### Chapter 4

# Subdomains and boundary conditions

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

# 4.1 Combining Dirichlet and Neumann conditions

Let's return to the Poisson problem from Chapter 2 and see how to extend the mathematics and the implementation to handle a Dirichlet condition in combination with a Neumann condition. The domain is still the unit square, but now we set the Dirichlet condition  $u=u_{\rm D}$  at the left and right sides, x=0 and x=1, while the Neumann condition

$$-\frac{\partial u}{\partial n} = g$$

is applied to the remaining sides y = 0 and y = 1.

#### 4.1.1 PDE problem

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

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

$$u = u_{\rm D} \text{ on } \Gamma_{\rm D},$$
 (4.2)

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

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

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

For ease of programming, we define g as a function over the whole domain  $\Omega$  such that g takes on the correct values at y=0 and y=1. One possible extension is

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

#### 4.1.2 Variational formulation

The first task is to derive the variational formulation. This time we cannot omit the boundary term arising from the integration by parts, because v is only zero on  $\Gamma_{\rm D}$ . We have

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

and since v = 0 on  $\Gamma_{\rm D}$ ,

$$-\int_{\partial \varOmega} \frac{\partial u}{\partial n} v \, \mathrm{d}s = -\int_{\varGamma_{\mathbf{N}}} \frac{\partial u}{\partial n} v \, \mathrm{d}s = \int_{\varGamma_{\mathbf{N}}} g v \, \mathrm{d}s,$$

by applying the boundary condition on  $\Gamma_{\rm N}.$  The resulting weak form reads

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

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

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

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

#### 4.1.3 FEniCS implementation

How does the Neumann condition impact the implementation? Let us revisit our previous implementation ft01\_poisson.py from Section 2.2 and examine which changes we need to make to incorporate the Neumann condition. It turns out that only two changes are necessary:

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

The first adjustment can be coded as

```
tol = 1E-14

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

A more compact implementation reads

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

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

```
g = Expression('4*x[1]', degree=1)
L = f*v*dx - g*v*ds
```

The ds variable implies a boundary integral, while dx implies an integral over the domain  $\Omega$ . No other modifications are necessary.

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

# 4.2 Setting multiple Dirichlet conditions

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## 4.3 Defining subdomains for different materials

Solving PDEs in domains made up of different materials is a frequently encountered task. In FEniCS, these kinds of problems are handled by defining subdomains inside the domain. A simple example with two materials (subdomains) in 2D will demonstrate the idea. We consider the following variable-coefficient extension of the Poisson equation from Chapter 2:

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

in some domain  $\Omega$ . Physically, this problem may be viewed as a model of heat conduction, with variable heat conductivity  $\kappa(x,y) \ge \kappa > 0$ .

For illustration purposes, we consider the domain  $\Omega = [0,1] \times [0,1]$  and divide it into two equal subdomains, as depicted in Figure 4.1:

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

We define  $\kappa(x,y) = \kappa_0$  in  $\Omega_0$  and  $\kappa(x,y) = \kappa_1$  in  $\Omega_1$ , where  $\kappa_0, \kappa_1 > 0$  are given constants.

$$\Omega_1: \kappa(x,y) = \kappa_1$$

$$\Omega_0: \kappa(x,y) = \kappa_0$$

Fig. 4.1 Two subdomains with different material parameters.

The variational formulation may be easily expressed in FEniCS as follows:

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

In the remainder of this section, we will discuss different strategies for defining the coefficient kappa as an Expression that takes on different values in the two subdomains.

#### 4.3.1 Using expressions to define subdomains

The simplest way to implement a variable coefficient  $\kappa = \kappa(x,y)$  is to define an Expression which depends on the coordinates x and y. We have previously used the Expression class to define expressions based on simple formulas. Attentively, an Expression can be defined as a Python class which allows for more complex logic. The following code snippet illustrates this construction:

```
class K(Expression):
    def set_k_values(self, k_0, k_1):
        self.k_0, self.k_1 = k_0, k_1

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

# Initialize kappa
kappa = K()
kappa.set_k_values(1, 0.01)</pre>
```

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

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

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

### 4.3.2 Using mesh functions to define subdomains

We now address how to specify the subdomains  $\Omega_0$  and  $\Omega_1$  using a more general technique. This technique involves the use of two classes that are essential in FEniCS when working with subdomains: SubDomain and MeshFunction. Consider the following definition of the boundary x=0:

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

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

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

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

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

We will use two SubDomain subclasses to define the two subdomains  $\Omega_0$  and  $\Omega_1$ :

```
tol = 1E-14

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

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

Notice the use of <= and >= in both tests. FEniCS will call the inside function for each vertex in a cell to determine whether or not the cell belongs to a particular subdomain. For this reason, it is important that the test holds for all vertices in cells aligned with the boundary. In addition, we use a tolerance to make sure that vertices on the internal boundary at y=0.5 will belong to both subdomains. This is a little counter-intuitive, but is necessary to make the cells both above and below the internal boundary belong to either  $\Omega_0$  or  $\Omega_1$ .

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

is parameterized both over its data type (like integers or booleans) and its dimension (0 = vertex, 1 = edge etc.). Special subclasses VertexFunction, EdgeFunction etc. are provided for easy definition of a MeshFunction of a particular dimension.

Since we need to define subdomains of  $\Omega$  in the present example, we make use of a CellFunction. The constructor is given two arguments: (1) the type of value: 'int' for integers, 'size\_t' for non-negative (unsigned) integers, 'double' for real numbers, and 'bool' for logical values; (2) a Mesh object. Alternatively, the constructor can take just a filename and initialize the CellFunction from data in a file.

We first create a CellFunction with non-negative integer values ('size t'):

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

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

```
subdomain_0 = Omega_0()
subdomain_1 = Omega_1()
subdomain_0.mark(materials, 0)
subdomain_1.mark(materials, 1)
```

This will set the values of the mesh function materials to 0 on each cell belonging to  $\Omega_0$  and 1 on all cells belonging to  $\Omega_1$ . Alternatively, we can use the following equivalent code to mark the cells:

```
materials.set_all(0)
subdomain_1.mark(materials, 1)
```

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

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

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

```
File('materials.xml.gz') << materials</pre>
```

which can later be read back from file as follows:

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

Now, to use the values of the mesh function materials to define the variable coefficient  $\kappa$ , we create a FEniCS Expression:

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

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

```
values[0] = self.k_0
else:
    values[0] = self.k_1
kappa = K(materials, k_0, k_1, degree=0)
```

This is similar to the Expression subclass we defined above, but we make use of the member function eval\_cell in place of the regular eval function. This version of the evaluation function has an additional cell argument which we can use to check on which cell we are currently evaluating the function. We also defined the special function \_\_init\_\_ (the constructor) so that we can pass all data to the Expression when it is created.

Since we make use of geometric tests to define the two SubDomains for  $\Omega_0$  and  $\Omega_1$ , the MeshFunction method may seem like an unnecessary complication of the simple method using an Expression with an if-test. However, in general the definition of subdomains may be available as a MeshFunction (from a data file), perhaps generated as part of the mesh generation process, and not as a simple geometric test. In such cases the method demonstrated here is the recommended way to work with subdomains.

#### 4.3.3 Using C++ code snippets to define subdomains

The SubDomain and Expression Python classes are very convenient, but their use leads to function calls from C++ to Python for each node in the mesh. Since this involves a significant cost, we need to make use of C++ code if performance is an issue.

Instead of writing the SubDomain subclass in Python, we may instead use the CompiledSubDomain tool in FEniCS to specify the subdomain in C++ code and thereby speed up our code. Consider the definition of the classes Omega\_0 and Omega\_1 above in Python. The key strings that define these subdomains can be expressed in C++ syntax and given as arguments to CompiledSubDomain as follows:

```
tol = 1E-14
subdomain_0 = CompiledSubDomain('x[1] <= 0.5 + tol', tol=tol)
subdomain_1 = CompiledSubDomain('x[1] >= 0.5 - tol', tol=tol)
```

As seen, parameters can be specified using keyword arguments. The resulting objects, subdomain\_0 and subdomain\_1, can be used as ordinary SubDomain objects.

Compiled subdomain strings can be applied for specifying boundaries as well:

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

It is also possible to feed the C++ string (without parameters) directly as the third argument to DirichletBC without explicitly constructing a CompiledSubDomain object:

```
bc1 = DirichletBC(V, value, 'on_boundary && near(x[0], 1, tol)')
```

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

```
cppcode = """
class K : public Expression
public:
  void eval(Array<double>& values,
            const Array<double>& x,
            const ufc::cell& cell) const
  {
    if ((*materials)[cell.index] == 0)
     values[0] = k_0;
    else
     values[0] = k_1;
  }
  std::shared_ptr<MeshFunction<std::size_t>> materials;
  double k 0:
  double k 1;
};
....
kappa = Expression(cppcode=cppcode, degree=0)
kappa.materials = materials
kappa.k_0 = k_0
kappa.k_1 = k_1
```

# 4.4 Setting multiple Dirichlet, Neumann, and Robin conditions

Consider again the variable-coefficient Poisson problem from Section 4.3. We will now discuss how to implement general combinations of boundary conditions of Dirichlet, Neumann, and Robin type for this model problem.

#### 4.4.1 Three types of boundary conditions

We extend our repertoire of boundary conditions to three types: Dirichlet, Neumann, and Robin. Dirichlet conditions apply to some parts  $\Gamma_D^0, \Gamma_D^1, \ldots$ , of the boundary:

$$u = u_D^0$$
 on  $\Gamma_D^0$ ,  $u = u_D^1$  on  $\Gamma_D^1$ , ...,

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

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

Finally, we have *Robin conditions*:

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

where r and s are specified functions. The Robin condition is most often used to model heat transfer to the surroundings and arise naturally from Newton's cooling law. In that case, r is a heat transfer coefficient, and s is the temperature of the surroundings. Both can be space and time-dependent. The Robin conditions apply at some parts  $\Gamma_{\rm R}^0, \Gamma_{\rm R}^1, \ldots$ , of the boundary:

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

#### 4.4.2 PDE problem

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

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

$$u = u_{\mathrm{D}}^{i}$$
 on  $\Gamma_{\mathrm{D}}^{i}$ ,  $i = 0, 1, \dots$  (4.9)

$$-\kappa \frac{\partial u}{\partial n} = g_i$$
 on  $\Gamma_N^i$ ,  $i = 0, 1, \dots$  (4.10)

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

#### 4.4.3 Variational formulation

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

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

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

$$-\int_{\partial\Omega} \kappa \frac{\partial u}{\partial n} v \, \mathrm{d}s = -\sum_{i} \int_{\Gamma_{\mathrm{N}}^{i}} \kappa \frac{\partial u}{\partial n} \, \mathrm{d}s - \sum_{i} \int_{\Gamma_{\mathrm{R}}^{i}} \kappa \frac{\partial u}{\partial n} \, \mathrm{d}s$$
$$= \sum_{i} \int_{\Gamma_{\mathrm{N}}^{i}} g_{i} \, \mathrm{d}s + \sum_{i} \int_{\Gamma_{\mathrm{R}}^{i}} r_{i} (u - s_{i}) \, \mathrm{d}s.$$

We thus obtain the following variational problem:

$$F = \int_{\Omega} \kappa \nabla u \cdot \nabla v \, \mathrm{d}x + \sum_{i} \int_{\Gamma_{\mathbf{N}}^{i}} g_{i} v \, \mathrm{d}s + \sum_{i} \int_{\Gamma_{\mathbf{R}}^{i}} r_{i} (u - s_{i}) v \, \mathrm{d}s - \int_{\Omega} f v \, \mathrm{d}x = 0.$$

$$(4.12)$$

We have been used to writing this variational formulation in the standard notation a(u,v) = L(v), which requires that we identify all integral depending on the trial function u, and collect these in a(u,v), while the remaining integrals go into L(v). The integrals from the Robin condition must for this reason be split into two parts:

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

We then have

$$a(u,v) = \int_{\Omega} \kappa \nabla u \cdot \nabla v \, dx + \sum_{i} \int_{\Gamma_{\mathbf{R}}^{i}} r_{i} u v \, ds, \qquad (4.13)$$

$$L(v) = \int_{\Omega} f v \, \mathrm{d}x - \sum_{i} \int_{\Gamma_{\mathrm{N}}^{i}} g_{i} v \, \mathrm{d}s + \sum_{i} \int_{\Gamma_{\mathrm{R}}^{i}} r_{i} s_{i} v \, \mathrm{d}s. \tag{4.14}$$

Alternatively, we may keep the formulation (4.12) and either solve the variational problem as a nonlinear problem (F == 0) in FEniCS or use the FEniCS functions 1hs and rhs to extract the bilinear and linear parts of F:

```
L = rhs(F)
```

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

#### 4.4.4 FEniCS implementation

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

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

A general approach to the first task is to mark each of the desired boundary parts with markers 0, 1, 2, and so forth. Here we aim at the four sides of the unit square, marked with 0 (x=0), 1 (x=1), 2 (y=0), and 3 (y=1). The markers will be defined using a MeshFunction, but contrary to Section 4.3, this is not a function over cells, but a function over the facets of the mesh. We use a FacetFunction for this purpose:

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

As in Section 4.3 we use a subclass of SubDomain to identify the various parts of the mesh function. Problems with domains of more complicated geometries may set the mesh function for marking boundaries as part of the mesh generation. In our case, the boundary x=0 can be marked as follows:

```
class BoundaryX0(SubDomain):
    tol = 1E-14
    def inside(self, x, on_boundary):
        return on_boundary and near(x[0], 0, tol)

bx0 = BoundaryX0()
bx0.mark(boundary_markers, 0)
```

Similarly, we create the classes BoundaryX1 (x = 1), BoundaryY0 (y = 0), and BoundaryY1 (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,

specifies

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

As explained in Section 4.2, multiple Dirichlet conditions must be collected in a list of DirichletBC objects. Based on the boundary\_conditions data structure above, we can construct this list by the following code snippet:

A new aspect of the variational problem is the two distinct boundary integrals over  $\Gamma_{\rm N}^i$  and  $\Gamma_{\rm R}^i$ . Having a mesh function over exterior cell facets (our boundary\_markers object), where subdomains (boundary parts) are numbered as  $0,1,2,\ldots$ , the special symbol ds(0) implies integration over subdomain (part) 0, ds(1) denotes integration over subdomain (part) 1, and so on. The idea of multiple ds-type objects generalizes to volume integrals too: dx(0), dx(1), etc., are used to integrate over subdomain 0, 1, etc., inside  $\Omega$ 

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

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

Similarly, if we want integration over different parts of the domain, we redefine  $\mathtt{dx}$  as

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

where domain\_markers is a CellFunction defining subdomains in  $\Omega$ .

Suppose we have a Robin condition with values  ${\tt r}$  and  ${\tt s}$  on subdomain R, and a Neumann condition with value  ${\tt g}$  on subdomain N. The variational form can then be written

```
a = kappa*dot(grad(u), grad(v))*dx + r*u*v*ds(R)
L = f*v*dx - g*v*ds(N) + r*s*v*ds(R)
```

In our case, things get a bit more complicated since the information about integrals in Neumann and Robin conditions are in the boundary\_conditions data structure. We can collect all Neumann conditions by the following code snippet:

```
integrals_N = []
for i in boundary_conditions:
```

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

Applying sum(integrals\_N) will apply the + operator to the variational forms in the integrals\_N list and result in the integrals we need for the right-hand side L of the variational form.

The integrals in the Robin condition can similarly be collected in lists:

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

We are now in a position to define the  $\mathtt{a}$  and  $\mathtt{L}$  expressions in the variational formulation:

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

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

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

F = kappa*dot(grad(u), grad(v))*dx + \
        sum(integrals_R) - f*v*dx + sum(integrals_N)
a, L = lhs(F), rhs(F)
```

This time we can more naturally define the integrals from the Robin condition as r\*(u - s)\*v\*ds(i).

The complete code can be found in the function solver\_bcs in the program ft10\_poisson\_extended.py.

### 4.4.5 Test problem

We will use the same exact solution  $u_e = 1 + x^2 + 2y^2$  as in Chapter 2, and thus take  $\kappa = 1$  and f = -6. Our domain is the unit square, and we assign Dirichlet conditions at x = 0 and x = 1, a Robin condition at y = 0, and a Neumann condition at y = 1. With the given exact solution  $u_e$ , we realize that the Neumann condition at y = 1 is  $-\partial u/\partial n = -\partial u/\partial y = 4y = 4$ , while the Robin condition at y = 0 can be selected in many ways. Since  $-\partial u/\partial n = \partial u/\partial y = 0$ 

at y = 0, we can select  $s = u_e$  and specify  $r \neq 0$  arbitrarily in the Robin condition. We will set r = 1000 and  $s = u_e$ .

The boundary parts are thus  $\Gamma^0_{\rm D}$ :  $x=0,\ \Gamma^1_{\rm D}$ :  $x=1,\ \Gamma^0_{\rm R}$ : y=0, and  $\Gamma^0_{\rm N}$ : y=1.

When implementing this test problem, and especially other test problems with more complicated expressions, it is advantageous to use symbolic computing. Below we define the exact solution as a sympy expression and derive other functions from their mathematical definitions. Then we turn these expressions into C/C++ code, which can then be used to define Expression objects.

```
# Define manufactured solution in sympy and derive f, g, etc.
import sympy as sym
x, y = sym.symbols('x[0], x[1]')
                                                                                                           # needed by UFL
u = 1 + x**2 + 2*v**2
                                                                                                            # exact solution
u_e = u
                                                                                                            # exact solution
u_00 = u.subs(x, 0)
                                                                                                            # restrict to x = 0
u_01 = u.subs(x, 1)
                                                                                                            # restrict to x = 1
f = -sym.diff(u, x, 2) - sym.diff(u, y, 2) # -Laplace(u)
f = sym.simplify(f)
                                                                                                            # simplify f
g = -sym.diff(u, y).subs(y, 1)
                                                                                                            \# compute g = -du/dn
                                                                                                           # Robin data, arbitrary
r = 1000
s = u
                                                                                                            # Robin data, u = s
# Collect variables
variables = [u_e, u_00, u_01, f, g, r, s]
# Turn into C/C++ code strings
variables = [sym.printing.ccode(var) for var in variables]
# Turn into FEniCS Expressions
variables = [Expression(var, degree=2) for var in variables]
# Extract variables
u_e, u_0, u_0, u_1, u_1, u_2, u_1, u_2, u_3, u_4, u_1, u_2, u_3, u_4, u_4, u_4, u_5, 
# Define boundary conditions
boundary_conditions = {0: {'Dirichlet': u_00}, #x = 0
                                                         1: {'Dirichlet': u_01}, # x = 1
                                                         2: {'Robin': (r, s)}, # y = 0
                                                         3: {'Neumann': g}} # y = 1
```

The complete code can be found in the function demo\_bcs in the program ft10\_poisson\_extended.py.

### 4.4.6 Debugging boundary conditions

It is easy to make mistakes when implementing a problem with many different types of boundary conditions, as in the present case. One method to debug boundary conditions is to run through all vertex coordinates and check if the SubDomain.inside method marks the vertex as on the boundary. Another useful method is to list which degrees of freedom that are subject to Dirichlet conditions, and for first-order Lagrange  $(P_1)$  elements, print the corresponding vertex coordinates as illustrated by the following code snippet:

```
if debug1:
    # Print all vertices that belong to the boundary parts
    for x in mesh.coordinates():
        if bx0.inside(x, True): print('%s is on x = 0' % x)
        if bx1.inside(x, True): print('%s is on x = 1' % x)
        if by0.inside(x, True): print('%s is on y = 0' % x)
        if by1.inside(x, True): print('%s is on y = 1' % x)
    # Print the Dirichlet conditions
    print('Number of Dirichlet conditions:', len(bcs))
    if V.ufl_element().degree() == 1: # P1 elements
        d2v = dof_to_vertex_map(V)
        coor = mesh.coordinates()
        for i, bc in enumerate(bcs):
            print('Dirichlet condition %d' % i)
            boundary_values = bc.get_boundary_values()
            for dof in boundary_values:
                print('
                          dof %2d: u = %g' % (dof, boundary_values[dof]))
                if V.ufl_element().degree() == 1:
                    print('
                             at point %s' %
                          (str(tuple(coor[d2v[dof]].tolist()))))
```

#### Calls to the inside method

In the code snippet above, we call the inside method for each coordinate of the mesh. We could also place a printout inside the inside method. Then it will be surprising to see that this method is called not only for the points assoicated with degrees of freedom. For  $P_1$  elements the method is also called for each midpoint on each facet of the cells. This is because a Dirichlet condition is by default set only if the entire facet can be said to be subject to the condition defining the boundary.

### 4.5 Generating meshes with subdomains

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

look at how to use the FEniCS mesh generation tool mshr to generate meshes and define subdomains.

#### 4.5.1 PDE problem

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

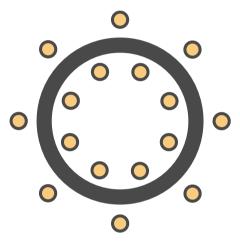


Fig. 4.2 Cross-section of an iron cylinder with copper wires wound around the cylinder, here with n=8 windings. The inner circles are cross-sections of the copper wire coming up ("north") and the outer circles are cross-sections of the copper wire going down into the plane ("south").

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

#### 4.5.2 Variational formulation

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

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

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

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

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

#### 4.5.3 FEniCS implementation

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

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

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

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

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

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

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

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

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

A detail of the mesh is shown in Figure 4.3.

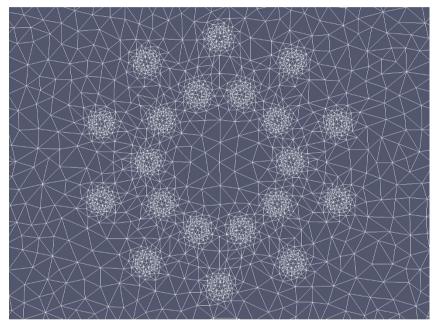


Fig. 4.3 Plot of (part of) the mesh generated for the magnetostatics test problem. The subdomains for the iron cylinder and copper wires are clearly visible

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

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

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

We can now use the markers as we have done before to redefine the integration measure  $\mathtt{dx}$ :

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

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

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

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

```
class Permeability(Expression):
    def __init__(self, mesh, **kwargs):
        self.markers = markers

def eval_cell(self, values, x, ufc_cell):
    if markers[ufc_cell.index] == 0:
        values[0] = 4*pi*1e-7 # vacuum
    elif markers[ufc_cell.index] == 1:
        values[0] = 1e-5 # iron (should really be 2.5e-1)
    else:
        values[0] = -6.4e-6 # copper (yes, it's negative!)

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

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

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

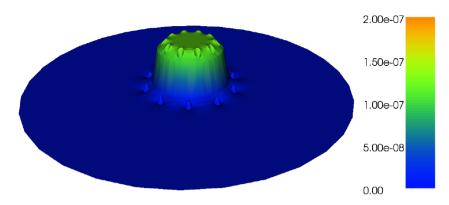
```
W = VectorFunctionSpace(mesh, 'P', 1)
B = project(as_vector((A_z.dx(1), -A_z.dx(0))), W)
```

We use as\_vector to interpret  $(A_z.dx(1), -A_z.dx(0))$  as a vector in the sense of the UFL form language, and not as a Python tuple. The resulting plots of the magnetic vector potential and magnetic field are shown in Figures 4.4 and 4.5.

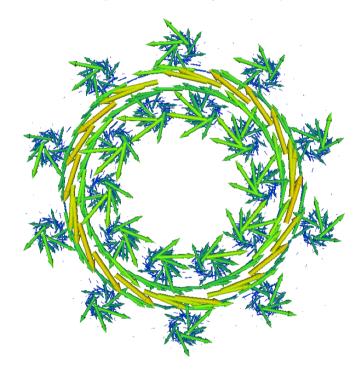
The complete code for computing the magnetic field follows below.

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

a = 1.0  # inner radius of iron cylinder
b = 1.2  # outer radius of iron cylinder
```



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



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

```
c_1 = 0.8 # radius for inner circle of copper wires
c_2 = 1.4 # radius for outer circle of copper wires
r = 0.1 # radius of copper wires
R = 5.0 # radius of domain
n = 10 # number of windings
# Define geometry for background
```

```
domain = Circle(Point(0, 0), R)
# Define geometry for iron cylinder
cylinder = Circle(Point(0, 0), b) - Circle(Point(0, 0), a)
# Define geometry for wires (N = North (up), S = South (down))
angles_N = [i*2*pi/n for i in range(n)]
angles_S = [(i + 0.5)*2*pi/n \text{ for } i \text{ in } range(n)]
wires_N = [Circle(Point(c_1*cos(v), c_1*sin(v)), r) for v in angles_N]
wires_S = [Circle(Point(c_2*cos(v), c_2*sin(v)), r) for v in angles_S]
# Set subdomain for iron cylinder
domain.set_subdomain(1, cylinder)
# Set subdomains for wires
for (i, wire) in enumerate(wires N):
    domain.set_subdomain(2 + i, wire)
for (i, wire) in enumerate(wires S):
    domain.set_subdomain(2 + n + i, wire)
# Create mesh
mesh = generate mesh(domain, 32)
# Define function space
V = FunctionSpace(mesh, 'P', 1)
# Define boundary condition
bc = DirichletBC(V, Constant(0), 'on_boundary')
# Define subdomain markers and integration measure
markers = MeshFunction('size_t', mesh, 2, mesh.domains())
dx = Measure('dx', domain=mesh, subdomain_data=markers)
# Define current densities
J_N = Constant(1.0)
J_S = Constant(-1.0)
# Define magnetic permeability
class Permeability(Expression):
    def __init__(self, mesh, **kwargs):
        self.markers = markers
    def eval_cell(self, values, x, cell):
        if markers[cell.index] == 0:
            values[0] = 4*pi*1e-7 # vacuum
        elif markers[cell.index] == 1:
                               # iron (should really be 2.5e-1)
            values[0] = 1e-5
        else:
            values[0] = -6.4e-6 # copper (yes, it's negative!)
mu = Permeability(mesh, degree=1)
# Define variational problem
A z = TrialFunction(V)
v = TestFunction(V)
```

```
a = (1 / mu)*dot(grad(A_z), grad(v))*dx
L_N = sum(J_N*v*dx(i) \text{ for i in range}(2, 2 + n))
L_S = sum(J_S*v*dx(i) \text{ for i in range}(2 + n, 2 + 2*n))
L = L_N + L_S
# Solve variational problem
A_z = Function(V)
solve(a == L, A_z, bc)
# Compute magnetic field (B = curl A)
W = VectorFunctionSpace(mesh, 'P', 1)
B = project(as\_vector((A\_z.dx(1), -A\_z.dx(0))), W)
# Plot solution
plot(A_z)
plot(B)
# Save solution to file
vtkfile_A_z = File('magnetostatics/potential.pvd')
vtkfile_B = File('magnetostatics/field.pvd')
vtkfile_A_z << A_z
vtkfile B << B
# Hold plot
interactive()
```

This example program can be found in the file ft11\_magnetostatics.py.

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