)
            for value, boundaries, index
            in Dirichlet_cond]

    # Update A
    self.dt = self.problem.time_step(t)
    A = self.M + self.dt*self.K

    # Update right-hand side
    f_k = interpolate(self.f, self.V)
    F_k = f_k.vector()
    b = self.M*self.u_1.vector() + self.dt*self.M*F_k + \
        self.dt*self.b_surface_int
    self.problem.update_boundary_conditions(t)

    # Solve linear system
    [bc.apply(A, b) for bc in self.bcs]

```

```

if linear_solver == 'direct':
    solve(A, self.u.vector(), b)
else:
    solver = KrylovSolver('gmres', 'ilu')
    solver.solve(A, self.u.vector(), b)

def solve(self):
    """Run time loop."""
    self.dt = self.problem.time_step(0)
    t = self.dt
    while t <= self.T:
        self.step(t)
        self.problem.user_action(t, self.u)
        t += self.dt
        self.u_1.assign(self.u)

```

- Think about Crank-Nicolson as subclass!
- Some simple diffusion problems with varying Δt , focus on a flux at a part of the boundary, etc. Can also be exercises.

4.3.2 A physical example

With the basic programming techniques for time-dependent problems from Sections 4.1.2 and 2.3.2 we are ready to attack more physically realistic examples. The next example concerns the question: How is the temperature in the ground affected by day and night variations at the earth's surface? We consider some box-shaped domain Ω in d dimensions with coordinates x_0, \dots, x_{d-1} (the problem is meaningful in 1D, 2D, and 3D). At the top of the domain, $x_0 = 0$, we have an oscillating temperature

$$T_0(t) = T_R + T_A \sin(\omega t),$$

where T_R is some reference temperature, T_A is the amplitude of the temperature variations at the surface, and ω is the frequency of the temperature oscillations. At all other boundaries we assume that the temperature does not change anymore when we move away from the boundary, i.e., the normal derivative is zero. Initially, the temperature can be taken as T_R everywhere. The heat conductivity properties of the soil in the ground may vary with space so we introduce a variable coefficient κ reflecting this property. Figure 4.1 shows a sketch of the problem, with a small region where the heat conductivity is much lower. **hpl 22:** All parameters ϱ , c , and κ are different!

The initial-boundary value problem for this problem reads

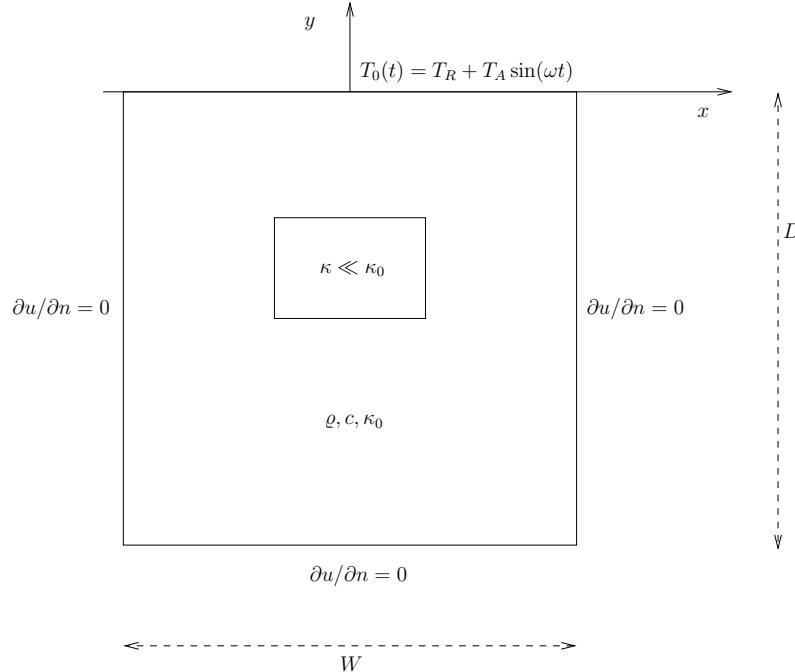


Fig. 4.1 Sketch of a (2D) problem involving heating and cooling of the ground due to an oscillating surface temperature.

$$\varrho c \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) \text{ in } \Omega \times (0, t_{\text{stop}}], \quad (4.4)$$

$$T = T_0(t) \text{ on } \Gamma_0, \quad (4.5)$$

$$\frac{\partial T}{\partial n} = 0 \text{ on } \partial\Omega \setminus \Gamma_0, \quad (4.6)$$

$$T = T_R \text{ at } t = 0. \quad (4.7)$$

Here, ϱ is the density of the soil, c is the heat capacity, κ is the thermal conductivity (heat conduction coefficient) in the soil, and Γ_0 is the surface boundary $x_0 = 0$.

We use a θ -scheme in time, i.e., the evolution equation $\partial P / \partial t = Q(t)$ is discretized as

$$\frac{P^k - P^{k-1}}{\Delta t} = \theta Q^k + (1 - \theta) Q^{k-1},$$

where $\theta \in [0, 1]$ is a weighting factor: $\theta = 1$ corresponds to the backward difference scheme, $\theta = 1/2$ to the Crank-Nicolson scheme, and $\theta = 0$ to a forward difference scheme. The θ -scheme applied to our PDE results in

$$\varrho c \frac{T^k - T^{k-1}}{\Delta t} = \theta \nabla \cdot (\kappa \nabla T^k) + (1-\theta) \nabla \cdot (k \nabla T^{k-1}).$$

Bringing this time-discrete PDE into weak form follows the technique shown many times earlier in this tutorial. In the standard notation $a(T, v) = L(v)$ the weak form has

$$a(T, v) = \int_{\Omega} (\varrho c T v + \theta \Delta t \kappa \nabla T \cdot \nabla v) dx, \quad (4.8)$$

$$L(v) = \int_{\Omega} \left(\varrho c T^{k-1} v - (1-\theta) \Delta t \kappa \nabla T^{k-1} \cdot \nabla v \right) dx. \quad (4.9)$$

Observe that boundary integrals vanish because of the Neumann boundary conditions.

The size of a 3D box is taken as $W \times W \times D$, where D is the depth and $W = D/2$ is the width. We give the degree of the basis functions at the command line, then D , and then the divisions of the domain in the various directions. To make a box, rectangle, or interval of arbitrary (not unit) size, we have the classes `BoxMesh`, `RectangleMesh`, and `IntervalMesh` at our disposal. The mesh and the function space can be created by the following code:

```
degree = int(sys.argv[1])
D = float(sys.argv[2])
W = D/2.0
divisions = [int(arg) for arg in sys.argv[3:]]
d = len(divisions) # no of space dimensions
if d == 1:
    mesh = IntervalMesh(divisions[0], -D, 0)
elif d == 2:
    mesh = RectangleMesh(-W/2, -D, W/2, 0, divisions[0], divisions[1])
elif d == 3:
    mesh = BoxMesh(-W/2, -W/2, -D, W/2, W/2, 0,
                  divisions[0], divisions[1], divisions[2])
V = FunctionSpace(mesh, 'P', degree)
```

The `RectangleMesh` and `BoxMesh` objects are defined by the coordinates of the "minimum" and "maximum" corners.

Setting Dirichlet conditions at the upper boundary can be done by

```
T_R = 0; T_A = 1.0; omega = 2*pi
T_0 = Expression('T_R + T_A*sin(omega*t)', T_R=T_R, T_A=T_A, omega=omega, t=0.0)

def surface(x, on_boundary):
    return on_boundary and abs(x[d-1]) < 1E-14

bc = DirichletBC(V, T_0, surface)
```

The κ function can be defined as a constant κ_1 inside the particular rectangular area with a special soil composition, as indicated in Figure 4.1. Outside this area κ is a constant κ_0 . The domain of the rectangular area is taken as

$$[-W/4, W/4] \times [-W/4, W/4] \times [-D/2, -D/2 + D/4]$$

in 3D, with $[-W/4, W/4] \times [-D/2, -D/2 + D/4]$ in 2D and $[-D/2, -D/2 + D/4]$ in 1D. Since we need some testing in the definition of the $\kappa(\mathbf{x})$ function, 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 Kappa(Expression):
    def eval(self, value, x):
        """x: spatial point, value[0]: function value."""
        d = len(x) # no of space dimensions
        material = 0 # 0: outside, 1: inside
        if d == 1:
            if -D/2. < x[d-1] < -D/2. + D/4.:
                material = 1
        elif d == 2:
            if -D/2. < x[d-1] < -D/2. + D/4. and \
               -W/4. < x[0] < W/4.:
                material = 1
        elif d == 3:
            if -D/2. < x[d-1] < -D/2. + D/4. and \
               -W/4. < x[0] < W/4. and -W/4. < x[1] < W/4.:
                material = 1
        value[0] = kappa_0 if material == 0 else kappa_1
```

The `eval` method gives great flexibility in defining functions, but a downside is that C++ calls up `eval` in Python for each point \mathbf{x} , which is a slow process, and the number of calls is proportional to the number of numerical integration points in the mesh (about the number of degrees of freedom). Function expressions in terms of strings are compiled to efficient C++ functions, being called from C++, so we should try to express functions as string expressions if possible. (The `eval` method can also be defined through C++ code, but this is much more complicated and not covered here.) Using inline if-tests in C++, we can make string expressions for κ , here stored in a Python dictionary so that `kappa_str[d-1]` is the proper test in a d dimensional problem:

```
kappa_str = {}
kappa_str[1] = 'x[0] > -D/2 && x[0] < -D/2 + D/4 ? kappa_1 : kappa_0'
kappa_str[2] = 'x[0] > -W/4 && x[0] < W/4 \
               && x[1] > -D/2 && x[1] < -D/2 + D/4 ? \
               kappa_1 : kappa_0'
kappa_str[3] = 'x[0] > -W/4 && x[0] < W/4 \
               'x[1] > -W/4 && x[1] < W/4 \
               && x[2] > -D/2 && x[2] < -D/2 + D/4 ? \
               kappa_1 : kappa_0'
```

```
kappa = Expression(kappa_str[d],
                    D=D, W=W, kappa_0=kappa_0, kappa_1=kappa_1)
```

Let T denote the unknown spatial temperature function at the current time level, and let T_{-1} be the corresponding function at one earlier time level. We are now ready to define the initial condition and the a and L forms of our problem:

```
T_prev = interpolate(Constant(T_R), V)

rho = 1
c = 1
period = 2*pi/omega
t_stop = 5*period
dt = period/20 # 20 time steps per period
theta = 1

T = TrialFunction(V)
v = TestFunction(V)
f = Constant(0)
a = rho*c*T*v*dx + theta*dt*kappa*\
    dot(grad(T), grad(v))*dx
L = (rho*c*T_prev*v + dt*f*v -
      (1-theta)*dt*kappa*dot(grad(T_1), grad(v)))*dx

A = assemble(a)
b = None # variable used for memory savings in assemble calls
T = Function(V) # unknown at the current time level
```

We could, alternatively, break a and L up in subexpressions and assemble a mass matrix and stiffness matrix, as exemplified in Section 4.1.2, to avoid assembly of b at every time level. This modification is straightforward and left as an exercise. The speed-up can be significant in 3D problems.

The time loop is very similar to what we have displayed in Section 2.3.2:

```
T = Function(V) # unknown at the current time level
t = dt
while t <= t_stop:
    b = assemble(L, tensor=b)
    T_0.t = t
    bc.apply(A, b)
    solve(A, T.vector(), b)
    # visualization statements
    t += dt
    T_prev.assign(T)
```

The complete code in `ft11_sin_daD.py` contains several statements related to visualization and animation of the solution, both as a finite element field (`plot` calls) and as a curve in the vertical direction. The code also plots the exact analytical solution,

$$T(x, t) = T_R + T_A e^{ax} \sin(\omega t + ax), \quad a = \sqrt{\frac{\omega \rho c}{2\kappa}},$$

which is valid when $\kappa = \kappa_0 = \kappa_1$.

Implementing this analytical solution as a Python function taking scalars and numpy arrays as arguments requires a word of caution. A straightforward function like

```
def T_exact(x):
    a = sqrt(omega*rho*c/(2*kappa_0))
    return T_R + T_A*exp(a*x)*sin(omega*t + a*x)
```

will not work and result in an error message from UFL. The reason is that the names `exp` and `sin` are those imported by the `from fenics import *` statement, and these names come from UFL and are aimed at being used in variational forms. In the `T_exact` function where `x` may be a scalar or a numpy array, we therefore need to explicitly specify `np.exp` and `np.sin` (if numpy is imported under the common name `np`):

```
def T_exact(x):
    a = sqrt(omega*rho*c/(2*kappa_0))
    return T_R + T_A*np.exp(a*x)*np.sin(omega*t + a*x)
```

The complete code is found in the file `exact.py`. The reader is encouraged to play around with the code and test out various parameter sets:

1. $T_R = 0$, $T_A = 1$, $\kappa_0 = \kappa_1 = 0.2$, $\varrho = c = 1$, $\omega = 2\pi$
2. $T_R = 0$, $T_A = 1$, $\kappa_0 = 0.2$, $\kappa_1 = 0.01$, $\varrho = c = 1$, $\omega = 2\pi$
3. $T_R = 0$, $T_A = 1$, $\kappa_0 = 0.2$, $\kappa_1 = 0.001$, $\varrho = c = 1$, $\omega = 2\pi$
4. $T_R = 10$ C, $T_A = 10$ C, $\kappa_0 = 2.3 \text{ K}^{-1}\text{Ns}^{-1}$, $\kappa_1 = 100 \text{ K}^{-1}\text{Ns}^{-1}$, $\varrho = 1500 \text{ kg/m}^3$, $c = 1480 \text{ Nm} \cdot \text{kg}^{-1}\text{K}^{-1}$, $\omega = 2\pi/24$ 1/h = $7.27 \cdot 10^{-5}$ 1/s, $D = 1.5$ m
5. As above, but $\kappa_0 = 12.3 \text{ K}^{-1}\text{Ns}^{-1}$ and $\kappa_1 = 10^4 \text{ K}^{-1}\text{Ns}^{-1}$

Data set number 4 is relevant for real temperature variations in the ground (not necessarily the large value of κ_1), while data set number 5 exaggerates the effect of a large heat conduction contrast so that it becomes clearly visible in an animation.

Chapter 5

The nonlinear Poisson solver revisited

FEniCS can be used in alternative ways for solving a nonlinear PDE problem. We shall in the following subsections go through three solution strategies:

- a simple Picard-type iteration
- a Newton method at the algebraic level
- a Newton method at the PDE level

The examples will show how tailored solution algorithms can easily be implemented in a FEniCS solver. (The exposition will hopefully also help newcomers to the finite element method to understand the method better.) However, first we provide more information for using the built-in automated Newton solver that was demonstrated in Section 2.4.2.

Test problem. We continue to address the nonlinear Poisson problem $-\nabla \cdot (q(u)\nabla u) = f$. To be able to easily verify our implementation, we choose the domain, $q(u)$, f , and the boundary conditions such that we have a simple, exact solution u . Let Ω be the unit hypercube $[0,1]^d$ in d dimensions, $q(u) = (1+u)^m$, $f = 0$, $u = 0$ for $x_0 = 0$, $u = 1$ for $x_0 = 1$, and $\partial u / \partial n = 0$ at all other boundaries $x_i = 0$ and $x_i = 1$, $i = 1, \dots, d-1$. The coordinates are now represented by the symbols x_0, \dots, x_{d-1} . The exact solution is then

$$u(x_0, \dots, x_{d-1}) = ((2^{m+1} - 1)x_0 + 1)^{1/(m+1)} - 1. \quad (5.1)$$

We refer to Section 3.2.4 for details on formulating a PDE problem in d space dimensions.

5.1 The built-in automated Newton solver

Solving nonlinear problems in FEniCS is a matter of defining the nonlinear variational form F and calling `solve(F == 0, ...)` as explained in Section 2.4.2. However, in real problems we will at least have control of the

tolerance used in the stopping criterion in Newton's method. Sometimes we also want to derive the Jacobian ourselves or provide approximations. Such customizations are shown next.

5.1.1 Computing the Jacobian

We may provide the Jacobian for Newton's method as argument to `solve`: `solve(F == 0, u, bcs=bcs, J=J)`. However, if you have several nonlinear problems within the same code and want different solvers for them, it is better to use these objects:

```
problem = NonlinearVariationalProblem(F, u, bcs, J)
solver = NonlinearVariationalSolver(problem)
solver.solve()
```

Here, `F` corresponds to the nonlinear form $F(u; v)$, `u` is the unknown `Function` object, `bcs` represents the essential boundary conditions (in general a list of `DirichletBC` objects), and `J` is a variational form for the Jacobian of `F`.

The `F` form corresponding to (2.34) is straightforwardly defined as follows, assuming `q(u)` is coded as a Python function (see Section 2.4.2 for code):

```
u_ = Function(V)      # most recently computed solution
v = TestFunction(V)
F = dot(q(u_)*grad(u_), grad(v))*dx
```

Note here that `u_` is a `Function` and not a `TrialFunction`. An alternative and perhaps more intuitive formula for F is to define $F(u; v)$ directly in terms of a trial function for u and a test function for v , and then create the proper `F` by

```
u = TrialFunction(V)
v = TestFunction(V)
F = dot(q(u)*grad(u), grad(v))*dx
u_ = Function(V)      # the most recently computed solution
F = action(F, u_)
```

The latter statement is equivalent to $F(u = u_-; v)$, where u_- is an existing finite element function representing the most recently computed approximation to the solution. (Note that u^k and u^{k+1} in the previous notation correspond to u_- and u in the present notation. We have changed notation to better align the mathematics with the associated UFL code.)

The derivative J (`J`) of F (`F`) is formally the Gateaux derivative $DF(u^k; \delta u, v)$ of $F(u; v)$ at $u = u_-$ in the direction of δu . Technically, this Gateaux derivative is derived by computing

$$\lim_{\epsilon \rightarrow 0} \frac{d}{d\epsilon} F_i(u_- + \epsilon \delta u; v). \quad (5.2)$$

The δu is now the trial function and u_- is the previous approximation to the solution u . We start with

$$\frac{d}{d\epsilon} \int_{\Omega} \nabla v \cdot (q(u_- + \epsilon\delta u) \nabla(u_- + \epsilon\delta u)) \, dx$$

and obtain

$$\int_{\Omega} \nabla v \cdot [q'(u_- + \epsilon\delta u)\delta u \nabla(u_- + \epsilon\delta u) + q(u_- + \epsilon\delta u)\nabla\delta u] \, dx,$$

which leads to

$$\int_{\Omega} \nabla v \cdot [q'(u_-)\delta u \nabla(u_-) + q(u_-)\nabla\delta u] \, dx, \quad (5.3)$$

as $\epsilon \rightarrow 0$. This last expression is the Gateaux derivative of F . We may use J or $a(\delta u, v)$ for this derivative, the latter having the advantage that we easily recognize the expression as a bilinear form. However, in the forthcoming code examples J is used as variable name for the Jacobian.

The specification of J goes as follows if du is the `TrialFunction`:

```
du = TrialFunction(V)
v = TestFunction(V)
u_ = Function(V)      # the most recently computed solution
F = dot(q(u_)*grad(u_), grad(v))*dx

J = dot(q(u_)*grad(du), grad(v))*dx +
    dot(Dq(u_)*du*grad(u_), grad(v))*dx
```

The alternative specification of F , with u as `TrialFunction`, leads to

```
u = TrialFunction(V)
v = TestFunction(V)
u_ = Function(V)      # the most recently computed solution
F = dot(q(u)*grad(u), grad(v))*dx
F = action(F, u)

J = dot(q(u_)*grad(u), grad(v))*dx +
    dot(Dq(u_)*u*grad(u_), grad(v))*dx
```

The UFL language, used to specify weak forms, supports differentiation of forms. This feature facilitates automatic *symbolic* computation of the Jacobian J by calling the function `derivative` with F , the most recently computed solution (`Function`), and the unknown (`TrialFunction`) as parameters:

```
du = TrialFunction(V)
v = TestFunction(V)
u_ = Function(V)      # the most recently computed solution
F = dot(q(u_)*grad(u_), grad(v))*dx

J = derivative(F, u_, du)  # Gateaux derivative in dir. of du
```

or

```

u = TrialFunction(V)
v = TestFunction(V)
u_ = Function(V)      # the most recently computed solution
F = dot(q(u)*grad(u), grad(v))*dx
F = action(F, u_)

J = derivative(F, u_, u)  # Gateaux derivative in dir. of u

```

The `derivative` function is obviously very convenient in problems where differentiating `F` by hand implies lengthy calculations.

5.1.2 Setting solver parameters

The following code defines the nonlinear variational problem and an associated solver based on Newton's method. We here demonstrate how key parameters in Newton's method can be set, as well as the choice of solver and preconditioner, and associated parameters, for the linear system occurring in the Newton iterations.

```

problem = NonlinearVariationalProblem(F, u_, bcs, J)
solver = NonlinearVariationalSolver(problem)
prm = solver.parameters
prm_n = prm['newton_solver']
prm_n['absolute_tolerance'] = abs_tol_Newton
prm_n['relative_tolerance'] = rel_tol_Newton
prm_n['maximum_iterations'] = max_iter_Newton
prm_n['relaxation_parameter'] = relaxation_prm_Newton
if linear_solver == 'Krylov':
    prec = 'jacobi' if 'jacobi' in \
        list(zip(*krylov_solver_preconditioners()))[0] \
        else 'ilu'
    prm_n['linear_solver'] = 'gmres'
    prm_n['preconditioner'] = prec
    prm_nk = prm_n['krylov_solver']
    prm_nk['absolute_tolerance'] = abs_tol_Krylov
    prm_nk['relative_tolerance'] = rel_tol_Krylov
    prm_nk['maximum_iterations'] = max_iter_Krylov
    prm_nk['monitor_convergence'] = True
    prm_nk['nonzero_initial_guess'] = False
    prm_nk['gmres']['restart'] = 40
    prm_nk['preconditioner']['structure'] = \
        'same_nonzero_pattern'
    prm_nk['preconditioner']['ilu']['fill_level'] = 0

```

A list of available parameters and their default values can as usual be printed by calling `info(prm, True)`. The `u_` we feed to the nonlinear variational problem object is filled with the solution by the call `solver.solve()`.

5.1.3 Implementation

The preferred implementation of F and J , depending on whether \mathbf{du} or \mathbf{u} is the `TrialFunction` object, is a matter of personal taste. Derivation of the Gateaux derivative by hand, as shown above, is most naturally matched by an implementation where \mathbf{du} is the `TrialFunction`, while use of automatic symbolic differentiation with the aid of the `derivative` function is most naturally matched by an implementation where \mathbf{u} is the `TrialFunction`. We have implemented both approaches in a `solver` function in the file `ft12_np_anyD.py`. An argument `TrialFunction_object` can be set to \mathbf{u} if we want to have \mathbf{u} as `TrialFunction`, otherwise it set to \mathbf{du} .

```
def solver(
    q, Dq, f, divisions, degree=1,
    TrialFunction_object='u',
    J_comp='manual',
    linear_solver='Krylov', # Alt: 'direct'
    abs_tol_Krylov=1E-5,
    rel_tol_Krylov=1E-5,
    abs_tol_Newton=1E-5,
    rel_tol_Newton=1E-5,
    max_iter_Krylov=1000,
    max_iter_Newton=50,
    relaxation prm_Newton=1.0,
    log_level=PROGRESS,
    dump_parameters=False,
):
```

Let us run the code for $m = 2$ and three meshes corresponding to `divisions` as 10 10, 20 20, and 40 40. The maximum errors are then $5 \cdot 10^{-3}$, $1.7 \cdot 10^{-3} \approx \frac{1}{4}5 \cdot 10^{-3}$, $4.5 \cdot 10^{-4} \approx \frac{1}{4}1.7 \cdot 10^{-3}$, and $1.2 \cdot 10^{-4} \approx \frac{1}{4}4.5 \cdot 10^{-4}$, demonstrating second-order convergence in the cell size as expected for P1 elements. This test is turned into a proper unit test in the `test_solver` function.

5.2 Manual implementation of solution algorithms

We now show how we can implement the solution algorithm for handling nonlinear PDEs from scratch. First, we treat the common and popular Picard iteration method. Second, we look at a standard Newton method for solving nonlinear algebraic equations. And third, we demonstrate application of the Newton method directly to the PDE, which is an approach that is more attractive to FEniCS programmers than the second one.

5.2.1 Picard iteration

Picard iteration is an easy way of handling nonlinear PDEs: we simply use a known, previous solution in the nonlinear terms so that these terms become linear in the unknown u . The strategy is also known as the method of successive substitutions. For our particular problem, we use a known, previous solution in the coefficient $q(u)$. More precisely, given a solution u^k from iteration k , we seek a new (hopefully improved) solution u^{k+1} in iteration $k+1$ such that u^{k+1} solves the *linear problem*,

$$\nabla \cdot (q(u^k) \nabla u^{k+1}) = 0, \quad k = 0, 1, \dots \quad (5.4)$$

The iterations require an initial guess u^0 . The hope is that $u^k \rightarrow u$ as $k \rightarrow \infty$, and that u^{k+1} is sufficiently close to the exact solution u of the discrete problem after just a few iterations.

We can easily formulate a variational problem for u^{k+1} from (5.4). Equivalently, we can approximate $q(u)$ by $q(u^k)$ in (2.34) to obtain the same linear variational problem. In both cases, the problem consists of seeking $u^{k+1} \in V$ such that

$$\tilde{F}(u^{k+1}; v) = 0 \quad \forall v \in \hat{V}, \quad k = 0, 1, \dots, \quad (5.5)$$

with

$$\tilde{F}(u^{k+1}; v) = \int_{\Omega} q(u^k) \nabla u^{k+1} \cdot \nabla v \, dx. \quad (5.6)$$

Since this is a linear problem in the unknown u^{k+1} , we can equivalently use the formulation

$$a(u^{k+1}, v) = L(v), \quad (5.7)$$

with

$$a(u, v) = \int_{\Omega} q(u^k) \nabla u \cdot \nabla v \, dx \quad (5.8)$$

$$L(v) = 0. \quad (5.9)$$

The iterations can be stopped when $\epsilon \equiv \|u^{k+1} - u^k\| < \text{tol}$, where tol is a small tolerance, say 10^{-5} , or when the number of iterations exceed some critical limit. The latter case will pick up divergence of the method or unacceptable slow convergence.

In the solution algorithm we only need to store u^k and u^{k+1} , called `u_k` and `u` in the code below. The algorithm can then be expressed as follows:

```
def q(u):
```

```

        return (1+u)**m

# Define variational problem for Picard iteration
u = TrialFunction(V)
v = TestFunction(V)
u_k = interpolate(Constant(0.0), V) # previous (known) u
a = dot(q(u_k)*grad(u), grad(v))*dx
f = Constant(0.0)
L = f*v*dx

# Picard iterations
u = Function(V)      # new unknown function
eps = 1.0            # error measure ||u-u_k||
tol = 1.0E-5         # tolerance
iter = 0              # iteration counter
maxiter = 25          # max no of iterations allowed
while eps > tol and iter < maxiter:
    iter += 1
    solve(a == L, u, bcs)
    diff = u.vector().array() - u_k.vector().array()
    eps = numpy.linalg.norm(diff, ord=numpy.Inf)
    print('iter=%d: norm=%g' % (iter, eps))
    u_k.assign(u)    # update for next iteration

```

We need to define the previous solution in the iterations, u_k , as a finite element function so that u_k can be updated with u at the end of the loop. We may create the initial `Function` u_k by interpolating an `Expression` or a `Constant` to the same vector space as u lives in (V).

In the code above we demonstrate how to use `numpy` functionality to compute the norm of the difference between the two most recent solutions. Here we apply the maximum norm (ℓ_∞ norm) on the difference of the solution vectors (`ord=1` and `ord=2` give the ℓ_1 and ℓ_2 vector norms - other norms are possible for `numpy` arrays, see `pydoc numpy.linalg.norm`).

The file `ft13_picard_np.py` contains the complete code for this nonlinear Poisson problem. The implementation is d dimensional, with mesh construction and setting of Dirichlet conditions as explained in Section 3.2.4. For a 33×33 grid with $m = 2$ we need 9 iterations for convergence when the tolerance is 10^{-5} .

5.2.2 A Newton method at the algebraic level

After having discretized our nonlinear PDE problem, we may use Newton's method to solve the system of nonlinear algebraic equations. From the continuous variational problem (2.33), the discrete version (2.35) results in a system of equations for the unknown parameters U_1, \dots, U_N (by inserting $u = \sum_{j=1}^N U_j \phi_j$ and $v = \hat{\phi}_i$ in (2.35)):

$$F_i(U_1, \dots, U_N) \equiv \sum_{j=1}^N \int_{\Omega} \left(q \left(\sum_{\ell=1}^N U_{\ell} \phi_{\ell} \right) \nabla \phi_j U_j \right) \cdot \nabla \hat{\phi}_i \, dx = 0, \quad i = 1, \dots, N. \quad (5.10)$$

Newton's method for the system $F_i(U_1, \dots, U_j) = 0, i = 1, \dots, N$ can be formulated as

$$\sum_{j=1}^N \frac{\partial}{\partial U_j} F_i(U_1^k, \dots, U_N^k) \delta U_j = -F_i(U_1^k, \dots, U_N^k), \quad i = 1, \dots, N, \quad (5.11)$$

$$U_j^{k+1} = U_j^k + \omega \delta U_j, \quad j = 1, \dots, N, \quad (5.12)$$

where $\omega \in [0, 1]$ is a relaxation parameter, and k is an iteration index. An initial guess u^0 must be provided to start the algorithm.

The original Newton method has $\omega = 1$, but in problems where it is difficult to obtain convergence, so-called *under-relaxation* with $\omega < 1$ may help. It means that one takes a smaller step than what is suggested by Newton's method.

We need, in a program, to compute the Jacobian matrix $\partial F_i / \partial U_j$ and the right-hand side vector $-F_i$. Our present problem has F_i given by (5.10). The derivative $\partial F_i / \partial U_j$ becomes

$$\int_{\Omega} \left[q' \left(\sum_{\ell=1}^N U_{\ell}^k \phi_{\ell} \right) \phi_j \nabla \left(\sum_{j=1}^N U_j^k \phi_j \right) \cdot \nabla \hat{\phi}_i + q \left(\sum_{\ell=1}^N U_{\ell}^k \phi_{\ell} \right) \nabla \phi_j \cdot \nabla \hat{\phi}_i \right] \, dx. \quad (5.13)$$

The following results were used to obtain (5.13):

$$\frac{\partial u}{\partial U_j} = \frac{\partial}{\partial U_j} \sum_{j=1}^N U_j \phi_j = \phi_j, \quad \frac{\partial}{\partial U_j} \nabla u = \nabla \phi_j, \quad \frac{\partial}{\partial U_j} q(u) = q'(u) \phi_j. \quad (5.14)$$

We can reformulate the Jacobian matrix in (5.13) by introducing the short notation $u^k = \sum_{j=1}^N U_j^k \phi_j$:

$$\frac{\partial F_i}{\partial U_j} = \int_{\Omega} \left[q'(u^k) \phi_j \nabla u^k \cdot \nabla \hat{\phi}_i + q(u^k) \nabla \phi_j \cdot \nabla \hat{\phi}_i \right] \, dx. \quad (5.15)$$

In order to make FEniCS compute this matrix, we need to formulate a corresponding variational problem. Looking at the linear system of equations in Newton's method,

$$\sum_{j=1}^N \frac{\partial F_i}{\partial U_j} \delta U_j = -F_i, \quad i = 1, \dots, N,$$

we can introduce v as a general test function replacing $\hat{\phi}_i$, and we can identify the unknown $\delta u = \sum_{j=1}^N \delta U_j \phi_j$. From the linear system we can now go "backwards" to construct the corresponding linear discrete weak form to be solved in each Newton iteration:

$$\int_{\Omega} \left[q'(u^k) \delta u \nabla u^k \cdot \nabla v + q(u^k) \nabla \delta u \cdot \nabla v \right] dx = - \int_{\Omega} q(u^k) \nabla u^k \cdot \nabla v dx. \quad (5.16)$$

This variational form fits the standard notation $a(\delta u, v) = L(v)$ with

$$\begin{aligned} a(\delta u, v) &= \int_{\Omega} \left[q'(u^k) \delta u \nabla u^k \cdot \nabla v + q(u^k) \nabla \delta u \cdot \nabla v \right] dx \\ L(v) &= - \int_{\Omega} q(u^k) \nabla u^k \cdot \nabla v dx. \end{aligned}$$

Note the important feature in Newton's method that the previous solution u^k replaces u in the formulas when computing the matrix $\partial F_i / \partial U_j$ and vector F_i for the linear system in each Newton iteration.

We now turn to the implementation. To obtain a good initial guess u^0 , we can solve a simplified, linear problem, typically with $q(u) = 1$, which yields the standard Laplace equation $\nabla^2 u^0 = 0$. The recipe for solving this problem appears in Sections 2.1.2, 2.1.5, and 3.4.1. The code for computing u^0 becomes as follows:

```
tol = 1E-14
def left_boundary(x, on_boundary):
    return on_boundary and abs(x[0]) < tol

def right_boundary(x, on_boundary):
    return on_boundary and abs(x[0]-1) < tol

Gamma_0 = DirichletBC(V, Constant(0.0), left_boundary)
Gamma_1 = DirichletBC(V, Constant(1.0), right_boundary)
bcs = [Gamma_0, Gamma_1]

# Define variational problem for initial guess (q(u)=1, i.e., m=0)
u = TrialFunction(V)
v = TestFunction(V)
a = dot(grad(u), grad(v))*dx
f = Constant(0.0)
L = f*v*dx
A, b = assemble_system(a, L, bcs)
u_k = Function(V)
U_k = u_k.vector()
solve(A, U_k, b)
```

Here, u_k denotes the solution function for the previous iteration, so that the solution after each Newton iteration is $u = u_k + \omega * du$. Initially, u_k is the initial guess we call u^0 in the mathematics.

The Dirichlet boundary conditions for δu , in the problem to be solved in each Newton iteration, are somewhat different than the conditions for u . Assuming that u^k fulfills the Dirichlet conditions for u , δu must be zero at the boundaries where the Dirichlet conditions apply, in order for $u^{k+1} = u^k + \omega \delta u$ to fulfill the right boundary values. We therefore define an additional list of Dirichlet boundary conditions objects for δu :

```
Gamma_0_du = DirichletBC(V, Constant(0), left_boundary)
Gamma_1_du = DirichletBC(V, Constant(0), right_boundary)
bcs_du = [Gamma_0_du, Gamma_1_du]
```

The nonlinear coefficient and its derivative must be defined before coding the weak form of the Newton system:

```
def q(u):
    return (1+u)**m

def Dq(u):
    return m*(1+u)**(m-1)

du = TrialFunction(V) # u = u_k + omega*du
a = dot(q(u_k)*grad(du), grad(v))*dx + \
    dot(Dq(u_k)*du*grad(u_k), grad(v))*dx
L = -dot(q(u_k)*grad(u_k), grad(v))*dx
```

The Newton iteration loop is very similar to the Picard iteration loop in Section 5.2.1:

```
du = Function(V)
u = Function(V) # u = u_k + omega*du
omega = 1.0      # relaxation parameter
eps = 1.0
tol = 1.0E-5
iter = 0
maxiter = 25
while eps > tol and iter < maxiter:
    iter += 1
    A, b = assemble_system(a, L, bcs_du)
    solve(A, du.vector(), b)
    eps = numpy.linalg.norm(du.vector().array(), ord=numpy.Inf)
    print('Norm:', eps)
    u.vector()[:] = u_k.vector() + omega*du.vector()
    u_k.assign(u)
```

There are other ways of implementing the update of the solution as well:

```
u.assign(u_k) # u = u_k
u.vector().axpy(omega, du.vector())

# or
u.vector()[:] += omega*du.vector()
```

The `axpy(a, y)` operation adds a scalar `a` times a `Vector` `y` to a `Vector` object. It is usually a fast operation calling up an optimized BLAS routine for the calculation.

Mesh construction for a d -dimensional problem with arbitrary degree of the Lagrange elements can be done as explained in Section 3.2.4. The complete program appears in the file `ft14_alg_newton_np.py`.

5.2.3 A Newton method at the PDE level

Although Newton's method in PDE problems is normally formulated at the linear algebra level, i.e., as a solution method for systems of nonlinear algebraic equations, we can also formulate the method at the PDE level. This approach yields a linearization of the PDEs before they are discretized. FEniCS users will probably find this technique simpler to apply than the more standard method in Section 5.2.2.

Given an approximation to the solution field, u^k , we seek a perturbation δu so that

$$u^{k+1} = u^k + \delta u \quad (5.17)$$

fulfills the nonlinear PDE. However, the problem for δu is still nonlinear and nothing is gained. The idea is therefore to assume that δu is sufficiently small so that we can linearize the problem with respect to δu . Inserting u^{k+1} in the PDE, linearizing the q term as

$$q(u^{k+1}) = q(u^k) + q'(u^k)\delta u + \mathcal{O}((\delta u)^2) \approx q(u^k) + q'(u^k)\delta u, \quad (5.18)$$

and dropping nonlinear terms in δu , we get

$$\nabla \cdot (q(u^k) \nabla u^k) + \nabla \cdot (q(u^k) \nabla \delta u) + \nabla \cdot (q'(u^k) \delta u \nabla u^k) = 0.$$

We may collect the terms with the unknown δu on the left-hand side,

$$\nabla \cdot (q(u^k) \nabla \delta u) + \nabla \cdot (q'(u^k) \delta u \nabla u^k) = -\nabla \cdot (q(u^k) \nabla u^k), \quad (5.19)$$

The weak form of this PDE is derived by multiplying by a test function v and integrating over Ω , integrating as usual the second-order derivatives by parts:

$$\int_{\Omega} (q(u^k) \nabla \delta u \cdot \nabla v + q'(u^k) \delta u \nabla u^k \cdot \nabla v) dx = - \int_{\Omega} q(u^k) \nabla u^k \cdot \nabla v dx. \quad (5.20)$$

The variational problem reads: find $\delta u \in V$ such that $a(\delta u, v) = L(v)$ for all $v \in \hat{V}$, where

$$a(\delta u, v) = \int_{\Omega} \left(q(u^k) \nabla \delta u \cdot \nabla v + q'(u^k) \delta u \nabla u^k \cdot \nabla v \right) dx, \quad (5.21)$$

$$L(v) = - \int_{\Omega} q(u^k) \nabla u^k \cdot \nabla v dx. \quad (5.22)$$

The function spaces V and \hat{V} , being continuous or discrete, are as in the linear Poisson problem from Section 2.1.2.

We must provide some initial guess, e.g., the solution of the PDE with $q(u) = 1$. The corresponding weak form $a_0(u^0, v) = L_0(v)$ has

$$a_0(u, v) = \int_{\Omega} \nabla u \cdot \nabla v dx, \quad L_0(v) = 0.$$

Thereafter, we enter a loop and solve $a(\delta u, v) = L(v)$ for δu and compute a new approximation $u^{k+1} = u^k + \delta u$. Note that δu is a correction, so if u^0 satisfies the prescribed Dirichlet conditions on some part Γ_D of the boundary, we must demand $\delta u = 0$ on Γ_D .

Looking at (5.21) and (5.22), we see that the variational form is the same as for the Newton method at the algebraic level in Section 5.2.2. Since Newton's method at the algebraic level required some "backward" construction of the underlying weak forms, FEniCS users may prefer Newton's method at the PDE level, which this author finds more straightforward, although not so commonly documented in the literature on numerical methods for PDEs. There is seemingly no need for differentiations to derive a Jacobian matrix, but a mathematically equivalent derivation is done when nonlinear terms are linearized using the first two Taylor series terms and when products in the perturbation δu are neglected.

The implementation is identical to the one in Section 5.2.2 and is found in the file `ft15_pde_newton_np.py`. The reader is encouraged to go through this code to be convinced that the present method actually ends up with the same program as needed for the Newton method at the linear algebra level in Section 5.2.2.

Chapter 6

More old stuff

6.1 Creating more complex domains

Up to now we have been very fond of the unit square as domain, which is an appropriate choice for initial versions of a PDE solver. The strength of the finite element method, however, is its ease of handling domains with complex shapes. This section shows some methods that can be used to create different types of domains and meshes.

Domains of complex shape must normally be constructed in separate pre-processor programs. Two relevant preprocessors are Triangle for 2D domains and NETGEN for 3D domains.

6.1.1 Built-in mesh generation tools

DOLFIN has a few tools for creating various types of meshes over domains with simple shape: `UnitIntervalMesh`, `UnitSquareMesh`, `UnitCubeMesh`, `IntervalMesh`, `RectangleMesh`, and `BoxMesh`. Some of these names have been briefly met in previous sections. The hopefully self-explanatory code snippet below summarizes typical constructions of meshes with the aid of these tools:

```
# 1D domains
mesh = UnitIntervalMesh(20)      # 20 cells, 21 vertices
mesh = IntervalMesh(20, -1, 1)   # domain [-1,1]

# 2D domains (6x10 divisions, 120 cells, 77 vertices)
mesh = UnitSquareMesh(6, 10)    # 'right' diagonal is default
# The diagonals can be right, left or crossed
mesh = UnitSquareMesh(6, 10, 'left')
mesh = UnitSquareMesh(6, 10, 'crossed')
```

```
# Domain [0,3]x[0,2] with 6x10 divisions and left diagonals
mesh = RectangleMesh(0, 0, 3, 2, 6, 10, 'left')

# 6x10x5 boxes in the unit cube, each box gets 6 tetrahedra:
mesh = UnitCubeMesh(6, 10, 5)

# Domain [-1,1]x[-1,0]x[-1,2] with 6x10x5 divisions
mesh = BoxMesh(-1, -1, -1, 1, 0, 2, 6, 10, 5)
```

6.1.2 Transforming mesh coordinates

Coordinate stretching. A mesh that is denser toward a boundary is often desired to increase accuracy in that region. Given a mesh with uniformly spaced coordinates x_0, \dots, x_{M-1} in $[a, b]$, the coordinate transformation $\xi = (x - a)/(b - a)$ maps x onto $\xi \in [0, 1]$. A new mapping $\eta = \xi^s$, for some $s > 1$, stretches the mesh toward $\xi = 0$ ($x = a$), while $\eta = \xi^{1/s}$ makes a stretching toward $\xi = 1$ ($x = b$). Mapping the $\eta \in [0, 1]$ coordinates back to $[a, b]$ gives new, stretched x coordinates,

$$\bar{x} = a + (b - a) \left(\frac{x - a}{b - a} \right)^s \quad (6.1)$$

toward $x = a$, or

$$\bar{x} = a + (b - a) \left(\frac{x - a}{b - a} \right)^{1/s} \quad (6.2)$$

toward $x = b$. Figure 6.1 shows the effect of making a rectangular mesh denser toward $x = 0$ (prior to the coordinate transformation below).

Rectangle to hollow circle mapping. One way of creating more complex geometries is to transform the vertex coordinates in a rectangular mesh according to some formula. Say we want to create a part of a hollow cylinder of Θ degrees, with inner radius a and outer radius b . A standard mapping from polar coordinates to Cartesian coordinates can be used to generate the hollow cylinder. Given a rectangle in (\bar{x}, \bar{y}) space such that $a \leq \bar{x} \leq b$ and $0 \leq \bar{y} \leq 1$, the mapping

$$\hat{x} = \bar{x} \cos(\Theta \bar{y}), \quad \hat{y} = \bar{x} \sin(\Theta \bar{y}),$$

takes a point in the rectangular (\bar{x}, \bar{y}) geometry and maps it to a point (\hat{x}, \hat{y}) in a hollow cylinder.

The corresponding Python code for first stretching the mesh and then mapping it onto a hollow cylinder looks as follows:

```
Theta = pi/2
a, b = 1, 5.0
```

```

nr = 10 # divisions in r direction
nt = 20 # divisions in theta direction
mesh = RectangleMesh(a, 0, b, 1, nr, nt, 'crossed')

# First make a denser mesh towards r=a
x = mesh.coordinates()[:,0]
y = mesh.coordinates()[:,1]
s = 1.3

def denser(x, y):
    return [a + (b-a)*((x-a)/(b-a))**s, y]

x_bar, y_bar = denser(x, y)
xy_bar_coor = numpy.array([x_bar, y_bar]).transpose()
mesh.coordinates()[:] = xy_bar_coor
plot(mesh, title='stretched mesh')

def cylinder(r, s):
    return [r*numpy.cos(Theta*s), r*numpy.sin(Theta*s)]

x_hat, y_hat = cylinder(x_bar, y_bar)
xy_hat_coor = numpy.array([x_hat, y_hat]).transpose()
mesh.coordinates()[:] = xy_hat_coor
plot(mesh, title='hollow cylinder')
interactive()

```

The result of calling `denser` and `cylinder` above is a list of two vectors, with the x and y coordinates, respectively. Turning this list into a `numpy` array object results in a $2 \times M$ array, M being the number of vertices in the mesh. However, `mesh.coordinates()` is by a convention an $M \times 2$ array so we need to take the transpose. The resulting mesh is displayed in Figure 6.1.

Setting boundary conditions in meshes created from mappings like the one illustrated above is most conveniently done by using a mesh function to mark parts of the boundary. The marking is easiest to perform before the mesh is mapped since one can then conceptually work with the sides in a pure rectangle.

6.2 A General d -Dimensional multi-material test problem

This section is in a preliminary state!

The purpose of the present section is to generalize the basic ideas from the previous section to a problem involving an arbitrary number of materials in 1D, 2D, or 3D domains. The example also highlights how to build more general and flexible FEniCS applications.

More to be done:

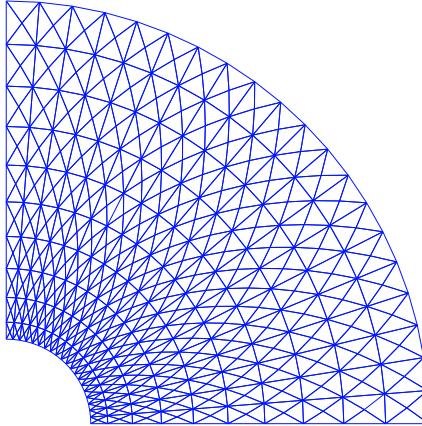


Fig. 6.1 Hollow cylinder generated by mapping a rectangular mesh, stretched toward the left side.

- Batch compilation of subdomains, see mailinglist.txt, lots of useful stuff in Hake's example with "pointwise", see what the bcs are etc.
- Use of `near` or similar function (better: user-adjusted tolerance)

6.2.1 The PDE problem

We generalize the problem in Section 3.4.3 to the case where there are s materials $\Omega_0, \dots, \Omega_{s-1}$, with associated constant k values k_0, k_1, \dots, k_{s-1} , as illustrated in Figure 6.2.

Although the sketch of the domain is in two dimensions, we can easily define this problem in any number of dimensions, using the ideas of Section 3.2.4, but the layer boundaries are planes $x_0 = \text{const}$ and u varies with x_0 only.

The PDE reads

$$\nabla \cdot (k \nabla u) = 0. \quad (6.3)$$

To construct a problem where we can find an analytical solution that can be computed to machine precision regardless of the element size, we choose Ω as a hypercube $[0, 1]^d$, and the materials as layers in the x_0 direction, as depicted in Figure 6.2 for a 2D case with four materials. The boundaries $x_0 = 0$ and $x_0 = 1$ have Dirichlet conditions $u = 0$ and $u = 1$, respectively,

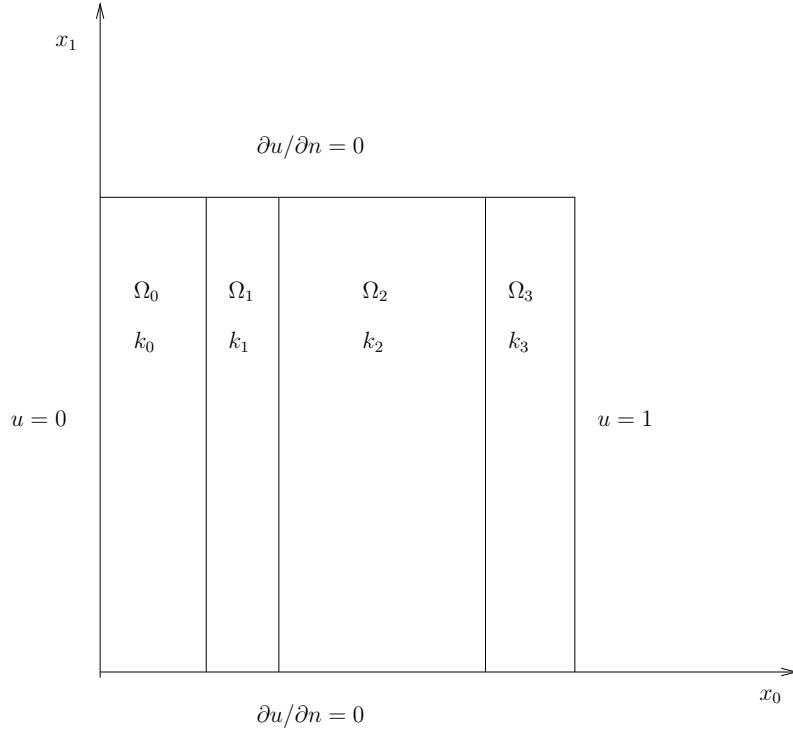


Fig. 6.2 Sketch of a multi-material problem.

while Neumann conditions $\partial u / \partial n = 0$ are set on the remaining boundaries. The complete boundary-value problem is then

$$\begin{aligned} \nabla \cdot (k(x_0) \nabla u(x_0, \dots, x_{d-1})) &= 0 \text{ in } \Omega, \\ u &= 0 \text{ on } \Gamma_0, \\ u &= 1 \text{ on } \Gamma_1, \\ \frac{\partial u}{\partial n} &= 0 \text{ on } \Gamma_N. \end{aligned} \tag{6.4}$$

The domain Ω is divided into s materials Ω_i , $i = 0, \dots, s - 1$, where

$$\Omega_i = \{(x_0, \dots, x_{d-1}) \mid L_i \leq x_0 < L_{i+1}\}$$

for given x_0 values $0 = L_0 < L_1 < \dots < L_s = 1$ of the material (subdomain) boundaries. The $k(x_0)$ function takes on the value k_i in Ω_i .

The exact solution of the basic PDE in (6.4)

$$u(x_0, \dots, x_{d-1}) = \frac{\int_0^{x_0} (k(\tau))^{-1} d\tau}{\int_0^1 (k(\tau))^{-1} d\tau}.$$

For a piecewise constant $k(x_0)$ as explained, we get

$$u(x_0, \dots, x_{d-1}) = \frac{(x_0 - L_i)k_i^{-1} + \sum_{j=0}^{i-1} (L_{j+1} - L_j)k_j^{-1}}{\sum_{j=0}^{s-1} (L_{j+1} - L_j)k_j^{-1}}, \quad L_i \leq x_0 \leq L_{i+1}. \quad (6.5)$$

That is, $u(x_0, \dots, x_{d-1})$ is piecewise linear in x_0 and constant in all other directions. If L_i coincides with the element boundaries, Lagrange elements will reproduce this exact solution to machine precision, which is ideal for a test case.

6.2.2 Preparing a mesh with subdomains

Our first task is to generate a mesh for $\Omega = [0, 1]^d$ and divide it into subdomains

$$\Omega_i = \{(x_0, \dots, x_{d-1}) \mid L_i < x_0 < L_{i+1}\}$$

for given subdomain boundaries $x_0 = L_i$, $i = 0, \dots, s$, $L_0 = 0$, $L_s = 1$. Note that the boundaries $x_0 = L_i$ are points in 1D, lines in 2D, and planes in 3D.

Let us, on the command line, specify the polynomial degree of Lagrange elements and the number of element divisions in the various space directions, as explained in detail in Section 3.2.4. This results in an object `mesh` representing the interval $[0, 1]$ in 1D, the unit square in 2D, or the unit cube in 3D.

Specification of subdomains (and boundary parts, if desired) is done using a user-defined subclass of `SubDomain`, as explained in Section 3.4.3. We could, in principle, introduce one subclass of `SubDomain` for each subdomain, and this would be feasible if one has a small and fixed number of subdomains as in the example in Section 3.4.3 with two subdomains. Our present case is more general as we have s subdomains. It then makes sense to create one subclass `Material` of `SubDomain` and have an attribute to reflect the subdomain (material) number. We use this number in the test whether a spatial point x is inside a subdomain or not:

```
class Material(SubDomain):
    """Define material (subdomain) no. i."""
    def __init__(self, subdomain_number, subdomain_boundaries):
        self.number = subdomain_number
        self.boundaries = subdomain_boundaries
        SubDomain.__init__(self)

    def inside(self, x, on_boundary):
        i = self.number
        L = self.boundaries           # short form (cf. the math)
        if L[i] <= x[0] <= L[i+1]:
            return True
```

```
    else:
        return False
```

The `<=` in the test if a point is inside a subdomain is important as x will equal vertex coordinates in the cells, and all vertices of a cell must lead to a `True` return value from the `inside` method for the cell to be a part of the actual subdomain. That is, the more mathematically natural test $L[i] \leq x[0] < L[i+1]$ fails to include elements with $x = L_{i+1}$ as boundary in subdomain Ω_i .

The marking and numbering of all subdomains goes as follows:

```
cell_entity_dim = mesh.topology().dim() # = d
subdomains = MeshFunction('uint', mesh, cell_entity_dim)
# Mark subdomains with numbers i=0,1,\ldots,s (=len(L)-1)
for i in range(s):
    material_i = Material(i, L)
    material_i.mark(subdomains, i)
```

We have now all the geometric information about subdomains in a `MeshFunction` object `subdomains`. The subdomain number of mesh entity number e , here cell e , is given by `subdomains.array() [e]`.

The code presented so far had the purpose of preparing a mesh and a mesh function defining the subdomain. It is smart to put this code in a separate file, say `ft16_define_layers.py`, and view the code as a preprocessing step. We must then store the computed mesh and mesh function in files. Another program may load the files and perform the actually solve the boundary-value problem.

Storing the mesh itself and the mesh function in XML format is done by

```
file = File('hypercube_mesh.xml.gz')
file << mesh
file = File('layers.xml.gz')
file << subdomains
```

This preprocessing code knows about the layer geometries and the corresponding k , which must be propagated to the solver code. One idea is to let the preprocessing code write a Python module containing the L and k lists as well as an implementation of a function that evaluates the exact solution. The solver code can import this module to get access to L , k , and the exact solution (for comparison). The relevant Python code for generating a Python module may take the form

```
f = open('u_layered.py', 'w')
f.write("""
import numpy
L = numpy.array(
#s, float)
k = numpy.array(
#s, float)
s = len(L)-1
```

```

def u_e(x):
    # First find which subdomain x0 is located in
    for i in range(len(L)-1):
        if L[i] <= x <= L[i+1]:
            break

    # Vectorized implementation of summation:
    s2 = sum((L[1:s+1] - L[0:s])*(1.0/k[:]))
    if i == 0:
        u = (x - L[i])*(1.0/k[0])/s2
    else:
        s1 = sum((L[1:i+1] - L[0:i])*(1.0/k[0:i]))
        u = ((x - L[i])*(1.0/k[i]) + s1)/s2
    return u

if __name__ == '__main__':
    # Plot the exact solution
    from scitools.std import linspace, plot, array
    x = linspace(0, 1, 101)
    u = array([u_e(xi) for xi in x])
    print(u)
    plot(x, u)
"""

# (L, k)
f.close()

```

6.2.3 Solving the PDE problem

The solver program starts with loading a prepared mesh with a mesh function representing the subdomains:

```

mesh = Mesh('hypercube_mesh.xml.gz')
subdomains = MeshFunction('uint', mesh, 'layers.xml.gz')

```

The next task is to define the k function as a finite element function. As we recall from Section 3.4.3, a k that is constant in each element is suitable. We then follow the recipe from Section 3.4.3 to compute k :

```

V0 = FunctionSpace(mesh, 'DG', 0)
k = Function(V0)

# Vectorized calculation
help = numpy.asarray(subdomains.array(), dtype=numpy.int32)
k.vector()[:] = numpy.choose(help, k_values)

```

The essential boundary conditions are defined in the same way as in `dn2_p2D.py` from Section 3.4.2 and therefore not repeated here. The variational problem is defined and solved in a standard manner,

```

u = TrialFunction(V)

```

```

v = TestFunction(V)
f = Constant(0)
a = k*dot(grad(u), grad(v))*dx
L = f*v*dx

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

```

Plotting the discontinuous k is often desired. Just a `plot(k)` makes a continuous function out of k , which is not what we want. Making a `MeshFunction` over cells and filling in the right k values results in an object that can be displayed as a discontinuous field. A relevant code is

```

k_meshfunc = MeshFunction('double', mesh, mesh.topology().dim())

# Scalar version
for i in range(len(subdomains.array())):
    k_meshfunc.array()[i] = k_values[subdomains.array()[i]]

# Vectorized version
help = numpy.asarray(subdomains.array(), dtype=numpy.int32)
k_meshfunc.array()[:] = numpy.choose(help, k_values)

plot(k_meshfunc, title='k as mesh function')

```

The file `ft17_Poisson_layers.py` contains the complete code.

6.3 More Examples

Many more topics could be treated in a FEniCS tutorial, e.g., how to solve systems of PDEs, how to work with mixed finite element methods, how to create more complicated meshes and mark boundaries, and how to create more advanced visualizations. However, to limit the size of this tutorial, the examples end here. There are, fortunately, a rich set of FEniCS demos. The FEniCS documentation explains a collection of PDE solvers in detail: the Poisson equation, the mixed formulation for the Poisson equation, the Biharmonic equation, the equations of hyperelasticity, the Cahn-Hilliard equation, and the incompressible Navier-Stokes equations. Both Python and C++ versions of these solvers are explained. An eigenvalue solver is also documented. In the `fenics/demo` directory of the DOLFIN source code tree you can find programs for these and many other examples, including the advection-diffusion equation, the equations of elastodynamics, a reaction-diffusion equation, various finite element methods for the Stokes problem, discontinuous Galerkin methods for the Poisson and advection-diffusion equations, and an eigenvalue problem arising from electromagnetic waveguide problem with Nedelec elements. There are also numerous demos on how to apply various functionality in FEniCS, e.g., mesh refinement and error control, moving meshes (for ALE

methods), computing functionals over subsets of the mesh (such as lift and drag on bodies in flow), and creating separate subdomain meshes from a parent mesh.

The project `cbc.solve` (<https://launchpad.net/cbc.solve>) offers more complete PDE solvers for the Navier-Stokes equations, the equations of hyperelasticity, fluid-structure interaction, viscous mantle flow, and the bidomain model of electrophysiology. Most of these solvers are described in the "FEniCS book" [20] (<https://launchpad.net/fenics-book>). Another project, `cbc.rans` (<https://launchpad.net/cbc.rans>), offers an environment for very flexible and easy implementation of Navier-Stokes solvers and turbulence [21, 22]. For example, `cbc.rans` contains an elliptic relaxation model for turbulent flow involving 18 nonlinear PDEs. FEniCS proved to be an ideal environment for implementing such complicated PDE models. The easy construction of systems of nonlinear PDEs in `cbc.rans` has been further generalized to simplify the implementation of large systems of nonlinear PDEs in general. The functionality is found in the `cbc.pdesys` package (<https://launchpad.net/cbc.pdesys>).

6.4 Miscellaneous topics

hpl 23: Needs to be cleaned up.

6.4.1 Glossary

Below we explain some key terms used in this tutorial.

FEniCS: name of a software suite composed of many individual software components (see fenicsproject.org). Some components are DOLFIN and Viper, explicitly referred to in this tutorial. Others are FFC and FIAT, heavily used by the programs appearing in this tutorial, but never explicitly used from the programs.

DOLFIN: a FEniCS component, more precisely a C++ library, with a Python interface, for performing important actions in finite element programs. DOLFIN makes use of many other FEniCS components and many external software packages.

Viper: a FEniCS component for quick visualization of finite element meshes and solutions.

UFL: a FEniCS component implementing the *unified form language* for specifying finite element forms in FEniCS programs. The definition of the forms, typically called `a` and `L` in this tutorial, must have legal UFL syntax. The same applies to the definition of functionals (see Section 3.3.1).

Class (Python): a programming construction for creating objects containing a set of variables and functions. Most types of FEniCS objects are defined through the class concept.

Instance (Python): an object of a particular type, where the type is implemented as a class. For instance, `mesh = UnitIntervalMesh(10)` creates an instance of class `UnitIntervalMesh`, which is reached by the name `mesh`. (Class `UnitIntervalMesh` is actually just an interface to a corresponding C++ class in the DOLFIN C++ library.)

Class method (Python): a function in a class, reached by dot notation: `instance_name.method_name`

argument `self` (Python): required first parameter in class methods, representing a particular object of the class. Used in method definitions, but never in calls to a method. For example, if `method(self, x)` is the definition of `method` in a class `Y`, `method` is called as `y.method(x)`, where `y` is an instance of class `Y`. In a call like `y.method(x)`, `method` is invoked with `self=y`.

Class attribute (Python): a variable in a class, reached by dot notation: `instance_name.attribute_name`

6.4.2 Handy methods in key FEniCS objects

In general, `pydoc fenics.X` shows the documentation of any name `X` and lists all the methods (i.e.g, functions in the class) that can be called. Below, we list just a few, but very useful, methods in the most central FEniCS classes.

Mesh. Let `mesh` be a `Mesh` object.

- `mesh.coordinates()` returns an array of the coordinates of the vertices in the mesh.
- `mesh.num_cells()` returns the number of cells (triangles) in the mesh,
- `mesh.num_vertices()` returns the number of vertices in the mesh (with our choice of linear Lagrange elements this equals the number of nodes, `len(u_array)`, or dimension of the space `V.dim()`),
- `mesh.cells()` returns the vertex numbers of the vertices in each cell as a `numpy` array with shape (*number of cells, number of vertices in a cell*),
- `mesh.hmin()` returns the minimum cell diameter (“smallest cell”),
- `mesh.hmax()` returns the maximum cell diameter (“largest cell”).
- `mesh.topology().dim()` returns the number of physical dimensions of the mesh.

Writing `print(mesh)` dumps a short, pretty-print description of the mesh (`print(mesh)` actually displays the result of `str(mesh)`, which defines the pretty print):

```
<Mesh of topological dimension 2 (triangles) with
16 vertices and 18 cells, ordered>
```

Function space. Let `V` be a `FunctionSpace` object.

- `V.mesh()` returns the associated mesh.
- `V.dim()` returns the dimension (number of degrees of freedom).
- `V.ufl_element()` returns the associated finite element.

Function. Let `u` be a `Function` object.

- `u.function_space()` returns the associated function space.
- `u.vector()` returns the vector object of degrees of freedom.
- `u.vector().array()` returns a copy of the degrees of freedom in a `numpy` array.

6.4.3 Overview of objects and functions

Most classes in FEniCS have an explanation of the purpose and usage that can be seen by using the general documentation command `pydoc` for Python objects. You can type

Terminal

```
pydoc fenics.X
```

to look up documentation of a Python class `X` from the DOLFIN library (`X` can be `UnitSquareMesh`, `Function`, `Viper`, etc.). Below is an overview of the most important classes and functions in FEniCS programs, in the order they typically appear within programs.

`UnitSquareMesh(nx, ny)`: generate mesh over the unit square $[0, 1] \times [0, 1]$ using `nx` divisions in x direction and `ny` divisions in y direction. Each of the $nx*ny$ squares are divided into two cells of triangular shape.

`UnitIntervalMesh`, `UnitCubeMesh`, `UnitCircleMesh`, `UnitSphere`, `IntervalMesh`, `RectangleMesh`, and `BoxMesh`: generate mesh over domains of simple geometric shape, see Section 6.1.

`FunctionSpace(mesh, element_type, degree)`: a function space defined over a mesh, with a given element type (e.g., '`Lagrange`' or '`DG`'), with basis functions as polynomials of a specified degree.

`Expression(formula, p1=v1, p2=v2, ...)`: a scalar- or vector-valued function, given as a mathematical expression `formula` (string) written in C++ syntax. The spatial coordinates in the expression are named `x[0]`, `x[1]`, and `x[2]`, while time and other physical parameters can be represented as symbols `p1`, `p2`, etc., with corresponding values `v1`, `v2`, etc., initialized through keyword arguments. These parameters become attributes, whose values can be modified when desired.

`Function(V)`: a scalar- or vector-valued finite element field in the function space `V`. If `V` is a `FunctionSpace` object, `Function(V)` becomes a scalar field,

and with `V` as a `VectorFunctionSpace` object, `Function(V)` becomes a vector field.

`SubDomain`: class for defining a subdomain, either a part of the boundary, an internal boundary, or a part of the domain. The programmer must subclass `SubDomain` and implement the `inside(self, x, on_boundary)` function (see Section 2.1.5) for telling whether a point `x` is inside the subdomain or not.

`Mesh`: class for representing a finite element mesh, consisting of cells, vertices, and optionally faces, edges, and facets.

`MeshFunction`: tool for marking parts of the domain or the boundary. Used for variable coefficients ("material properties", see Section 3.4.3) or for boundary conditions (see Section 3.4.4).

`DirichletBC(V, value, where)`: specification of Dirichlet (essential) boundary conditions via a function space `V`, a function `value(x)` for computing the value of the condition at a point `x`, and a specification `where` of the boundary, either as a `SubDomain` subclass instance, a plain function, or as a `MeshFunction` instance. In the latter case, a 4th argument is provided to describe which subdomain number that describes the relevant boundary.

`TestFunction(V)`: define a test function on a space `V` to be used in a variational form.

`TrialFunction(V)`: define a trial function on a space `V` to be used in a variational form to represent the unknown in a finite element problem.

`assemble(X)`: assemble a matrix, a right-hand side, or a functional, given a from `X` written with UFL syntax.

`assemble_system(a, L, bcs)`: assemble the matrix and the right-hand side from a bilinear (`a`) and linear (`L`) form written with UFL syntax. The `bcs` parameter holds one or more `DirichletBC` objects.

`LinearVariationalProblem(a, L, u, bcs)`: define a variational problem, given a bilinear (`a`) and linear (`L`) form, written with UFL syntax, and one or more `DirichletBC` objects stored in `bcs`.

`LinearVariationalSolver(problem)`: create solver object for a linear variational problem object (`problem`).

`solve(A, U, b)`: solve a linear system with `A` as coefficient matrix (`Matrix` object), `U` as unknown (`Vector` object), and `b` as right-hand side (`Vector` object). Usually, `U = u.vector()`, where `u` is a `Function` object representing the unknown finite element function of the problem, while `A` and `b` are computed by calls to `assemble` or `assemble_system`.

`plot(q)`: quick visualization of a mesh, function, or mesh function `q`, using a built-in, VTK-based component in FEniCS.

`interpolate(func, V)`: interpolate a formula or finite element function `func` onto the function space `V`.

`project(func, V)`: project a formula or finite element function `func` onto the function space `V`.

6.4.4 Linear solvers and preconditioners

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

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

Possible choices of preconditioners include

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

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

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

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

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

6.4.5 Using a backend-specific solver

Warning

The linear algebra backends in FEniCS have recently changed. This section is not yet up-to-date.

The linear algebra backend determines the specific data structures that are used in the `Matrix` and `Vector` classes. For example, with the PETSc backend, `Matrix` encapsulates a PETSc matrix storage structure, and `Vector` encapsulates a PETSc vector storage structure. Sometimes one wants to perform operations directly on (say) the underlying PETSc objects. These can be fetched by

```
A_PETSc =
down_cast(A).mat() b_PETSc = down_cast(b).vec() U_PETSc =
down_cast(u.vector()).vec()
```

Here, `u` is a `Function`, `A` is a `Matrix`, and `b` is a `Vector`. The same syntax applies if we want to fetch the underlying Epetra, uBLAS, or MTL4 matrices and vectors.

Sometimes one wants to implement tailored solution algorithms, using special features of the underlying numerical packages. Here is an example where we create an ML preconditioned Conjugate Gradient solver by programming with Trilinos-specific objects directly. Given a linear system $AU = b$, represented by a `Matrix` object `A`, and two `Vector` objects `U` and `b` in a Python program, the purpose is to set up a solver using the Aztec Conjugate Gradient method from Trilinos' Aztec library and combine that solver with the algebraic multigrid preconditioner ML from the ML library in Trilinos. Since the various parts of Trilinos are mirrored in Python through the PyTrilinos package, we can operate directly on Trilinos-specific objects.

```
try:
    from PyTrilinos import Epetra, AztecOO, TriUtils, ML
except:
    print(''You Need to have PyTrilinos with
Epetra, AztecOO, TriUtils and ML installed
for this demo to run'')
    exit()

from fenics import *

if not has_la_backend('Epetra'):
    print('Warning: Dolfin is not compiled with Trilinos')
    exit()

parameters['linear_algebra_backend'] = 'Epetra'

# create matrix A and vector b in the usual way
```

```
# u is a Function

# Fetch underlying Epetra objects
A_epetra = down_cast(A).mat()
b_epetra = down_cast(b).vec()
U_epetra = down_cast(u.vector()).vec()

# Sets up the parameters for ML using a python dictionary
ML_param = {"max levels" : 3,
             "output" : 10,
             "smoother: type" : "ML symmetric Gauss-Seidel",
             "aggregation: type" : "Uncoupled",
             "ML validate parameter list" : False
            }

# Create the preconditioner
prec = ML.MultiLevelPreconditioner(A_epetra, False)
prec.SetParameterList(ML_param)
prec.ComputePreconditioner()

# Create solver and solve system
solver = AztecOO.AztecOO(A_epetra, U_epetra, b_epetra)
solver.SetPrecOperator(prec)
solver.SetAztecOption(AztecOO.AZ_solver, AztecOO.AZ_cg)
solver.SetAztecOption(AztecOO.AZ_output, 16)
solver.Iterate(MaxIters=1550, Tolerance=1e-5)

plot(u)
```

Chapter 7

Troubleshooting

7.1 Compilation Problems

Expressions and variational forms in a FEniCS program need to be compiled to C++ and linked with libraries if the expressions or forms have been modified since last time they were compiled. The tool Instant, which is part of the FEniCS software suite, is used for compiling and linking C++ code so that it can be used with Python.

Sometimes the compilation fails. You can see from the series of error messages which statement in the Python program that led to a compilation problem. Make sure to scroll back and identify whether the problematic line is associated with an expression, variational form, or the solve step.

The final line in the output of error messages points to a log file from the compilation where one can examine the error messages from the compiler. It is usually the last lines of this log file that are of interest. Occasionally, the compiler's message can quickly lead to an understanding of the problem. A more fruitful approach is normally to examine the below list of common compilation problems and their remedies.

7.1.1 Problems with the Instant cache

Instant remembers information about previous compilations and versions of your program. Sometimes removal of this information can solve the problem. Just run

instant-clean

in a terminal window whenever you encounter a compilation problem.

7.1.2 Syntax errors in expressions

If the compilation problem arises from line with an `Expression` object, examine the syntax of the expression carefully. Section 2.1.7 contains some information on valid syntax. You may also want to examine the log file, pointed to in the last line in the output of error messages. The compiler's message about the syntax problem may lead you to a solution.

Some common problems are

1. using `a**b` for exponentiation (illegal in C++) instead of `pow(a, b)`,
2. forgetting that the spatial coordinates are denoted by a vector `x`,
3. forgetting that the x , y , and z coordinates in space correspond to `x[0]`, `x[1]`, and `x[2]`, respectively.

Failure to initialize parameters in the expressions lead to a compilation error where this problem is explicitly pointed out.

Example. The implementation

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

fails with compilation error

```
RuntimeError: In instant.recompile: The module did not compile with
command 'make VERBOSE=1', see '/some/path/.../compile.log'
```

Looking up the `compile.log` file and searching for `error`, we see the following message from the C++ compiler:

```
error: expected `*' before `p_0'
values[0] = x[1] <= 0.5? 2*x[1]*p_1/(p_0 + p_1) :
((2*x[1]-1)p_0 + p_1)/(p_0 + p_1);
```

Now we realize that a `*` symbol is missing between `)` and `p_0`.

7.1.3 Problems in the solve step

Sometimes the problem lies in the solve step where a variational form is turned into a system of algebraic equations. The error message *Unable to extract all indicies* points to a problem with the variational form. Common errors include

1. missing either the `TrialFunction` or the `TestFunction` object,
2. no terms without `TrialFunction` objects.
3. mathematically invalid operations in the variational form.

The first problem implies that one cannot make a matrix system or system of nonlinear algebraic equations out of the variational form. The second problem means that there is no "right-hand side" terms in the PDE with known quantities. Sometimes this is seemingly the case mathematically because the "right-hand side" is zero. Variational forms must represent this case as `Constant(0)*v*dx` where `v` is a `TestFunction` object. An example of the third problem is to take the `inner` product of a scalar and a vector (causing in this particular case the error message to be "Shape mismatch").

The message *Unable to extract common cell; missing cell definition in form or expression* will typically arise from a term in the form where a test function (holding mesh and cell information) is missing. For example, a zero right-hand side `Constant(0)*dx` will generate this error.

7.1.4 Unable to convert object to a UFL form

One common reason for the above error message is that a form is written without being multiplied by `dx` or `ds`.

7.1.5 UFL reports that a numpy array cannot be converted to any UFL type

One reason may be that there are mathematical functions like `sin` and `exp` operating on `numpy` arrays. The problem is that the

```
from fenics import *
```

statement imports `sin`, `cos`, and similar mathematical functions from UFL and these are aimed at taking `Function` or `TrialFunction` objects as arguments and not `numpy` arrays. The remedy is to use prefix mathematical functions aimed at `numpy` arrays with `numpy`, or `np` if `numpy` is imported as `np: numpy.exp` or `np.exp`, for instance. Normally, boundary conditions and analytical solutions are represented by `Expression` objects and then this problem does not arise. The problem usually arises when pure Python functions with, e.g., analytical solutions are introduced for, e.g., plotting.

7.1.6 All programs fail to compile

When encountering a compilation problem where the Instant log file says something about missing double quote in an `Expression`, try compiling a previously working program. If that program faces the same problem, reboot

Ubuntu and try again. If the problem persists, try running the Update Manager (because unfinished updates can cause compiler problems), reboot and try again.

7.2 Problems with Expression Objects

7.2.1 There seems to be some bug in an Expression object

Run the command `instant-clean` to ensure that everything is (re)compiled. Check the formulas in string expressions carefully, and make sure that divisions do not lead to integer division (i.e., at least one of the operands in a division must be a floating-point variable).

7.2.2 Segmentation fault when using an Expression object

One reason may be that the point vector `x` has indices out of bounds, e.g., that you access `x[2]` but the mesh is only a 2D mesh. Also recall that the components of `x` are `x[0]`, `x[1]`, etc. Accessing `x[2]` as the "y" coordinate is a common error.

7.3 Other Problems

7.3.1 Very strange error message involving a `mesh` variable

If you encounter a really strange error message, and the statement in question involves a variable with name `mesh`, check if this is really your mesh variable. When doing `from fenics import *`, you get a `mesh` variable, which is actually a module, and sending this module to functions creates a `TypeError`. Substitute with the actual name of your mesh object.

One should also note other names that get imported by `from fenics import *: e, f, i, j, k, l, p, q, r, s`. It is easy to use such variables without initializing them, and strange error message arises (since the mentioned names are UFL `Index` objects).

7.3.2 The plot disappears quickly from the screen

You have forgotten to insert `interactive()` as the last statement in the program.

7.3.3 Only parts of the program are executed

Check if a call to `interactive()` appears in the middle of the program. The computations are halted by this call and not continued before you press `q` in a plot window. Most people thus prefer to have `interactive()` as the last statement.

7.3.4 Error in the definition of the boundary

Consider this code and error message:

```
class DirichletBoundary(SubDomain): # define the Dirichlet boundary
    def inside(self, x, on_boundary):
        return on_boundary and abs(x) < 1E-14

bc = DirichletBC(V, u0, xleft_boundary)

Error: ValueError: The truth value of an array with more than
one element is ambiguous. Use a.any() or a.all()
```

The reason for this error message is that `x` is a point vector, not just a number. In the `inside` function one must work with the components of `x`: `x[0]`, `x[1]`, etc.

7.3.5 The solver in a nonlinear problems does not converge

There can be many reasons for this common problem:

1. The form (variational formulation) is not consistent with the PDE(s).
2. The boundary conditions in a Newton method are wrong. The correction vector must have vanishing essential conditions where the complete solution has zero or non-zero values.
3. The initial guess for the solution is not appropriate. In some problems, a simple function equal to 0 just leads to a zero solution or a divergent

solver. Try 1 as initial guess, or (better) try to identify a linear problem that can be used to compute an appropriate initial guess, see Section 5.2.2.

7.4 How To Debug a FEniCS Program?

Here is an action list you may follow.

Step 1. Examine the weak form and its implementation carefully. Check that all terms are multiplied by `dx` or `ds`, and that the terms do not vanish; check that at least one term has both a `TrialFunction` and a `TestFunction` (term with unknown); and check that at least one term has no `TrialFunction` (known term).

Step 2. Check that Dirichlet boundary conditions are set correctly.

```
# bcs is list of DirichletBC objects
for bc in bcs:
    bc_dict = bc.get_boundary_values()
    for dof in bc_dict:
        print('dof %d: value=%s' % (dof, bc_dict[dof]))
```

See also an expanded version of this snippet in the `solvers_bc_ft06_poisson_vc.py` file located in the directory `poisson`.

A next step in the debugging, if these values are wrong, is to call the functions that define the boundary parts. For example,

```
for coor in mesh.coordinates():
    if my_boundary_function(coor, True):
        print('%s is on the boundary' % coor)

# or, in case of a SubDomain subclass my_subdomain_object,
for coor in mesh.coordinates():
    if my_subdomain_object.inside(coor, True):
        print('%s is on the boundary' % coor)
```

You may map the solution to a structured grid with structured data, i.e., a `BoxField`, see Chapters 2.2.8 and 4.3.2, and then examine the solution field along grid lines in x and y directions. For example, you can easily check that correct Dirichlet conditions are set, e.g., at the upper boundary (check `u_box[:, -1]`).

Step 4. Switching to a simple set of coefficients and boundary conditions, such that the solution becomes simple too, but still obeys the same PDE, may help since it is then easier to examine numerical values in the solution array.

Step 5. Formulate a corresponding 1D problem. Often this can be done by just running the problem with a 1D mesh. Doing hand calculations of element matrices and vectors, and comparing the assembled system from these hand calculations with the assembled system from the FEniCS program can uncover bugs. For nonlinear problems, or problems with variable coefficients, it is usually wise to choose simple coefficients so that the problem becomes effectively linear and the hand calculations are doable.

7.5 To-do list

7.5.1 AL list

- Title?: Writing State-of-the-Art Finite Element Solvers in Minutes (HPL: Yes - let's have this for a while)
- Title: "Writing... in minutes" sounds more like a good subtitle than an actual title. We already have a good subtitle in "The FEniCS tutorial" so let's try to find a more "serious" main title. (HPL: What about switching?)
- Title?: Introduction to Finite Element Programming
- Add 2nd author
- Rewrite abstract to reflect new title and non-initial state of book
- Rename and expand Chapter 5: Boundary conditions, markers and sub-domains (many and confusing ways to do this, `MeshFunctions`, `MeshData`, etc) (HPL: This is important and confusing, but very much needed early on)
- DONE: Add chapter on installation (difficult, still in flux)
- Installation chapter should be number 0
- Remove capitalization of sections in Chapter 8
- Add new chapter: "Advanced example: Linear elasticity" (HPL: do this first - important for many courses)
- Add new chapter: "Advanced example: Hyperelasticity"
- Add new chapter: "Advanced example: Incompressible Navier-Stokes"
- Place these chapters near end of book so progression becomes:
 - Installation
 - Fundamentals (3 chapters: Fundamentals, Time-dependent, Nonlinear)
 - Misc technical chapters (boundary conditions, geometries etc) (HPL: Think we need these things before time-dependent, or maybe split the very simplest things from time-dependent (1st example) and nonlinear (`solve(F==0, ...)`) and place in fundamentals?)
 - Advanced examples (using previously discussed techniques)
- Add chapter on performance and profiling? HPL: Yes!

- Move source code links to <http://fenisproject.org/tutorial> (we can set up a cron job to copy files from `hplgit`)
- Number examples sequentially, something like
 - `fenics_tutorial_01_poisson_first.py`
 - `fenics_tutorial_05_poisson_nonlinear.py`

Hierarchic structure becomes complicated, better with flat structure (HPL: These filenames are too long, giving too long lines in the text and the need for lots of rewrites. We have an automated scheme to assign new filenames to the logical files that we use for the text. Right now the names are `ft01_poisson_flat.py`.)

- Add command `fenics-version`
- DONE: Use dot and grad in Poisson example (not `inner` and `nabla_grad`)
- Use new notation '`P`' instead of '`Lagrange`' in `FunctionSpace`. HPL: Done. (HPL: Not yet documented in `FunctionSpace` ;)
- DONE: Use `from fenics import *`
- Fix copyright footer so we avoid the linebreak. HPL: Fixed. This and similar adjustments in the latex file is easily done by auto editing in `make.sh`.
- How does doconce handle – and —? HPL: Like latex. Just use ndash if you want. ndash and mdash are ignored in other formats than latex and html where there is no support for this. Just introduce ndash where you like, as in Navier–Stokes.
- When to use . and when to use . ? HPL: Springer had a rule with thinspace. I don't know if it applies to the brief series, but it became a habit of mine since other styles demanded it.
- When to specify floats as 2 or 2.0? HPL: In code? Anytime there is a danger of integer division.

7.5.2 HPL list

Remember: cannot exceed 150 pages (as reported at the end of `ftut.log`). Solutions to exercises will not appear in the printed book. If we run out of pages, we can also remove the exercises by putting if-else constructs around them. There will be one short printed tutorial and then extended e-versions with exercises (and optionally solution) on our github web site.

Regarding layout, we must use `svmono.cls` for the printed book, but are allowed to use gray background in code boxes and `lmodern` instead of `Courier` for monospace font. Springer's official ebook has exactly the same layout. For all other versions on our github web site, we can choose whatever layout we want.

- `mshr` must align subdomains with cell facets!! Important feature.

- Programs are now flat demos. Educate the reader with better software engineering habits: functions, classes, unit tests. Avoid copy-and-edit flat programs implied by today's collection. (HPL)
- Find successful exercises from various tutorials (AL) and add as exercises in the book (HPL/AL). Exercises are key for learning software so having them (in an extended version?) sends an important signal about their relevance.
- Meshr domains. Set up some common continuum mechanics examples first. (HPL/AL)
- Decide on an elasticity problem.
- Simple Navier-Stokes solver. Do backward facing step and flow around a cylinder.
- According to the `plot` doc string, it should be easy to plot the element a la `plot(u.function_space().ufl_element())` but I did not get this to work. Not crucial, but plotting the element is a nice feature :-)
- Show how the definition of boundaries can be done via strings compiled to C++ (as soon as we have an example with non-trivial boundary segments), cf. Navier-Stokes FEniCS demo.
- Comment regarding FEniCS demos: The documented demos mention a lot of packages: DOLFIN, FFC, Fiat, ... Make sure the reader of the tutorial does not get lost in the jungle of packages and make sure the names are explained somewhere in the text such that the tutorial is a good background for understanding every demo in every detail.
- Should we say "in this book" or "in this tutorial"?
- Introduce `near(x, x0, eps)` earlier? Not used until it got the `eps` argument, but is more readable. Important to understand the underlying problem with rounding which is more explicit when doing `abs(x-x0) < eps`.
- Can we change the value of `DOLFIN_EPS`? `import fenics; fenics.DOLFIN_EPS=...` will work, but then all modules in the simulator must do `import fenics`. Note that its value is very strict, e.g., $10.1+10.2$ has rounding 3.510^{-15} , so `DOLFIN_EPS` is strictly for scaled problems only, where all variables are in $[0,1]$.

7.5.3 HPL questions

Iterative linear solvers info. We can get this printed out on the screen, but is there any method to extract this text inside the program, such that we can see how many Krylov iterations we do etc.? Any way for Python to capture the standard output stream in C++?

Easy to write a script that post-processes the output, but we have to wait until the simulator has terminated, or we can pipe to a script `process.py`

that treats the output in some desired way (could append some into to a file and that is reopened by the simulator):

Terminal

```
Terminal> python mysolver.py | process.py
```

where the simplest `process.py` is

```
import sys, time
t0 = time.clock()
while True:
    line = sys.stdin.readline()
    if not line:
        break
    t1 = time.clock()
    print 'after %g seconds: %s' % (t1-t0, line.rstrip())
print 'END'
```

References

- [1] M. S. AlnÄes, A. Logg, K. B. ÃYlgaard, M. E. Rognes, and G. N. Wells. Unified Form Language: A domain-specific language for weak formulations of partial differential equations. *ACM Transactions on Mathematical Software*, 40(2), 2014. doi:10.1145/2566630, arXiv:1211.4047.
- [2] Douglas N. Arnold and Anders Logg. Periodic table of the finite elements. *SIAM News*, 2014.
- [3] W. B. Bickford. *A First Course in the Finite Element Method*. Irwin, 2nd edition, 1994.
- [4] Dietrich Braess. *Finite Elements*. Cambridge University Press, Cambridge, third edition, 2007.
- [5] Susanne C. Brenner and L. Ridgway Scott. *The Mathematical Theory of Finite Element Methods*, volume 15 of *Texts in Applied Mathematics*. Springer, New York, third edition, 2008.
- [6] Philippe G. Ciarlet. *The Finite Element Method for Elliptic Problems*, volume 40 of *Classics in Applied Mathematics*. SIAM, Philadelphia, PA, 2002. Reprint of the 1978 original [North-Holland, Amsterdam; MR0520174 (58 #25001)].
- [7] J. Donea and A. Huerta. *Finite Element Methods for Flow Problems*. Wiley Press, 2003.
- [8] K. Eriksson, D. Estep, P. Hansbo, and C. Johnson. *Computational Differential Equations*. Cambridge University Press, 1996.
- [9] A. Ern and J.-L. Guermond. *Theory and Practice of Finite Elements*. Springer, 2004.
- [10] Python Software Foundation. The Python tutorial.
<http://docs.python.org/2/tutorial>.
- [11] M. Gockenbach. *Understanding and Implementing the Finite Element Method*. SIAM, 2006.
- [12] T. J. R. Hughes. *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall, 1987.
- [13] J. M. Kinder and P. Nelson. *A Student's Guide to Python for Physical Modeling*. Princeton University Press, 2015.

- [14] J. Kiusalaas. *Numerical Methods in Engineering With Python*. Cambridge University Press, 2005.
- [15] R. H. Landau, M. J. Paez, and C. C. Bordeianu. *Computational Physics: Problem Solving with Python*. Wiley, third edition, 2015.
- [16] H. P. Langtangen. *Python Scripting for Computational Science*. Springer, third edition, 2009.
- [17] H. P. Langtangen. *A Primer on Scientific Programming With Python*. Texts in Computational Science and Engineering. Springer, fifth edition, 2016.
- [18] H. P. Langtangen and L. R. Hellevik. Brief tutorials on scientific Python. <http://hplgit.github.io/bumpy/doc/web/index.html>.
- [19] H. P. Langtangen and G. K. Pedersen. *Scaling of Differential Equations*. Simula Springer Brief Series. Springer, 2016. <http://tinyurl.com/qfjgxmfw>.
- [20] A. Logg, K.-A. Mardal, and G. N. Wells. *Automated Solution of Partial Differential Equations by the Finite Element Method*. Springer, 2012.
- [21] M. Mortensen, H. P. Langtangen, and J. Myre. Cbc.rans - a new flexible, programmable software framework for computational fluid dynamics. In H. I. Andersson and B. Skallerud, editors, *Sixth National Conference on Computational Mechanics (MekIT'11)*. Tapir, 2011.
- [22] M. Mortensen, H. P. Langtangen, and G. N. Wells. A FEniCS-based programming framework for modeling turbulent flow by the Reynolds-averaged Navier-Stokes equations. *Advances in Water Resources*, 2011. doi: 10.1016/j.advwatres.2011.02.013.
- [23] M. Pilgrim. *Dive into Python*. Apress, 2004. <http://www.diveintopython.net>.
- [24] A. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations*. Springer Series in Computational Mathematics. Springer, 1994.
- [25] A. Henderson Squillacote. *The Paraview Guide*. Kitware, 2007.

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