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# Finite Elements in Computational Mechanics

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## Not included

- Liftint
- Hdiv, Hcurl elements
- $\text{frac}(A)$  observation
- time-discretization
- least squares
- adjoint



## Chapter 1

# Elliptic equations and the finite element method

### 1.1 Introduction

As a starting point for the finite element method, let us consider the mother problem of partial differential equations, the elliptic problem: Find the solution  $u$  of the problem

$$-\nabla \cdot (k \nabla u) = f \quad \text{in } \Omega, \quad (1.1)$$

$$u = g \quad \text{on } \partial\Omega_D, \quad (1.2)$$

$$k \frac{\partial u}{\partial n} = h \quad \text{on } \partial\Omega_N. \quad (1.3)$$

We include here both Dirichlet (1.2) and Neumann (1.3) boundary conditions and assume  $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$  and  $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ .

Unusual concepts like weak or variational formulations, trial and test functions, Sobolev spaces etc. show up in the finite element methods and many find them troublesome and strange. To motivate these concepts we start with some "philosophical" considerations that lead to three challenges which will be resolved by the finite element method. The first challenge: the above equation is the so-called strong formulation and its interpretation is (directly) that: For every point  $x \in \Omega$  the equation

$$-\nabla \cdot (k(x) \nabla u(x)) = f(x), \quad (1.4)$$

should be valid. Hence,  $u, f$  are functions and if we assume that  $f$  is a continuous function then  $u$  is continuous with two derivatives that are also continuous. More formally,  $f \in C(\Omega)$  directly leads to the requirement that  $u \in C^2(\Omega)$ . In general it is however well known, and we will meet many such solutions in this course, that  $u \notin C^2(\Omega)$  are also solutions to (1.1).

In this book, it will be central to compare differential operators with matrices in order to build intuition. So, let us assume that (1.4) is somehow (ignoring the boundary conditions for now) represented as a linear system, i.e.,

$$Au = b. \quad (1.5)$$

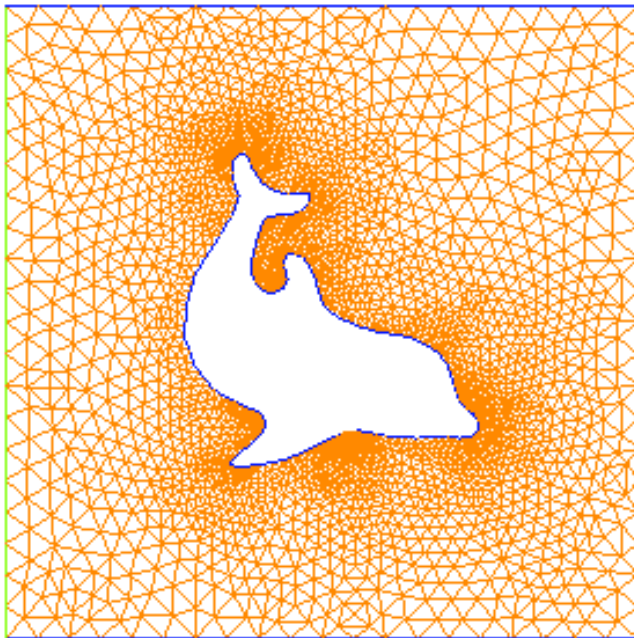
This leads us to our second challenge: In order to have a linear system with a well-defined solution we at least need the same number of equations and unknowns, ie.  $A$  is a  $\mathbb{R}^{N \times N}$  matrix and  $u, f$  are vectors in  $\mathbb{R}^N$ . How can we make numerical methods that ensure the same number of equations and unknowns? Is it ensured by the definition in (1.4). A direct comparison of (1.4) and (1.5) would for instance be to assume that  $i$ 'th equation of  $Au = b$  correspond to the point  $x_i$  in (1.4). Hence,  $\sum_j A_{ij}u_j = b_i$  corresponds to  $-\nabla \cdot (k(x_i)\nabla u(x_i)) = f(x_i)$ . Then the number of equations (or number of rows in  $A$ ) is  $N$  and equals the number of points in the domain. Assuming for instance that  $\Omega$  is the unit square with  $n$  internal points (as the boundary is currently ignored) in both the  $x$ - and  $y$ -direction gives that  $N = n^2$ . With a slight abuse of notation<sup>1</sup>, we may then enumerate the points as  $x_i = (x_j, y_k)$  where  $i = j(N-1) + k$  for  $i, j \in (1, N)$ . In order to get a non-singular matrix, the number of unknowns should equal the number of equations. We do obtain  $N$  unknowns if we assume that for every point in the domain we have an unknown  $u_k = u(x_i, y_j)$ ,  $k = j + i(N-1)$  corresponding to the equations  $-\nabla \cdot (k\nabla u(x_i, y_j)) = f(x_i, y_j)$ . It is however not clear how to make sense of  $u$  outside the points  $(x_i, y_j)$ . Furthermore, an obvious mathematical question is then to what extent we recover  $u \in C^2(\Omega)$ ,  $f \in C(\Omega)$  as  $n$  tends to  $\infty$  with this construction. In general, we will not recover the conditions set by the strong formulation, although a proper mathematical explanation of this is beyond the scope of this book. The reader is referred to [5] for a more detailed explanation of the strong formulation.

Computationally, we need to resort to finite resolutions and this brings us to our third challenge. In Figure 1.1 we see triangulation of domain outside a swimming dolphin. We can immediately see that it will be difficult to formulate a finite difference approach on this domain as the nodal points does not form

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<sup>1</sup> We avoid bold face notation for coordinates.





**Fig. 1.1** An example mesh of a swimming dolphin.

squares. Hence, a stencil like:

$$\frac{u(x+h, y) + u(x, y+h) - 4u(x, y) + u(x-h, y) + u(x, y-h)}{h^2} (\approx \Delta u)$$

will not be able to exploit the triangulation. Furthermore, the stencil will cross  $\partial\Omega$ .

## 1.2 The finite element method in a nutshell

The finite element method (FEM) resolves these three challenges by combining 1) the so-called weak formulations to reduced the demands of differentiability of the solution with 2) trial and test functions constructed by the same approach

leads to  $N \times N$  matrices and 3) a structured approach of integration adjusted to the underlying meshes. Hence, before we start with FEM, let us recap some fundamental results of calculus that will lead to the weak formulation, the Gauss-Green's lemma:

$$\int_{\Omega} -\nabla \cdot (k \nabla u) v \, dx = \int_{\Omega} (k \nabla u) \cdot \nabla v \, dx - \int_{\partial \Omega} k \frac{\partial u}{\partial n} v \, ds. \quad (1.6)$$

Here, we have two functions: the trial function  $u$  and the test function  $v$ , and we are able to move derivatives from  $u$  to  $v$  and hence reduce the strict requirement of  $u \in C^2(\Omega)$ .

Next, we apply the boundary conditions. That is, for the Dirichlet condition (1.2) we already know that  $u = g$ . Hence,  $u$  is not an unknown on that part of the boundary. Therefore, it is common to let  $v = 0$  at  $\partial \Omega_D$ . Hence, by inserting the Neumann condition, we obtain that

$$\int_{\partial \Omega} k \frac{\partial u}{\partial n} v \, ds = \int_{\partial \Omega_D} k \frac{\partial u}{\partial n} v \, ds + \int_{\partial \Omega_N} k \frac{\partial u}{\partial n} v \, ds \quad (1.7)$$

$$= \int_{\partial \Omega_D} k \frac{\partial u}{\partial n} 0 + \int_{\partial \Omega_N} h v \, ds \quad (1.8)$$

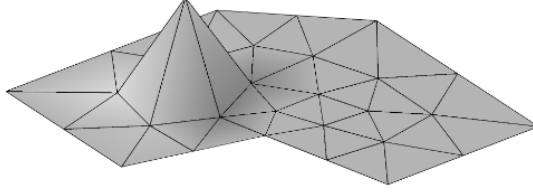
As such we arrive at the *weak formulation* of the elliptic problem: Find  $u$  such that

$$\int_{\Omega} k \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx + \int_{\partial \Omega_N} h v \, ds, \quad \forall v \quad (1.9)$$

Here, we assume as mentioned that  $u = g$  and  $v = 0$  on  $\partial \Omega_D$ . We will come back to what  $\forall v$  means in a more precise sense later.

At this point we *summarize how to obtain a weak formulation* as this will be done over and over again throughout this book. First, we multiply with a test function and integrate. Second, the Gauss-Green lemma (or a similar lemma) is applied and third we apply the boundary conditions.

*Remark 1.1* We remark that the test function  $v$  plays the role of pointwise evaluation in the strong formulation (1.4). That is, we evaluate (or test) the above equation with respect to many different test functions, which in the previous formulation corresponded to many different points. We notice that if the test functions are Dirac delta functions then we recover the strong formulation. However, since but we cannot differentiate the  $\delta$  functions (in a classical sense) we are only able to evaluate the left-hand side of (1.6). Using the  $\delta$  functions as test functions and avoiding the use of Gauss-Green is often called the *collocation method* and is used e.g. by the Runge-Kutta method. However,



**Fig. 1.2** One finite element basis function /pyramide function associated with a particular node.

it is seldom used for FEM because of the high demands on the differentiability on  $u$ .

The second challenge was to find formulations that lead to linear systems with  $N \times N$  matrices. The finite element method directly exploits the weak formulation. The finite element method resolves this challenge by employing the same basis functions for both the trial and the test functions. That is, let the trial and test functions be as follows:

$$u = \sum_{j=1}^N u_j N_j \quad \text{and} \quad v = N_i, \quad i = 1 \dots N. \quad (1.10)$$

Here  $\{N_i\}$  is a set of basis functions that needs to be chosen somehow. Furthermore, as the third challenge above mentioned, the basis functions need to adapt to a mesh. There are many possibilities and one may target the basis function to the problem at hand. The simplest basis function is shown in Fig 1.2. Here, the basis function is chosen as linear functions / pyramids associated with the nodal points, so-called Lagrange element of first order. There are many, many different finite element functions to choose from and they have different properties. Lists of common and unusual elements available in FEniCS can be found in [7].

The FEM problem is obtained by inserting (1.10) into the weak formulation (1.9), i.e.

$$\int_{\Omega} k \nabla \sum_j u_j N_j \cdot \nabla N_i dx = \int_{\Omega} f N_i dx + \int_{\Omega_N} h N_i ds \quad \forall j.$$

We pull the summation out:

$$\sum_j u_j \int_{\Omega} k \nabla N_j \cdot \nabla N_i dx = \int_{\Omega} f N_i dx + \int_{\Omega_N} h N_i ds \quad \forall j.$$

Hence, with

$$A_{ij} = \int_{\Omega} k \nabla N_j \cdot \nabla N_i dx,$$

$$b_i = \int_{\Omega} f N_i dx + \int_{\Omega_N} h N_i ds$$

we arrive at the following linear system

$$Au = b$$

The following code solves the Poisson problem on the unit square consisting of  $32 \times 32$  rectangles, where each rectangle is divided in two and  $f = 1$ ,  $g = 0$  and  $h = x$ . Dirichlet conditions are set for  $y = 0$  and Neumann for the rest of  $\partial\Omega$ .

```
from dolfin import *

# Create mesh and define function space
mesh = UnitSquareMesh(32, 32)
V = FunctionSpace(mesh, "Lagrange", 1)

# Define Dirichlet boundary (x = 0 or x = 1)
def boundary(x): return x[0] < DOLFIN_EPS

# Define boundary condition
u0 = Constant(0.0)
bc = DirichletBC(V, g, boundary)

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Constant(1)
g = Expression("x[0]")
a = inner(grad(u), grad(v))*dx
L = f*v*dx + h*v*ds

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

# Save solution in VTK format
```

```
file = File("poisson.pvd")
file << u
```

### 1.3 Brief remark on the strange world of partial differential equations and their discretizations

A fundamental property in both the theory of partial differential equations and numerical analysis is the concept of well-posedness. In Hadamard's definition a problem is well-posed if three conditions are met for the given input. The solution 1) exists, is 2) unique and 3) depends continuously on the input. Hence, if we have two inputs to our problem,  $b_1$  and  $b_2$  then the difference between the unique solutions  $u_1$  and  $u_2$  should be bounded by the differences between  $b_1$  and  $b_2$ . In terms of linear algebra, we directly obtain well-posedness if  $A$  is a non-singular matrix. That is, we directly obtain

$$A(u_1 - u_2) = (b_1 - b_2)$$

which leads to

$$\|(u_1 - u_2)\| = \|A^{-1}(b_1 - b_2)\| \leq \|A^{-1}\| \|b_1 - b_2\|$$

and

$$\|(b_1 - b_2)\| = \|A(u_1 - u_2)\| \leq \|A\| \|u_1 - u_2\|$$

Hence, the difference between the solutions  $u_1$  and  $u_2$  in the sense  $\|u_1 - u_2\|$  is bounded continuously both above and below by the difference in data in the sense  $\|b_1 - b_2\|$ . In the above, the norms have not been specified, but then, in a finite dimensional setting, all vector norms are equivalent. These rather simple observations on the linear algebra level does not easily extend to the continuous setting of partial differential equations. For instance, an intuitive estimate given a point  $x$  is

$$\|(u_1(x) - u_2(x))\| \leq \|(-\Delta)^{-1}\| \|f_1(x) - f_2(x)\|$$

This bound is not trivial and in many cases not valid on the continuous level. Here,

Instead, it is useful to consider the square roots for matrices and operators. We will make it more precise later, but let us assume that we have a concept

of  $A^{1/2}$  and  $A^{-1/2}$ . The, as we will see, the notion

$$\|A^{1/2}(u_1 - u_2)\| = \|A^{-1/2}(b_1 - b_2)\|$$

is extraordinary useful and gives precise estimates in a wide range of situations. We remark that  $\Delta = \nabla \cdot \nabla$  and as such  $\nabla$  can be interpreted as some kind of square root of  $\Delta$ . There are however some difficulties that arise with this notion. Let us consider the problem in 1D, using FDM. The stencil is then

$$-u_{xx} \approx Au = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2},$$

where  $u_i = u(x_i)$  and  $x_i = ih$ ,  $i = 0, \dots, N$ . For a mesh with two internal degrees of freedom, the corresponding matrix is

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

Let  $B$

$$Bu = \frac{1}{h} \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}$$

Obviously,

$$A = B^T B$$

However,  $B$  is not unique. Furthermore, it is a rectangular matrix that makes it difficult to invert it. In particular, it has a one-dimensional kernel consisting of the constant vector  $c(1, 1, 1)^T$ , where  $c \in \mathbb{R}$ . Likewise in the continuous setting  $\nabla$  has a kernel of constant functions. However, and withough any mathematical rigour, the correct and actually quite practical variant of the above estimate is

$$\|\nabla(u_1 - u_2)\| = \|\nabla^{-1}(f_1 - f_2)\|$$

We do however need to make sense of the  $\nabla^{-1}$ . For now it is enough to think of it as some form of antiderivative. Here, for instance  $u_1, f_1$  may be the actual continuous solution and input data whereas the  $u_2, f_2$  are the numerical solution and input data.

## 1.4 Further reading

There are several excellent and highly recommended books on the finite element method [1, 2].

## 1.5 Exercises

**Exercise 1.1** Consider the problem  $-u''(x) = x^2$  on the unit interval with  $u(0) = u(1) = 0$ . Let  $u = \sum_{k=1}^N u_k \sin(\pi k x)$  and  $v = \sin(\pi l x)$  for  $l = 1, \dots, N$ , for e.g.  $N = 10, 20, 40$ . and solve (1.9). What is the error in  $L_2$  and  $L_\infty$ .

**Exercise 1.2** Consider the same problem as in the previous exercise, but using Bernstein polynomials. That is, the basis for the Bernstein polynomial of order  $N$  on the unit interval is  $B_k(x) = x^k(1-x)^{N-k}$  for  $k = 0, \dots, N$ . Let  $u = \sum_{k=0}^N u_k B_k(x)$  and  $v = B_l(x)$  for  $l = 1, \dots, N$  and solve (1.9). What is the error in  $L_2$  and  $L_\infty$  in terms of  $N$  for  $N = 1, 2, \dots, 10$ . Remark: Do the basis functions satisfy the boundary conditions? Should some of them be removed?

**Exercise 1.3** Consider the same problem as in the previous exercise, but with  $-u''(x) = \sin(k\pi x)$  for  $k = 1$  and  $k = 10$ .

**Exercise 1.4** Consider the same problem as in the previous exercise, but with the finite element method in for example FEniCS, FEniCSx or Firedrake, using Lagrange method of order 1, 2 and 3.





# Chapter 2

## Crash course in Sobolev Spaces

### 2.1 Introduction

Sobolev spaces are fundamental tools in the analysis of partial differential equations and also for finite element methods. Many books provide a detailed and comprehensive analysis of these spaces that in themselves deserve significant attention if one wishes to understand the foundation that the analysis of partial differential equations relies on. In this chapter we will however not provide a comprehensive mathematical description of these spaces, but rather try to provide insight into their use.

We will here provide the definition of these spaces. Further we will show typical functions, useful for finite element methods, that are in some but not all spaces. We also show how different norms capture different characteristics.

### 2.2 Sobolev spaces, norms and inner products

Sobolev spaces are generalizations of  $L^p$  spaces.  $L^p$  spaces are function spaces defined as follows. Let  $u$  be a scalar valued function on the domain  $\Omega$ , which for the moment will be assumed to be the unit interval  $(0, 1)$ . Then

$$\|u\|_p = \left( \int_0^1 |u|^p dx \right)^{1/p}.$$

$L^p(\Omega)$  consists of all functions for which  $\|u\|_p < \infty$ . Sobolev spaces generalize  $L^p$  spaces by also including the derivatives. On the unit interval, let

$$\|u\|_{p,k} = \left( \int_{\Omega} \sum_{i \leq k} \left| \left( \frac{\partial u}{\partial x} \right)^i \right|^p dx \right)^{1/p}. \quad (2.1)$$

Then the Sobolev space  $W_k^p(\Omega)$  consists of all functions with  $\|u\|_{p,k} < \infty$ .  $W_k^p$  is a so-called Banach space - that is a complete normed vector space. The corresponding semi-norm, that only include the highest order derivative is

$$|u|_{p,k} = \left( \int_{\Omega} \sum_{i=k} \left| \left( \frac{\partial}{\partial x} \right)^i u \right|^p dx \right)^{1/p}. \quad (2.2)$$

The case  $p = 2$  is special in the sense that (2.1) defines an inner product. The Banach space then forms a Hilbert space and these named with  $H$  in Hilbert's honor. That is  $H^k(\Omega) = W^{2,k}(\Omega)$ .

For the most part, we will employ the two spaces  $L^2(\Omega)$  and  $H^1(\Omega)$ , but also  $H^2$  and  $H^{-1}$  will be used. The difference between the norm in  $L^2(\Omega)$  and  $H^1(\Omega)$  is illustrated in the following example.

### Norms of $\sin(k\pi x)$

Consider the functions  $u_k = \sin(k\pi x)$  on the unit interval. Figure 2.1 shows the function for  $k = 1$  and  $k = 10$ . Clearly, the  $L^2$  and  $L^7$  behave similarly in the sense that they remain the same as  $k$  increases. On the other hand, the  $H^1$  norm of  $u_k$  increases dramatically as  $k$  increases. The following code shows how the norms are computed using FEniCS.

```
from dolfin import *

N = 10000
mesh = UnitInterval(N)
V = FunctionSpace(mesh, "Lagrange", 1)

for k in [1, 10]:
    u_ex = Expression("sin(k*pi*x[0])", k=k)
    u = project(u_ex, V)

    L2_norm = sqrt(assemble(u**2*dx))
    print "L2 norm of sin(%d pi x) %e " % (k, L2_norm)

    L7_norm = pow(assemble(abs(u)**7*dx), 1.0/7)
```

```

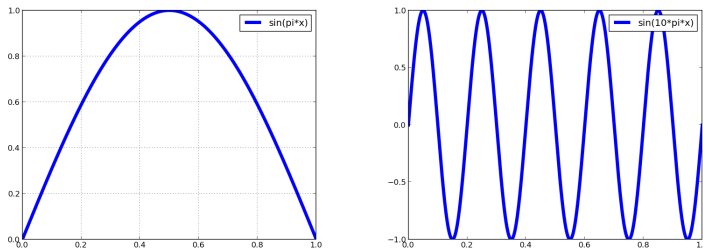
print "L7 norm of sin(%d pi x) %e " % (k, L7_norm)

H1_norm = sqrt(assemble(u*u*dx + inner(grad(u), grad(u))*dx
))
print "H1 norm of sin(%d pi x) %e" % (k, H1_norm)

```

$k \backslash \text{norm}$	$L^2$	$L^7$	$H^1$
1	0.71	0.84	2.3
10	0.71	0.84	22
100	0.71	0.84	222

**Table 2.1** The  $L^2$ ,  $L^7$ , and  $H^1$  norms of  $\sin(k\pi x)$  for  $k=1, 10$ , and  $100$ .



**Fig. 2.1** Left picture shows  $\sin(\pi x)$  on the unit interval, while the right picture shows  $\sin(10\pi x)$ .

## 2.3 Spaces and sub-spaces

The Sobolev space with  $k$  derivatives in  $L_2(\Omega)$  was denoted by  $H^k(\Omega)$ . The subspace of  $H^k$  with  $k-1$  derivatives equal to zero at the boundary is denoted  $H_0^k(\Omega)$ . For example,  $H_0^1(\Omega)$  consists of all functions in  $H^1$  that are zero at

the boundary. Similarly, we may also define a subspace  $H_g^1(\Omega)$  which consists of all functions in  $H^1(\Omega)$  that are equal to the function  $g$  on the boundary.

Mathematically, it is somewhat tricky to define that a function in  $H^1$  is equal to another function as it can not be done in a pointwise sense. This difficulty is resolved by the concept of a trace usually denoted by  $T$ . The concept of a trace is tricky, for example if  $T$  takes a function  $u$  in  $H^1(\Omega)$  and restrict it to  $\partial\Omega$  then  $Tu \notin H^1(\partial\Omega)$ . In fact, in general we only have  $Tu \in H^{1/2}(\partial\Omega)$ .

## 2.4 Norms and Semi-norms

The norm  $\|\cdot\|_{p,k}$  defined in 2.1 is a norm which means that  $\|u\|_{p,k} > 0$  for all  $u \neq 0$ . On the other hand  $|\cdot|_{p,k}$  is a semi-norm, meaning that  $|u|_{p,k} \geq 0$  for all  $u$ . The space  $H^1(\Omega)$  is defined by the norm

$$\|u\|_1 = \left( \int_{\Omega} u^2 + (\nabla u)^2 dx \right)^{1/2}$$

and contains all functions for which  $\|u\|_1 \leq \infty$ . Often we consider subspaces of  $H^1$  satisfying the Dirichlet boundary conditions. The most common space is denoted  $H_0^1$ . This space contains all functions in  $H^1$  that are zero on the boundary. The semi-norm  $|\cdot|_1$  defined as

$$|u|_1 = \left( \int_{\Omega} (\nabla u)^2 dx \right)^{1/2}$$

is a norm on the subspace  $H_0^1$ . In fact, as we will see later, Poincaré's lemma ensures that  $\|\cdot\|_1$  and  $|\cdot|_1$  are equivalent norms on  $H_0^1$  (see Exercise 2.5).

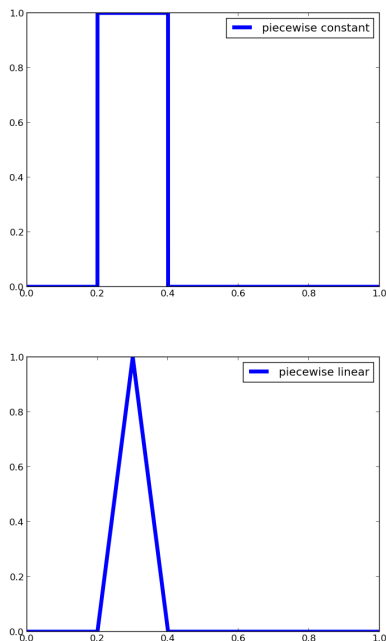
## 2.5 Examples of Functions in Different Spaces

The above functions  $\sin(k\pi x)$  are smooth functions that for any  $k$  are infinitely many times differentiable. They are therefore members of any Sobolev space.

On the other hand, the step function in upper picture in Figure 2.2 is discontinuous in  $x = 0.2$  and  $x = 0.4$ . Obviously, the function is in  $L^2(0,1)$ , but

the function is not in  $H^1(0,1)$  since the derivative of the function consists of Dirac's delta functions<sup>1</sup> that are  $\infty$  at  $x = 0.2$  and  $-\infty$  in  $x = 0.4$ .

The hat function in the lower picture in Figure 2.2 is a typical first order finite element function. The function is in both  $L^2(0,1)$  and  $H^1(0,1)$  (see Exercise 2.3). In general, functions in  $H^q$  are required to be in  $C^{q-1}$ , where  $C^k$  is the class where the  $k$ 'th derivatives exist and are continuous.



**Fig. 2.2** The upper picture shows a piecewise function, discontinuous at  $x = 0.2$  and  $x = 0.4$ , while the lower picture shows a linear function that is continuous.

---

<sup>1</sup> The Dirac's delta function  $\delta_x$  is 0 everywhere except at  $x$  where it is  $\infty$  and  $\int_{\Omega} \delta_x dx = 1$ . Hence, Dirac's delta function is in  $L^1(\Omega)$  but not in  $L^2(\Omega)$ .

## 2.6 Sobolev Spaces and Polynomial Approximation

From Taylor series we know that a  $f(x+h)$  may be approximated by  $f(x)$  and a polynomial in  $h$  that depends on the derivatives of  $f$ . To be precise,

$$|f(x+h) - (P_k f)(x)| \leq \mathcal{O}(h^{k+1}).$$

Here,  $(P_k f)(x)$  is a polynomial of degree  $k$  in  $h$ ,  $f^{(n)}$  denotes the  $n$ 'th derivative of  $f$ , and the error will be of order  $k+1$  in  $h$ . To be precise,

$$(P_k f)(x) = f(x) + \sum_{n=1}^k \frac{f^{(n)}(x)}{n!} h^n.$$

In general, approximation by Taylor series bears strong requirement on the smoothness of the solution which needs to be differentiable in a point-wise sense. However, in Sobolev spaces we have the very usefull approximation property

$$|u - P_k u|_{m,p} \leq C h^{k-m} |u|_{k,p} \quad \text{for } m = 0, 1, \dots, k \text{ and } k \geq 1.$$

This property is used extensively in analysis of finite element methods. The above approximation property is often called the Bramble-Hilbert lemma for  $k \geq 2$  and the case  $k = 1$  was included by a special interpolation operator by Clement, the so-called Clement interpolant. For proof, see e.g. [1, 2].

## 2.7 Eigenvalues and Finite Element Methods

We remember that for  $-\Delta$  on the unit interval  $(0,1)$ , the eigenvalues and eigenvectors are  $(\pi k)^2$  and  $\sin(\pi k x)$ ,  $k = 1, \dots, \infty$ , respectively. It is natural to expect that the eigenvalues in the discrete setting approximate the continuous eigenvalues such that the minimal eigenvalue is  $\approx \pi^2$ , while the maximal eigenvalue is  $\approx \pi^2/h^2$ , where  $k = 1/h$  is the largest  $k$  that may be represented on a mesh with element size  $h$ . Computing the eigenvalues of the finite element stiffness matrix in FEniCS as <sup>2</sup>,

---

<sup>2</sup> We use the `assemble_system` function to enforce the Dirichlet condition in symmetric fashion.

```
A = assemble_system(inner(grad(u), grad(v))*dx, Constant(0)*v*
                    dx, bc)
```

reveals that the eigenvalues are differently scaled. In fact, the minimal eigenvalue is  $\approx \pi^2 h$  and that the maximal eigenvalue is  $\approx \pi^2/h$ . The reason is that the finite element method introduces a mesh-dependent scaling. To estimate the continuous eigenvalues we instead compute the eigenvalues of the generalized eigenvalue problem,

$$Ax = \lambda Mx, \quad (2.3)$$

where  $A$  is the above mentioned stiffness matrix and  $M$  is the mass matrix (or the finite element identity matrix)

```
M = assemble_system(inner(u*v*dx, Constant(0)*v*dx, bc)
```

Figure 2.3 shows the eigenvalues of  $-\Delta$ ,  $A$ , and (2.3) based on the following code:

```
from dolfin import *
import numpy
from scipy import linalg, matrix

def boundary(x, on_boundary): return on_boundary

for N in [100, 1000]:
    mesh = UnitIntervalMesh(N)
    V = FunctionSpace(mesh, "Lagrange", 1)
    u = TrialFunction(V)
    v = TestFunction(V)

    bc = DirichletBC(V, Constant(0), boundary)
    A, _ = assemble_system(inner(grad(u), grad(v))*dx, Constant(
        0)*v*dx, bc)
    M, _ = assemble_system(u*v*dx, Constant(0)*v*dx, bc)

    AA = matrix(A.array())
    MM = matrix(M.array())

    k = numpy.arange(1, N, 1)
    eig = pi**2*k**2

    l1, v = linalg.eigh(AA)
    l2, v = linalg.eigh(AA, MM)

    print "l1 min, max ", min(l1), max(l1)
```

```

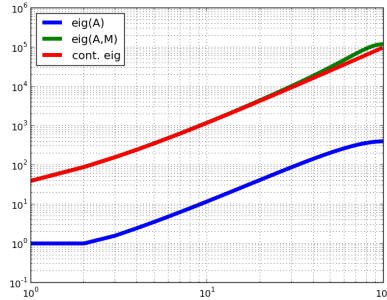
print "l2 min, max ", min(l2), max(l2)
print "eig min, max ", min(eig), max(eig)

import pylab
pylab.loglog(l1[2:], linewidth=5) # exclude the two
                                # smallest (they correspond to
                                # Dirichlet cond))

pylab.loglog(l2[2:], linewidth=5) # exclude the two
                                # smallest again

pylab.loglog(eig, linewidth=5)
pylab.legend(["eig(A)", "eig(A,M)", "cont. eig"], loc="upper
left")
pylab.show()

```



**Fig. 2.3** A log-log plot of the eigenvalues of  $A$ ,  $M^{-1}A$ , and  $-\Delta$ .

From Figure 2.3 we see that the eigenvalues of (2.3) and  $-\Delta$  are close, while the eigenvalues of  $A$  are differently scaled. We remark that we excluded the two smallest eigenvalues in the discretized problems as they correspond to the Dirichlet conditions.

## 2.8 Negative and Fractional Norms

As will be discussed more thoroughly later,  $-\Delta$  is a symmetric positive operator and can be thought of as an infinite dimensional matrix that is symmetric and positive. It is also known from the Riesz representation theorem that if  $u$  solves



the problem

$$\begin{aligned} -\Delta u &= f, & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega \end{aligned}$$

then

$$|u|_1 = \|f\|_{-1}. \quad (2.4)$$

This implicitly define the  $H^{-1}$  norm, although the definition then requires the solution of a Poisson problem. For example, in the previous example where  $u_k = \sin(k\pi x)$ , we have already estimated that  $|u_k|_1 = \frac{\pi k}{\sqrt{2}}$  and therefore  $\|u_k\|_{-1} = |(-\Delta)^{-1}u_k|_1 = \frac{1}{\sqrt{2}k\pi}$ .

Let us now generalize these considerations and consider a matrix (or differential operator)  $A$  which is symmetric and positive.  $A$  has positive and real eigenvalues and defines an inner product which may be represented in terms of eigenvalues and eigenfunctions. Let  $\lambda_i$  and  $u_i$  be the eigenvalues and eigenfunctions such that

$$Au_i = \lambda_i u_i$$

Then,  $x$  may be expanded in terms of the eigenfunctions  $u_i$  as  $x = \sum_i c_i u_i$ , where  $c_i = (x, u_i)$ , and we obtain

$$(x, x)_A = (Ax, x) = (A \sum_i c_i u_i, \sum_j c_j u_j) = (\sum_i \lambda_i c_i u_i, \sum_j c_j u_j)$$

Because  $A$  is symmetric, the eigenfunctions  $u_i$  are orthogonal to each other and we may choose a normalized basis such that  $(u_i, u_j) = \delta_{ij}$ . With this normalization, we simply obtain

$$\|x\|_A^2 = (x, x)_A = (Ax, x) = (A \sum_i c_i u_i, \sum_j c_j u_j) = \sum_i \lambda_i c_i^2$$

A generalization of the  $A$ -inner product (with corresponding norm) to a  $A^q$ -inner product that allow for both negative and fractional  $q$  is then as follows

$$\|x\|_{A,q}^2 = (x, x)_{A,q} = \sum_i \lambda_i^q c_i^2. \quad (2.5)$$

Clearly, this definition yields that  $|u_k|_1 = \frac{\pi k}{\sqrt{2}}$  and  $\|u_k\|_{-1} = \frac{1}{\sqrt{2}k\pi}$ , as above.

As mentioned in Section 2.7, care has to be taken in finite element methods if the discrete eigenvalues are to correspond with the continuous eigenvalues.

We will therefore detail the computation of negative and fractional norms in the following. Let  $\lambda_i$  and  $u_i$  be the eigenvalues and eigenvectors of the following generalized eigenvalue problem

$$Au_i = \lambda_i Mu_i \quad (2.6)$$

and let  $U$  be the matrix with the eigenvectors as columns. The eigenvalues are normalized in the sense that

$$U^T MU = I$$

where  $I$  is the identity matrix. We obtain

$$U^T AU = \Lambda \quad \text{or} \quad A = MU\Lambda(MU)^T,$$

where  $\Lambda$  is a matrix with the eigenvalues  $\lambda_i$  on the diagonal. Hence also in terms of the generalized eigenvalue problem (2.6) we obtain the  $A$ -norm as

$$\|x\|_A^2 = x^T MU\Lambda(MU)^T x$$

and we may define fractional and negative norms in the same manner as (2.5), namely that

$$\|x\|_{A,M,q}^2 = x^T MU\Lambda^q(MU)^T x.$$

Defining the negative and fractional norms in terms of eigenvalues and eigenvectors is convenient for small scale problems, but it is an expensive procedure because eigenvalue problems are computationally demanding. It may, however, be tractable on subdomains, surfaces, or interfaces of larger problems. We also remark that there are other ways of defining fractional and negative norms. For example, one often used technique is via the Fourier series, c.f. e.g. [11]. These different definitions do in general *not* coincide, in particular because they typically have different requirement on the domain or boundary conditions. One should also be careful when employing the above definition with integer  $q > 1$ , in particular because boundary conditions requirements will deviate from standard conditions in the Sobolev spaces for  $q > 1$ .

### Computing the $H^1$ , $L^2$ , and $H^{-1}$ norms

Let as before  $\Omega = (0, 1)$  and  $u_k = \sin(\pi kx)$ . Table 5.1 shows the  $H^1$ ,  $L^2$ , and  $H^{-1}$  norms as computed with (2.5) with  $q = 1, 0$ , and  $-1$ , respectively.

Comparing the computed norms with the norms  $L^2$  and  $H^1$  norms computed in Example 2.2, we see that the above definition (2.5) reproduces the  $H^1$  and  $L^2$  norms with  $q = 1$  and  $q = 0$ , respectively. We also remark that while the  $H^1$  norm increases as  $k$  increases, the  $H^{-1}$  norm demonstrates a corresponding decrease. Below we show the code for computing these norms.

$k \backslash \text{norm}$	$H^1, q = 1$	$L^2, q = 0$	$H^{-1}, q = -1$
1	2.2	0.71	0.22
10	22	0.71	0.022
100	222	0.71	0.0022

**Table 2.2** The  $L^2$ ,  $L^7$ , and  $H^1$  norms of  $\sin(k\pi x)$  for  $k=1, 10$ , and  $100$ .

```

from dolfin import *
from numpy import matrix, diagflat, sqrt
from scipy import linalg, random

def boundary(x, on_boundary): return on_boundary

mesh = UnitIntervalMesh(200)
V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
bc = DirichletBC(V, Constant(0), boundary)

A, _ = assemble_system(inner(grad(u), grad(v))*dx, Constant(0)
                        *v*dx, bc)
M, _ = assemble_system(u*v*dx, Constant(0)*v*dx, bc)
AA = matrix(A.array())
MM = matrix(M.array())

l, v = linalg.eigh(AA, MM)
v = matrix(v)
l = matrix(diagflat(l))

for k in [1, 10, 100]:
    u_ex = Expression("sin(k*pi*x[0])", k=k)
    u = interpolate(u_ex, V)
    x = matrix(u.vector().array())

    H1_norm = pi*k*sqrt(2)/2
    print "H1 norm of sin(%d pi x) %e (exact)          " % (k,
                                                              H1_norm)
    H1_norm = sqrt(assemble(inner(grad(u), grad(u))*dx))

```

```

print "H1 norm of sin(%d pi x) %e (|grad(u)|^2)      " % (k,
H1_norm)
H1_norm = sqrt(x*AA*x.T)
print "H1 norm of sin(%d pi x) %e (x A x' )          " % (k,
H1_norm)
W = MM.dot(v)
H1_norm = sqrt(x*W*1*W.T*x.T)
print "H1 norm of sin(%d pi x) %e (eig)              " % (k,
H1_norm)

print ""

L2_norm = sqrt(2)/2
print "L2 norm of sin(%d pi x) %e (exact)            " % (k,
L2_norm)
L2_norm = sqrt(assemble(u**2*dx))
print "L2 norm of sin(%d pi x) %e |u|^2             " % (k,
L2_norm)
L2_norm = sqrt(x*MM*x.T)
print "L1 norm of sin(%d pi x) %e (x M x' )          " % (k,
L2_norm)
W = MM.dot(v)
L2_norm = sqrt(x*W*1**0*W.T*x.T)
print "L2 norm of sin(%d pi x) %e (eig)              " % (k,
L2_norm)

print ""

Hm1_norm = sqrt(2)/2/k/pi
print "H^-1 norm of sin(%d pi x) %e (exact)          " % (k,
Hm1_norm)
Hm1_norm = sqrt(x*W*1**-1*W.T*x.T)
print "H^-1 norm of sin(%d pi x) %e (eig)            " % (k,
Hm1_norm)
Hm1_norm = sqrt(x*MM*linalg.inv(AA)*MM*x.T)
print "H^-1 norm of sin(%d pi x) %e (x inv(A) x')    " % (k,
Hm1_norm)

```

*Remark 2.1* **Norms for  $|q| > 1$ .**

The norm (2.5) is well defined for any  $|q| \geq 1$ , but will not correspond to the corresponding Sobolev spaces.

*Remark 2.2* **The standard definition of a dual norm**

Let  $(\cdot, \cdot)_A$  be an inner product over the Hilbert space  $V$ . The norm of the dual space is then defined by

$$\|f\|_{A^*} = \sup_{v \in V} \frac{(f, v)}{(v, v)_A}.$$

For example, the  $H^{-1}$  norm is defined as

$$\|f\|_{-1} = \sup_{v \in H^1} \frac{(f, v)}{(v, v)_1}.$$

## 2.9 Exercises

**Exercise 2.1** Compute the  $H^1$  and  $L^2$  norms of a random function with values in  $(0, 1)$  on meshes representing the unit interval of with 10, 100, and 1000 cells.

**Exercise 2.2** Compute the  $H^1$  and  $L^2$  norms of  $\sin(k\pi x)$  on the unit interval analytically and compare with the values presented in Table 2.2.

**Exercise 2.3** Compute the  $H^1$  and  $L^2$  norms of the hat function in Picture 2.2.

**Exercise 2.4** Consider the following finite element function  $u$  defined as

$$u = \begin{cases} \frac{1}{h}x - \frac{1}{h}(0.5 - h), & x = (0.5 - h, 0.5) \\ -\frac{1}{h}x + \frac{1}{h}(0.5 + h), & x = (0.5, 0.5 + h) \\ 0, & \text{elsewhere} \end{cases}$$

That is, it corresponds to the hat function in Figure 2.2, where  $u(0.5) = 1$  and the hat function is zero every where in  $(0, 0.5 - h)$  and  $(0.5 + h, 1)$ . Compute the  $H^1$  and  $L^2$  norms of this function analytically, and the  $L^2$ ,  $H^1$  and  $H^{-1}$  norms numerically for  $h = 10, 100$  and  $1000$ .

**Exercise 2.5** Let  $\Omega = (0, 1)$  then for all functions in  $H^1(\Omega)$  Poincaré's inequality states that

$$|u|_{L^2} \leq C \left| \frac{\partial u}{\partial x} \right|_{L^2}$$

Use this inequality to show that the  $H^1$  semi-norm defines a norm equivalent with the standard  $H^1$  norm on  $H_0^1(\Omega)$ .



## Chapter 3

# Discretization of a convection-diffusion problem

### 3.1 Introduction

This chapter concerns convection-diffusion equations of the form:

$$\begin{aligned} -\mu\Delta u + v \cdot \nabla u &= f & \text{in } \Omega \\ u &= g & \text{on } \partial\Omega \end{aligned}$$

Here  $v$  is typically a velocity,  $\mu$  is the diffusivity, and  $u$  is the unknown variable of interest. We assume the Dirichlet condition  $u = g$  on the boundary, while  $f$  is a source term.

The problem is a singular perturbation problem. That is, the problem is well-posed for  $\mu > 0$  but becomes over-determined as  $\mu$  tends to zero. For  $\mu = 0$  the Dirichlet conditions should only be set on the inflow domain  $\Gamma$ ; that is, where  $n \cdot v < 0$  for the outward unit normal  $n$ .

For many practical situations  $\mu > 0$ , but small in the sense that  $\mu \ll |v|$ . For such problems, the solution will often be similar to the solution of the reduced problem with  $\mu = 0$  except close to the non-inflow boundary  $\partial\Omega \setminus \Gamma$ . Here, there will typically be a boundary layer  $\exp(\|v\|_\infty x / \mu)$ . Furthermore, discretizations often shows unphysical oscillations starting at this boundary layer.

The next example shows a 1D convection diffusion problem resulting in non-physical oscillations due to the use of a standard Galerkin approximation.

#### Standard Galerkin approximation

Consider the following 1D problem convection diffusion problem, where  $v = -1$  for simplicity:

$$-u_x - \mu u_{xx} = 0, \quad (3.1)$$

$$u(0) = 0, u(1) = 1. \quad (3.2)$$

The analytical solution is:

$$u(x) = \frac{e^{-x/\mu} - 1}{e^{-1/\mu} - 1}.$$

Hence, for  $\mu \rightarrow 0$ , both  $e^{-x/\mu}$  and  $e^{-1/\mu}$  will be small and  $u(x) \approx 1$  unless  $x \approx 0$ . However, close to the outflow boundary at  $x = 0$ , there will be a boundary layer where  $u$  has exponential growth.

We solve the problem with a standard Galerkin method using linear first order Lagrange elements. To be specific, the variational problem is:

Find  $u \in H^1_{(0,1)}$  such that

$$\int_0^1 -u_x v + \mu u_x v_x dx = 0, \quad \forall v \in H^1_{(0,0)}.$$

Here,  $H^1_{(0,1)}$  contains functions  $u \in H^1$  with  $u = 0$  at  $x = 0$  and  $u = 1$  and  $x = 1$ , while  $H^1_{(0,0)}$  contains functions that are zero both at  $x = 0$  and  $x = 1$ . We consider a  $\mu = 0.01$ , a relatively large  $\mu$ , to enable us to see the differences on a relatively coarse mesh.

Both the numerical and analytical solutions are shown in Figure 3.1. Clearly, the numerical solution is polluted by non-physical oscillations on the coarse mesh with 10 elements, while a good approximation is obtained for 100 elements.

Finally, we show the complete code for this example:

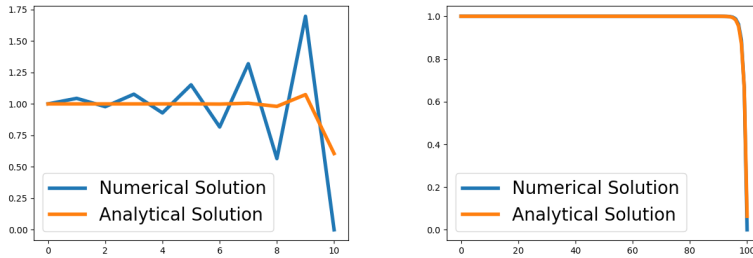
```
from dolfin import *
for N in [10, 100]:

    mesh = UnitInterval(N)
    V = FunctionSpace(mesh, "CG", 1)

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

    mu_value = 1.0e-2
```





**Fig. 3.1** Solution of the convection diffusion problem obtained with 10 and 100 elements. The left figure obtained on a mesh with 10 elements shows wild oscillations, while the mesh with 100 elements demonstrate a nicely converged solution.

```
mu = Constant(mu_value)
f = Constant(0)
h = mesh.hmin()

a = (-u.dx(0)*v + mu*u.dx(0)*v.dx(0))*dx
L = f*v*dx

u_analytical = Expression("(exp(-x[0]/e) - 1) / (exp(-1/%e) - 1)" % (mu_value, mu_value))

def boundary(x):
    return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS

bc = DirichletBC(V, u_analytical, boundary)

U = Function(V)
solve(a == L, U, bc)

U_analytical = project(u_analytical, V)

import pylab
pylab.plot(U.vector().array())
pylab.plot(U_analytical.vector().array())
pylab.legend(["Numerical Solution", "Analytical Solution"])
pylab.show()
```

□

To understand Example 3.1 we first remark that the discretization corresponds to the following central finite difference scheme:

$$-\frac{\mu}{h^2} [u_{i+1} - 2u_i + u_{i-1}] - \frac{v}{2h} [u_{i+1} - u_{i-1}] = 0, \quad i = 1, \dots, N-1$$

$$u_0 = 0, \quad u_N = 1$$

Above, we kept  $v$  as a variable such that we may discuss the directionality of upwinding in terms of the convection. Clearly, if  $\mu = 0$  then the scheme reduces to

$$-\frac{v}{2h} [u_{i+1} - u_{i-1}] = 0, \quad i = 1, \dots, N-1$$

$$u_0 = 0, \quad u_N = 1$$

Here, it is clear that  $u_{i+1}$  is coupled to  $u_{i-1}$ , but not to  $u_i$ . Hence, this scheme allow for an alternating sequence of  $u_{i+1} = u_{i-1} = \dots$ , while  $u_i = u_{i-2} = \dots$  resulting in oscillations.

One cure for these oscillations is upwinding. That is, instead of using a central difference scheme, we employ the following difference scheme:

$$\frac{du}{dx}(x_i) = \frac{1}{h} [u_{i+1} - u_i] \quad \text{if } v < 0,$$

$$\frac{du}{dx}(x_i) = \frac{1}{h} [u_i - u_{i-1}] \quad \text{if } v > 0.$$

Using this scheme, oscillations will disappear. The approximation will however only be first order.

There is a relationship between upwinding and artificial diffusion. If we discretize  $u_x$  with a central difference and add diffusion as  $\epsilon = h/2\Delta$  we get

$$\begin{aligned} & \frac{u_{i+1} - u_{i-1}}{2h} \quad \text{central scheme, first order derivative} \\ & + \frac{h}{2} \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} \quad \text{central scheme, second order derivate} \\ & = \frac{u_i - u_{i-1}}{h} \quad \text{upwind scheme} \end{aligned}$$

Hence, upwinding is equivalent to adding artificial diffusion with  $\epsilon = h/2$ ; that is, in both cases we actually solve the problem

$$-(\mu + \epsilon)u_{xx} + vu_x = f.$$

using a central difference scheme.

Finite difference upwinding is difficult to express using finite elements methods, but it is closely to adding some kind of diffusion to the scheme. The next example shows the solution of the problem in Example 3.1 with artificial diffusion added.

### Stabilization using artificial diffusion

Consider again the following 1D problem convection diffusion problem:

$$-u_x - \mu u_{xx} = 0, \quad (3.3)$$

$$u(0) = 0, u(1) = 1. \quad (3.4)$$

We solve the problem with a standard Galerkin method using linear first order Lagrange elements as before, but we add artificial diffusion. To be specific, the variational problem is:

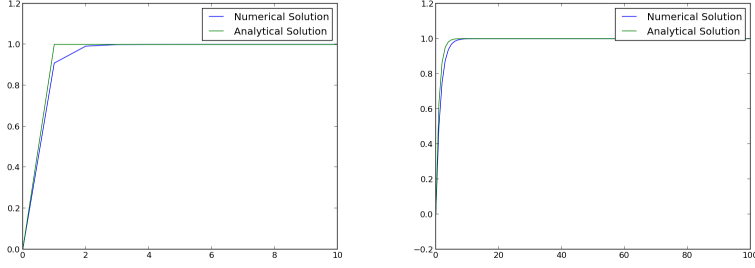
Find  $u \in H_{(0,1)}^1$  such that

$$\int_0^1 -u_x v + (\mu + \beta h) u_x v_x = 0, \quad \forall v \in H_{(0,0)}^1,$$

where  $\beta = 0.5$  corresponds to the finite difference scheme with artificial diffusion mentioned above. Below is the code for the changed variational form:

```
beta_value = 0.5
beta = Constant(beta_value)
f = Constant(0)
h = mesh.hmin()
a = (-u.dx(0)*v + mu*u.dx(0)*v.dx(0) + beta*h*u.dx(0)*v.dx(0)) * dx
```

Figure 3.2 shows the solution for 10 and 100 elements when using artificial diffusion stabilization. Clearly, the solution for the coarse grid has improved dramatically since the oscillations have vanished and the solution appear smooth. It is, however, interesting to note that the solution for the fine mesh is actually less accurate than the solution in Fig 3.2 for the corresponding fine mesh. The reason is that the scheme is now first order, while the scheme in Example 3.1 is second order.



**Fig. 3.2** Solution of the convection diffusion problem obtained with 10 and 100 elements using artificial diffusion to stabilize.

### 3.2 Streamline diffusion/Petrov-Galerkin methods

In the previous section we saw that artificial diffusion may be added to convection diffusion dominated problems to avoid oscillations. The diffusion was, however, added in a rather ad-hoc manner. Here, we will see how diffusion may be added in a consistent way; that is, without changing the solution as  $h \rightarrow 0$ . This leads us to streamline diffusion using the Petrov-Galerkin method. Our problem reads:

Find  $u$  such that

$$\begin{aligned} -\mu \Delta u + v \cdot \nabla u &= f \quad \text{in } \Omega, \\ u &= g \quad \text{on } \partial\Omega. \end{aligned}$$

The **weak formulation** reads:

Find  $u \in H_g^1$  such that

$$a(u, w) = b(w) \quad \forall w \in H_0^1,$$

where

$$\begin{aligned} a(u, w) &= \int_{\Omega} \mu \nabla u \cdot \nabla w \, dx + \int_{\Omega} v \cdot \nabla u w \, dx, \\ b(w) &= \int_{\Omega} f w \, dx. \end{aligned}$$

Here,  $H_g^1$  is the subspace of  $H^1$  where the trace equals  $g$  on the boundary  $\partial\Omega$ .

The *standard Galerkin* discretization is:

Find  $u_h \in V_{h,g}$  such that

$$a(u_h, v_h) = (f, v_h) \quad \forall v_h \in V_{h,0}. \quad (3.5)$$

Here,  $V_{h,g}$  and  $V_{h,0}$  are the subspaces with traces that equals  $g$  and 0 on the boundary, respectively.

Adding artificial diffusion to the standard Galerkin discretization, as was done in Example 3.1, can be done as:

Find  $u_h \in V_{h,g}$  such that

$$a(u_h, v_h) + \frac{h}{2}(\nabla u_h, \nabla v_h) = (f, v_h) \quad \forall v_h \in V_{h,0}.$$

Let

$$\tau(u, v_h) = a(u_h, v_h) - (f, v_h).$$

Then the *truncation error* is first order in  $h$ ; that is,

$$\tau(u) = \sup_{v \in V_h, v \neq 0} \frac{\tau(u, v_h)}{\|v\|_V} \sim \mathcal{O}(h).$$

Hence, the scheme is *consistent* in the sense that

$$\lim_{h \rightarrow 0} \tau(u) \rightarrow 0.$$

However, it is not *strongly consistent* in the sense that  $\tau(u) = 0$  for every discretization, which is what is obtained with the Galerkin method due to Galerkin-orthogonality:

$$\tau(u, v_h) = a(u_h, v_h) - (f, v_h) = a(u_h - h, v_h) = 0 \quad \forall v_h \in V_h.$$

The *Streamline diffusion/Petrov-Galerkin* method introduces a strongly consistent diffusion by employing alternative test functions. Let us therefore assume that we have a space of test functions  $W_h$ . Abstractly, the Petrov-Galerkin method appears very similar to the Galerkin method, that is:

Find  $u_h \in V_{h,g}$  such that

$$a(u_h, v_h) = (f, v_h) \quad \forall v_h \in W_{h,0}.$$

Again,  $V_{h,g}$  and  $W_{h,0}$  are the subspaces with traces that equals  $g$  and 0 on the boundary, respectively. Notice that the only difference from the standard Galerkin formulation is that test and trial functions differ.

On matrix form, the standard Galerkin formulation reads:

$$A_{ij} = a(N_i, N_j) = \int_{\Omega} \mu \nabla N_i \cdot \nabla N_j \, dx + \int_{\Omega} v \cdot \nabla N_i N_j \, dx, \quad (3.6)$$

while for the Petrov Galerkin method, we use the test functions  $L_j$ :

$$A_{ij} = a(N_i, L_j) = \int_{\Omega} \mu \nabla N_i \cdot \nabla L_j \, dx + \int_{\Omega} v \cdot \nabla N_i L_j \, dx$$

A clever choice of  $L_j$  will enable us to add diffusion in a consistent way. To make sure that the matrix is still quadratic, we should however make sure that the dimension of  $V_h$  and  $W_h$  are equal.

Let  $L_j$  be defined as  $L_j = N_j + \beta h v \cdot \nabla N_j$ . Writing out the matrix  $A_{ij}$  in (3.6) now gives

$$\begin{aligned} A_{ij} &= a(N_i, N_j + \beta h v \cdot \nabla N_j) \\ &= \int_{\Omega} \mu \nabla N_i \cdot \nabla (N_j + \beta h v \cdot \nabla N_j) \, dx + \int_{\Omega} v \cdot \nabla N_i \cdot (N_j + \beta h v \cdot \nabla N_j) \, dx \\ &= \underbrace{\int_{\Omega} \mu \nabla N_i \cdot \nabla N_j \, dx + \int_{\Omega} v \cdot \nabla N_i N_j \, dx}_{\text{standard Galerkin}} \\ &\quad + \underbrace{\beta h \int_{\Omega} \mu \nabla N_i \cdot \nabla (v \cdot \nabla N_j) \, dx}_{=0 \text{ third order term, for linear elements}} + \underbrace{\beta h \int_{\Omega} (v \cdot \nabla N_i)(v \cdot \nabla N_j) \, dx}_{\text{Artificial diffusion in } v \text{ direction}} \end{aligned}$$

Notice that also the righthand side changes

$$b(L_j) = \int_{\Omega} f L_j \, dx = \int_{\Omega} f (N_j + \beta h v \cdot \nabla N_j) \, dx$$

Thus, both the matrix and the righthand side are changed such that artificial diffusion is added in a consistent way.

We summarize this derivation by stating the SUPG problem. Find  $u_{h,sd} \in H_g^1$  such that

$$a_{sd}(u, w) = b_{sd}(w) \quad \forall w \in H_0^1, \quad (3.7)$$

where

$$\begin{aligned}
a_{sd}(u, w) &= \int_{\Omega} \mu \nabla u \cdot \nabla w \, dx + \int_{\Omega} v \cdot \nabla u w \, dx \\
&\quad + \beta h \int_{\Omega} (v \cdot \nabla u)(v \cdot \nabla w) \, dx + \beta h \mu \sum_e \int_{\Omega_e} -\Delta u (v \cdot \nabla w) \, dx, \\
b_{sd}(w) &= \int_{\Omega} f w \, dx + \beta h \int_{\Omega} f v \cdot \nabla w \, dx.
\end{aligned}$$

### 3.3 Well posedness of the continuous problem

Before we discuss error estimates of the discrete problem, we briefly describe the properties of the continuous problem.

**Theorem 3.1 *Lax-Milgram theorem***

Let  $V$  be a Hilbert space,  $a(\cdot, \cdot)$  be a bilinear form,  $L(\cdot)$  a linear form, and let the following three conditions be satisfied:

1.  $a(u, u) \geq \alpha \|u\|_V^2, \quad \forall u \in V,$
2.  $a(u, v) \leq C \|u\|_V \|v\|_V, \quad \forall u, v \in V,$
3.  $L(v) \leq D \|v\|_V, \quad \forall v \in V.$

Then the problem: Find  $u \in V$  such that

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

is well-posed in the sense that there exists a unique solution with the following stability condition

$$\|u\|_V \leq \frac{C}{\alpha} \|L\|_{V^*}.$$

Condition (1) is often referred to as coercivity or positivity, while (2) is called continuity or boundedness. Condition 3 simply states that the right-hand side should be in the dual space of  $V$ .

In the following we will use Lax-Milgram's theorem to show that the convection-diffusion problem is well-posed. The Lax-Milgram's theorem is well-suited since it does not require symmetry of the bilinear form.

We will only consider the homogeneous Dirichlet conditions in the current argument<sup>1</sup>. From Poincare's lemma we know that

$$\|u\|_0 \leq C_\Omega |u|_1.$$

Using Poincare, it is straightforward to show that the semi-norm

$$|u|_1 = \left( \int (\nabla u)^2 dx \right)^{1/2}$$

and the standard  $H^1$  norm

$$\|u\|_1 = \left( \int (\nabla u)^2 + u^2 dx \right)^{1/2}$$

are equivalent. Hence, on  $H_0^1$  the  $|\cdot|_1$  is a norm equivalent the  $H^1$ -norm. Furthermore, this norm will be easier to use for our purposes.

For the convection-diffusion problem, we will consider two cases 1) incompressible flow, where  $\nabla \cdot v = 0$  and 2) compressible flow, where  $\nabla \cdot v \neq 0$ . Let us for the begin with the incompressible case. Further, let

$$\begin{aligned} b(u, w) &= \int_{\Omega} \mu \nabla u \nabla w dx \\ c_v(u, w) &= \int_{\Omega} v \cdot \nabla u w dx \\ a(u, w) &= a(u, w) + b(u, w) \end{aligned}$$

Furthermore, assuming for the moment that  $u \in H_g^1, w \in H_0^1$ , we have

$$\begin{aligned} c_v(u, w) &= \int_{\Omega} v \cdot \nabla u w dx \\ &= - \int_{\Omega} v \cdot \nabla w u dx - \underbrace{\int_{\Omega} \nabla \cdot v u w dx}_{=0 \text{ (incompressibility)}} + \underbrace{\int_{\Gamma} u w v \cdot n}_{=0 \text{ (Dirichlet conditions)}} \\ &= -c_v(w, u). \end{aligned}$$

---

<sup>1</sup> Has the argument for reducing non-homogeneous Dirichlet conditions to homogeneous Dirichlet conditions been demonstrated elsewhere?



and therefore  $c_v(\cdot, \cdot)$  is skew-symmetric. Letting  $w = u$  we obtain that  $c_v(u, u) = -c_v(u, u)$ , which means that  $c_v(u, u) = 0$ . Therefore, the first condition in Lax-Milgram's theorem (1) is satisfied:

$$a(u, u) = b(u, u) \geq \mu |u|_1^2.$$

The second condition, the boundedness of  $a$  (2), follows by applying Cauchy-Schwartz inequality if we assume bounded flow velocities  $\|v\|_\infty$ .

$$\begin{aligned} a(u, v) &= \int_{\Omega} \mu \nabla u \nabla w \, dx + \int_{\Omega} v \nabla u w \, dx \\ &\leq \mu |u|_1 |w|_1 + \|v\|_\infty |u|_1 \|w\|_0 \\ &\leq (\mu + \|v\|_\infty C_\Omega) |u|_1 |v|_1. \end{aligned}$$

The third condition simply means that the right-hand side needs to be in the dual space of  $H_g^1$ . Hence, we obtain the following bounds by Lax-Milgram's theorem:

$$|u|_1 \leq \frac{\mu + C_\Omega \|v\|_\infty}{\mu} \|f\|_{-1}.$$

Notice that for convection-dominated problems  $C_\Omega \|v\|_\infty \gg \mu$  and the stability constant will therefore be large.

In the case where  $\nabla \cdot v \neq 0$ , we generally obtain that  $c_v(u, u) \neq 0$ . To ensure that  $a(u, u)$  is still positive, we must then put some restrictions on the flow velocities. That is, we need

$$|c_v(u, u)| \leq a(u, u).$$

If  $C_\Omega \|v\|_\infty \leq D\mu$  with  $D < 1$  we obtain

$$\begin{aligned} a(u, u) &= \int_{\Omega} \mu \nabla u \nabla u \, dx + \int_{\Omega} v \nabla u u \, dx \\ &\geq \mu |u|_1 |v|_1 - \|v\|_\infty |u|_1 \|u\|_0 \\ &\geq (\mu - \|v\|_\infty C_\Omega) |u|_1 |u|_1 \\ &\geq (\mu(1 - D)) |u|_1^2. \end{aligned}$$

Further, the second condition of Lax-Milgram's theorem still applies. However, that  $C_\Omega \|v\|_\infty \leq D\mu$  is clearly very restrictive compared to the incompressible case.

We remark that the Lax-Milgram conditions in the presence of the SUPG clearly will not be satisfied in the continuous case because of the third order

term  $-\Delta u(v \cdot \nabla w)$ . With this term, the second condition of Lax-Milgram is not satisfied with  $C \leq \infty$ .

Finally, in order to make the term  $c_v(u, u)$  skew-symmetric, it was required that the boundary integral  $\int_{\Gamma} u^2 w \cdot n$  was zero. This was a consequence of the Dirichlet conditions. In general, this is neither needed nor possible at Neumann boundaries. As long as  $\int_{\Gamma} u^2 w \cdot n \geq 0$ , the above argumentation is valid. From a physical point of view this means that there is outflow at the Neumann boundary, i.e., that  $w \cdot n \geq 0$ .

### 3.4 Error estimates

Finally, we provide some error estimates for the Galerkin method and the SUPG method applied to the convection-diffusion equation. Central in the derivation of both results are the following interpolation result.

**Theorem 3.2 *Approximation by interpolation***

*There exists an interpolation operator  $I_h : H^{t+1} \rightarrow V_h$  where  $V_h$  is a piecewise polynomial field of order  $t$  with the property that for any  $u \in H^t(\Omega)$*

$$\|u - I_h u\|_m \leq B h^{t+1-m} \|u\|_{t+1}.$$

*Proof* The bounds on the interpolation error is provided by the Bramble-Hilbert lemma for  $t \geq 1$  and Clement's result (the case  $t = 1$ ), cf. e.g. [1, 2].  $\square$

For the Galerkin method the general and elegant result of Cea's lemma provide us with error estimates. Cea's lemma applies to general conforming approximations, i.e. when  $V_h \subset V$ . In our case  $V = H_0^1(\Omega)$  and  $V_h$  is a finite element subspace such as for example a discretization in terms of the Lagrange elements (of any order). Hence, in our case  $\|\cdot\|_V = \|\cdot\|_1$  and the  $H^1$  semi-norm is equivalent with the full  $H^1$  norm due to Poincare's inequality.

**Theorem 3.3 *Cea's lemma***

*Suppose the conditions for Lax-Milgram's theorem is satisfied and that we solve the linear problem (3.5) on a finite element space of order  $t$ . Then,*

$$\|u - u_h\|_V \leq C_1 \frac{CB}{\alpha} h^t \|u\|_{t+1}.$$

Here  $C_1 = \frac{CB}{\alpha}$ , where  $B$  comes from the approximation property and  $\alpha$  and  $C$  are the constants of Lax-Milgram's theorem.

*Proof* The proof is straightforward and follows from the Galerkin orthogonality:

$$a(u - u_h, v) = 0, \quad \forall v \in V_h$$

Since  $V_h \subset V$ :

$$\begin{aligned} \alpha \|u - u_h\|_V^2 &\leq a(u - u_h, u - u_h) \\ &= a(u - u_h, u - v) - a(u - u_h, v - u_h) \\ &\leq C \|u - u_h\|_V \|u - v\|_V. \end{aligned}$$

Since  $v - u_h \in V_h$ . Furthermore,  $v$  is arbitrary and we may therefore choose  $v = I_h u$  and obtain:

$$|u - u_h|_1 \leq \frac{C}{\alpha} |u - I_h u|_1 \leq \frac{CB}{\alpha} h^t \|u\|_t,$$

where  $t - 1$  is the order of the polynomials of the finite elements.  $\square$

We remark, as mentioned above, that  $\frac{C}{\alpha}$  is large for convection dominated problems and that this is what causes the poor approximation on the coarse grid, shown in Example 3.1.

To obtain improved error estimates for the SUPG method, we introduce an alternative norm:

$$\|u\|_{sd} = (h \|v \cdot \nabla u\|^2 + \mu |\nabla u|^2)^{1/2} \quad (3.8)$$

**Theorem 3.4** *Suppose the conditions for Lax-Milgram's theorem is satisfied in the Hilbert space defined by the SUPG norm (3.8) and that we solve the SUPG problem (3.7) on a finite element space of order 1. Then,*

$$\|u - u_h\|_{sd} \leq Ch^{3/2} \|u\|_2$$

*Proof* The proof can be found in e.g. [4, 10].  $\square$

### 3.5 Exercises

**Exercise 3.1** Show that the matrix obtained from a central difference scheme applied to the operator  $Lu = u_x$  is skew-symmetric. Furthermore, show that the matrix obtained by linear continuous Lagrange elements are also skew-

symmetric. Remark: The matrix is only skew-symmetric in the interior of the domain, not at the boundary.

**Exercise 3.2** Estimate numerically the constant in Cea's lemma for various  $\alpha$  and  $h$  for the Example 3.1.

**Exercise 3.3** Implement the problem  $u = \sin(\pi x)$ , and  $f = -\alpha u_{xx} - u_x$  and estimate numerically the constant in Cea's lemma for various  $\alpha$ . Compare with the corresponding constant estimated from Example 3.1.

**Exercise 3.4** Implement the problem  $u = \sin(\pi x)$ , and  $f = -\alpha u_{xx} - u_x$  using SUPG and estimate the constants in the error estimate obtained by both the  $|\cdot|_1$  and the  $\|\cdot\|_v$  norms. Compare with the corresponding constant estimated from Example 3.1.

**Exercise 3.5** Investigate whether the coersivity condition holds when a homogeneous Neumann condition is assumed on the outflow. You may assume that  $v \cdot n > 0$ .

**Exercise 3.6** Consider the eigenvalues of the operators,  $L_1$ ,  $L_2$ , and  $L_3$ , where  $L_1 u = u_x$ ,  $L_2 u = -\alpha u_{xx}$ ,  $\alpha = 1.0e^{-5}$ , and  $L_3 = L_1 + L_2$ , with homogeneous Dirichlet conditions. For which of the operators are the eigenvalues positive and real? Repeat the exercise with  $L_1 = xu_x$ .

**Exercise 3.7** Compute the Soblev norms  $\|\cdot\|_m$  of the function  $\sin(k\pi x)$  on the unit interval. Assume that the Soblev norm is  $\|u\|_m = (-\Delta^m u, u)^{1/2}$ . What happens with negative  $m$ ? You may use either Fourier transformation or compute (eigenvalues of) powers of the stiffness matrix.

**Exercise 3.8** Perform numerical experiments to determine the order of approximation with respect to various Soblev norms and polynomial orders for the function  $\sin(k\pi x)$  on the unit interval.

# Chapter 4

## Stokes problem

### 4.1 Introduction

The Stokes problem describes the flow of a slowly moving viscous incompressible Newtonian fluid. Let the fluid domain be denoted  $\Omega$ . We assume that  $\Omega$  is a bounded domain in  $\mathbb{R}^n$  with a smooth boundary. Furthermore, let  $u : \Omega \rightarrow \mathbb{R}^n$  be the fluid velocity and  $p : \Omega \rightarrow \mathbb{R}$  be the fluid pressure. The strong form of the Stokes problem can then be written as

$$-\Delta u + \nabla p = f, \text{ in } \Omega, \quad (4.1)$$

$$\nabla \cdot u = 0, \text{ in } \Omega, \quad (4.2)$$

$$u = g, \text{ on } \partial\Omega_D, \quad (4.3)$$

$$\frac{\partial u}{\partial n} - pn = h, \text{ on } \partial\Omega_N. \quad (4.4)$$

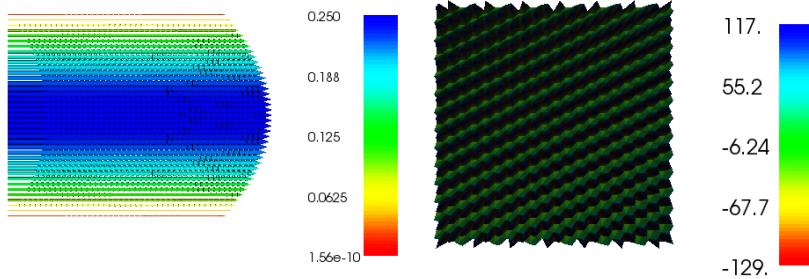
Here,  $f$  is the body force,  $\partial\Omega_D$  is the Dirichlet boundary, while  $\partial\Omega_N$  is the Neumann boundary. Furthermore,  $g$  is the prescribed fluid velocity on the Dirichlet boundary, and  $h$  is the surface force or stress on the Neumann boundary. These boundary condition leads to a well-posed problem provided that neither the Dirichlet nor Neumann boundaries are empty. In case of only Dirichlet conditions the pressure is only determined up to a constant, while only Neumann conditions leads to the velocity only being determined up to a constant.

These equations are simplifications of the Navier–Stokes equations for very slowly moving flow. In contrast to elliptic equations, many discretizations of this problem will lead to instabilities. These instabilities are particularly visible

as non-physical oscillations in the pressure. The following example illustrate such oscillations.

### Poiseuille flow

One of the most common examples of flow problems that can be solved analytically is Poiseuille flow. It describes flow in a straight channel (or cylinder in 3D). The analytical solution is  $u = (y(1-y), 0)$  and  $p = 1 - x$ . Since the solution is known, this flow problem is particularly useful for verifying that the code or numerical method. We therefore begin by discretizing the problem in the simplest way possible; that is, linear continuous/Lagrange elements for both velocity and pressure. The results are shown in Figure 4.1. Clearly, the velocity is approximated satisfactorily, but the pressure oscillates widely and is nowhere near the actual solution.



**Fig. 4.1** Poiseuille flow solution obtained with linear continuous elements for both velocity and pressure. The left figure shows the (well-represented) velocity while the right shows the pressure (with the wild oscillations).

```
from dolfin import *

def u_boundary(x):
    return x[0] < DOLFIN_EPS or x[1] > 1.0 - DOLFIN_EPS or x[1]
        < DOLFIN_EPS

def p_boundary(x):
    return x[0] > 1.0 - DOLFIN_EPS

mesh = UnitSquare(40,40)
```

```

V = VectorFunctionSpace(mesh, "Lagrange", 1)
Q = FunctionSpace(mesh, "Lagrange", 1)
#Q = FunctionSpace(mesh, "DG", 0)
W = MixedFunctionSpace([V, Q])

u, p = TrialFunctions(W)
v, q = TestFunctions(W)

f = Constant([0,0])

u_analytical = Expression(["x[1]*(1-x[1])", "0.0"])
p_analytical = Expression("-2+2*x[0]")

bc_u = DirichletBC(W.sub(0), u_analytical, u_boundary)
bc = [bc_u]

a = inner(grad(u), grad(v))*dx + div(u)*q*dx + div(v)*p*dx
L = inner(f, v)*dx

UP = Function(W)
A, b = assemble_system(a, L, bc)
solve(A, UP.vector(), b, "lu")

U, P = UP.split()

plot(U, title="Numerical velocity")
plot(P, title="Numerical pressure")

U_analytical = project(u_analytical, V)
P_analytical = project(p_analytical, Q)

plot(U_analytical, title="Analytical velocity")
plot(P_analytical, title="Analytical pressure")

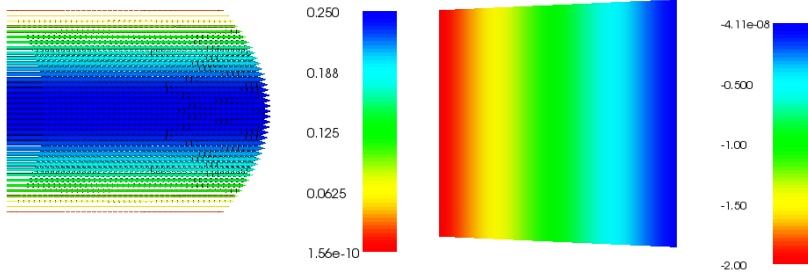
interactive()

```

However, when using the second order continuous elements for the velocity and first order continuous elements for the pressure, we obtain the perfect solution shown in Figure 4.2.

---

The previous example demonstrates that discretizations of the Stokes problem may lead to, in particular, strange instabilities in the pressure. In this chapter we will describe why this happens and several strategies to circumvent this behaviour.



**Fig. 4.2** Poiseuille flow solution obtained with quadratic continuous elements for the velocity and linear continuous elements for the pressure. The left figure shows the velocity while the right shows the pressure. Both the velocity and the pressure are correct.

## 4.2 Finite Element formulation

Let us first start with a weak formulation of Stokes problem: Find  $u \in H_{D,g}^1$  and  $p \in L^2$ .

$$\begin{aligned} a(u, v) + b(p, v) &= f(v), \quad v \in H_{D,0}^1 \\ b(q, u) &= 0, \quad q \in L^2, \end{aligned}$$

where

$$\begin{aligned} a(u, v) &= \int \nabla u : \nabla v \, dx, \\ b(p, v) &= \int p \nabla \cdot v \, dx, \\ f(v) &= \int f v \, dx + \int_{\Omega_N} h v \, ds. \end{aligned}$$

Here  $H_{D,g}^1$  contains functions in  $H^1$  with trace  $g$  on  $\partial\Omega_D$ . To obtain symmetry we have substituted  $\hat{p} = -p$  for the pressure and is referint to  $\hat{p}$  as  $p$ .

As before the standard finite element formulation follows directly from the weak formulation: Find  $u_h \in V_{g,h}$  and  $p_h \in Q_h$  such that



$$a(u_h, v_h) + b(p_h, v_h) = f(v_h), \quad \forall v_h \in V_{0,h}, \quad (4.5)$$

$$b(q_h, u_h) = 0, \quad \forall q_h \in Q_h. \quad (4.6)$$

Letting  $u_h = \sum_{i=1}^n u_i N_i$ ,  $p_h = \sum_{i=1}^m p_i L_i$ ,  $v_h = N_j$ , and  $q_h = L_j$  we obtain a linear system on the form

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} \quad (4.7)$$

Here

$$A_{ij} = a(N_i, N_j) = \int \nabla N_i \nabla N_j \, dx, \quad (4.8)$$

$$B_{ij} = b(L_i, N_j) = \int \nabla L_i N_j \, dx. \quad (4.9)$$

Hence,  $A$  is  $n \times n$ , while  $B$  is  $m \times n$ , where  $n$  is the number of degrees of freedom for the velocity field, while  $m$  is the number of degrees of freedom for the pressure.

Is the system (4.7) invertible? For the moment, we assume that the submatrix  $A$  is invertible. This is typically the case for Stokes problem. We may then perform blockwise Gauss elimination: That is, we multiply the first equation with  $A^{-1}$  to obtain

$$u = A^{-1}f - A^{-1}B^T p$$

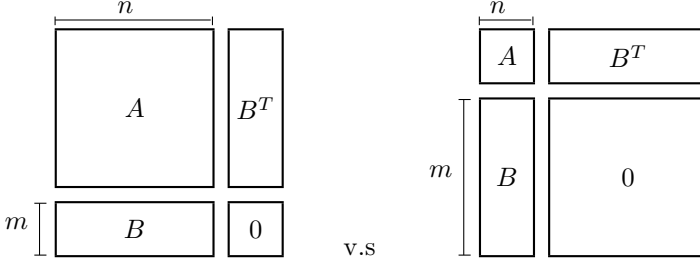
Then, we then insert  $u$  in the second equation to get

$$0 = Bu = BA^{-1}f - BA^{-1}B^T p$$

i.e we have removed  $v$  and obtained an equation only involving  $p$ :

$$BA^{-1}B^T p = BA^{-1}f$$

This equation is often called the pressure Schur complement. The question is then reduced to whether  $BA^{-1}B^T$  is invertible. Consider the following two situations:



Clearly, the right most figure is not invertible since  $n \ll m$  and the 0 in the lower right corner dominates. For the left figure one might expect that the matrix is non-singular since  $n \gg m$ , but it will depend on  $A$  and  $B$ . We have already assumed that  $A$  is invertible, and we therefore ignore  $A^{-1}$  in  $BA^{-1}B^T$ . The question is then whether  $BB^T$  is invertible.

$$\begin{array}{c}
 \begin{array}{|c|} \hline B \\ \hline \end{array}
 \begin{array}{|c|} \hline B^T \\ \hline \end{array}
 =
 \begin{array}{|c|} \hline m \times m \\ \hline \end{array}
 \end{array}$$

As illustrated above,  $BB^T$  will be a relatively small matrix compared to  $B^T$  and  $A$  as long as  $n \gg m$ . Therefore,  $BB^T$  may therefore be non-singular. To ensure that  $BB^T$  is invertible, it is necessary that

$$\text{kernel}(B^T) = 0, \text{ where } B \text{ is } m \times n$$

An equivalent statement is that

$$\max_v (v, B^T p) > 0 \quad \forall p. \quad (4.10)$$

Alternatively,

$$\max_v \frac{(v, B^T p)}{\|v\|} \geq \beta \|p\| \quad \forall p. \quad (4.11)$$

which obviously may be written

$$\max_v \frac{(Bv, p)}{\|v\|} \geq \beta \|p\| \quad \forall p. \quad (4.12)$$

Here,  $\beta > 0$ . We remark that (4.10) and (4.11) are equivalent for a finite dimensional matrix. However, in the infinite dimensional setting of PDEs (4.10) and (4.11) are different. Inequality (4.10) allow  $(v, B^T p)$  to approach zero, while (4.11) requires a lower bound. For the Stokes problem, the corresponding condition is crucial:

$$\sup_{v \in H_{D,g}^1} \frac{(p, \nabla \cdot u)}{\|u\|_1} \geq \beta \|p\|_0 > 0, \quad \forall p \in L^2 \quad (4.13)$$

Similarly, to obtain order optimal convergence rates, that is

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq Ch^k \|u\|_{k+1} + Dh^{\ell+1} \|p\|_{\ell+1}$$

where  $k$  and  $\ell$  are the ploynomial degree of the velocity and the pressure, respectively, the celebrated *Babuska-Brezzi condition* has to be satisfied:

$$\sup_{v \in V_{h,g}} \frac{(p, \nabla \cdot v)}{\|v\|_1} \geq \beta \|p\|_0 > 0, \quad \forall p \in Q_h \quad (4.14)$$

We remark that the discrete condition (4.14) does not follow from (4.13). In fact, it has been a major challenge in numerical analysis to determine which finite element pairs  $V_h$  and  $Q_h$  that meet this condition.

*Remark 4.1* For saddle point problems on the form (4.5)-(4.6) four conditions have to be satisfied in order to have a well-posed problem:

Boundedness of  $a$ :

$$a(u_h, v_h) \leq C_1 \|u_h\|_{V_h} \|v_h\|_{V_h}, \quad \forall u_h, v_h \in V_h, \quad (4.15)$$

and boundedness of  $b$ :

$$b(u_h, q_h) \leq C_2 \|u_h\|_{V_h} \|q_h\|_{Q_h}, \quad \forall u_h \in V_h, q_h \in Q_h, \quad (4.16)$$

Coersivity of  $a$ :

$$a(u_h, u_h) \geq C_3 \|u_h\|_{V_h}^2, \quad \forall u_h \in Z_h, \quad (4.17)$$

where  $Z_h = \{u_h \in V_h \mid b(u_h, q_h) = 0, \forall q_h \in Q_h\}$  and "coersivity" of  $b$ :

$$\sup_{u_h \in V_h} \frac{b(u_h, q_h)}{\|u_h\|_{V_h}} \geq C_4 \|q_h\|_{Q_h}, \quad \forall q_h \in Q_h. \quad (4.18)$$

For the Stokes problem, (4.15)-(4.17) are easily verified, while (4.18) often is remarkably difficult unless the elements are designed to meet this condition. We remark also that condition (4.17) strictly speaking only needs to be valid on a subspace of  $V_h$  but this is not important for the Stokes problem.

### 4.3 Examples of elements

#### 4.3.1 The Taylor-Hood element

The Taylor-Hood elements are quadratic for the velocity and linear for pressure, i.e., the  $i$ 'th basis function of the velocity and pressure are of the form

$$\begin{aligned} u : N_i &= a_i + b_i x + c_i y + d_i xy + e_i x^2 + f_i y^2, \\ p : L_i &= k_i + l_i x + m_i y. \end{aligned}$$

And the basis functions are continuous across elements. For the Taylor-Hood element we have the following error estimate:

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq Ch^2(\|u\|_3 + \|p\|_2).$$

The generalization of the Taylor-Hood element to higher order, that is  $P_k - P_{k-1}$ , satisfies the Brezzi conditions (on reasonable meshes). For the Taylor-Hood element of higher order we have the following error estimate:

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq Ch^k(\|u\|_{k+1} + \|p\|_k).$$

#### 4.3.2 The Crouzeix-Raviart element

This element is linear in velocity and constant in pressure. Hence, the  $i$ 'th basis functions are of the form:

$$\begin{aligned} v : N_i &= a_i + b_i x + c_i y \\ p : L_i &= a_i \end{aligned}$$

The  $v$  element is continuous *only* in the mid-point of each side, and the  $p$  element is discontinuous. The Crouzeix-Raviart element satisfies the inf-sup

condition, but is non-conforming because it is only continuous at the mid-point of each element. The non-conformity does not affect the approximation properties for the Stokes problem, but can not be used if the  $-\Delta u - \nabla p = f$  is replaced with the more "physically correct"  $-\nabla \cdot \epsilon(u) - \nabla p = f$ , where  $\epsilon = \frac{1}{2}(\nabla + \nabla^T)$  is the symmetric gradient. For the Crouzeix–Raviart element we have the following error estimate:

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq Ch(\|u\|_2 + \|p\|_1)$$

The element may be generalized to odd, but not even orders.

### 4.3.3 The P1-P0 element

The P1-P0 element is perhaps the most natural element to consider as it consists of combining continuous piecewise linear functions for the velocity with piecewise constants for the pressure. This combination often work quite well, and this puzzled the community for quite some time. However, this combination is not inf-sup stable and oscillations in the pressure may occur.

### 4.3.4 The P2-P0 element

$P_2 - P_0$  element is a popular element that satisfies the Brezzi conditions. An advantage with this approach is that mass conservation is maintained elementwise. However, the approximation properties of the pressure is one order lower than that for the Taylor-Hood element and consequently the velocity approximation is also formally, in general, reduced by one order, i.e.,

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq C_0 h^2 \|u\|_2 + C_1 h \|p\|_2$$

The  $P_2 - P_0$  element can be generalized to higher order. In fact,  $P_k - P_{k-2}$ , satisfies the Brezzi conditions for  $k \geq 2$ . Here, the pressure element  $P_{k-2}$  may in fact consist of both continuous and discontinuous polynomials. The discontinuous polynomials then has the advantage of providing mass conservation, albeit at the expanse of many degrees of freedom compared with the continuous variant.

### 4.3.5 The Mini element

The mini element is linear in both velocity and pressure, but with one degree of freedom added per element since it is well-known that elements that are linear in both  $v$  and  $p$  will not satisfy the inf-sup condition. The extra degree of freedom is in 2D constructed such it is a cubic polynomial which is zero at all element faces. For example, on the reference element, the barycentric coordinates  $x$ ,  $y$ , and  $1 - x - y$  are all zero at their respective faces. Hence, the composition  $xy(1 - x - y)$  is zero at all element faces. The barycentric coordinates can be used for this purpose on any element and also in higher dimensions. The function is often called the bubble function as its support is local to one element and is zero at the element faces. For the Mini element we have the following error estimate:

$$\|u - u_h\|_1 + \|p - p_h\|_0 \leq C_0 h \|u\|_2 + C_1 h^2 \|p\|_2$$

We notice that the convergence rate for the velocity is linear, hence the extra bubbles bring stability but does not increase approximation order.

## 4.4 Stabilization techniques to circumvent the Babuska-Brezzi condition

Stabilization techniques typically replace the system:

$$\begin{aligned} Au + B^T p &= f \\ Bu &= 0 \end{aligned}$$

with an alternative system

$$\begin{aligned} Au + B^T p &= f \\ Bu - \epsilon Dp &= \epsilon d, \end{aligned}$$

where  $\epsilon$  is properly chosen and  $D$  is a positive, but not necessarily positive definite, matrix.

To see that we obtain a nonsingular system we again multiply the first equation with  $A^{-1}$  and then factorize:

$$\begin{aligned}
u &= A^{-1}f - A^{-1}B^T p \\
Bu &= BA^{-1}f - BA^{-1}B^T p = \epsilon d + \epsilon Dp \\
(BA^{-1}B^T + \epsilon D)p &= BA^{-1}f - \epsilon d
\end{aligned}$$

If  $D$  is nonsingular then  $(BA^{-1}B^T + \epsilon D)$  will be nonsingular since both  $D$  and  $BA^{-1}B^T$  are positive (only  $D$  is positive definite however).

Factorizing for  $p$  we end up with a *Velocity-Schur complement*. Solving for  $p$  in the second equation and inserting the expression for  $p$  into the first equation we have

$$\begin{aligned}
p &= (-\epsilon D)^{-1}(\epsilon d - Bu) \\
&\Downarrow \\
Au + B^T(-\epsilon D)^{-1}(\epsilon d - Bu) &= f \\
(A + \frac{1}{\epsilon}B^T D^{-1}B)u &= f + D^{-1}d
\end{aligned}$$

$(A + \frac{1}{\epsilon}B^T D^{-1}B)$  is nonsingular since  $A$  is nonsingular and  $B^T D^{-1}B$  is positive.

At least, three techniques have been proposed for stabilization. These are:

1.  $\nabla \cdot v + \epsilon \Delta p = 0$ . Pressure stabilization. Motivated through mathematical intuition (from the convection-diffusion equation).
2.  $\nabla \cdot v - \epsilon p = 0$ . Penalty method. Typically, one uses the Velocity-Schur complement
3.  $\nabla \cdot -\epsilon \frac{\partial p}{\partial t} = 0$ . Artificial compressibility. A practical method as one adds the possibility for time stepping.

In other words, these techniques sets  $D$  to be

1.  $D = A$
2.  $D = M$
3.  $D = \frac{1}{\Delta t}M$

where  $A$  is the stiffness matrix (discrete laplace operator) and  $M$  is the mass matrix.

## 4.5 Exercises

**Exercise 4.1** Show that the conditions (4.15)-(4.17) are satisfied for  $V_h = H_0^1$  and  $Q_h = L^2$ .

**Exercise 4.2** Show that the conditions (4.15)-(4.17) are satisfied for Taylor–Hood and Mini discretizations. (Note that Crouzeix–Raviart is non-conforming so it is more difficult to prove these conditions for this case.)

**Exercise 4.3** Condition (4.18) is difficult to prove. However, if we assume that  $V_h = L^2$  and  $Q_h = H_0^1$ , you should be able to prove it. (Hint: This is closely related to Poincaré’s inequality.)

**Exercise 4.4** Test other finite elements for the Poiseuille flow problem. Consider  $P_1 - P_0$ ,  $P_2 - P_2$ ,  $P_2 - P_0$ , as well as the Mini and Crouzeix–Raviart element.

**Exercise 4.5** Implement stabilization for the Poiseuille flow problem and use first order linear elements for both velocity and pressure.

**Exercise 4.6** In the previous problem the solution was a second order polynomial in the velocity and first order in the pressure. We may therefore obtain the exact solution and it is therefore difficult to check order of convergence for higher order methods with this solution. In this exercise you should therefore implement the problem  $u = (\sin(\pi y), \cos(\pi x))$ ,  $p = \sin(2\pi x)$ , and  $f = -\Delta u - \nabla p$ . Test whether the approximation is of the expected order for  $P_4 - P_3$ ,  $P_4 - P_2$ ,  $P_3 - P_2$ , and  $P_3 - P_1$ .

**Exercise 4.7** Implement the Stokes problem with analytical solution  $u = (\sin(\pi y), \cos(\pi x))$ ,  $p = \sin(2\pi x)$ , and  $f = -\Delta u - \nabla p$  on the unit square. Consider the case where you have Dirichlet conditions on the sides ‘x=0’, ‘x=1’ and ‘y=1’ while Neumann is used on the last side (this way we avoid the singular system associated with either pure Dirichlet or pure Neumann problems). Then determine the order of the approximation of wall shear stress on the side ‘x=0’. The wall shear stress on the side ‘x=0’ is  $\nabla u \cdot t$  where  $t = (0, 1)$  is the tangent along ‘x=0’.



## Chapter 5

# Efficient Solution Algorithms: Iterative methods and Preconditioning

To compute the solution of a partial differential equation, we often need to solve a system of linear equations with a large number of unknowns. The accuracy of the solution increases with the number of unknowns used. Nowadays, unknowns in the order of millions to billions are routinely solved for without the use of (state-of-the-art) high-performance computing. Such computations are facilitated by the enormous improvements in numerical algorithms and scientific software the last decades.

It should be quite clear that naive Gaussian elimination can not be employed. For a naive Gaussian elimination implementation, the number of required floating point operations (FLOPS) scales as the cube of the number of unknowns. Hence, solving a problem with  $10^6$  unknowns would then require  $10^{18}$  FLOPS which on a modern computer with e.g. 3 GHz still would take about 10 years. As we will see later, such problems may in common cases be solved in just a few seconds. There are two ingredients in such efficient algorithms: *iterative methods* and *preconditioning*.

Lets therefore consider the numerical solution of large linear systems,

$$Au = b,$$

where the linear system comes from discretization of PDEs. That is,  $A$  is a  $N \times N$  matrix, and  $N$  is between  $10^6$  and  $10^9$  in typical simulations. Furthermore, the matrix is normally extremely sparse and contains only  $\mathcal{O}(N)$  nonzeros (see Exercise 5.1). It is important to notice that even though  $A$  is sparse  $A^{-1}$  will in general be full. This is a main reason to consider iterative methods.

## 5.1 The simplest iterative method: the Richardson iteration

The Richardson iteration<sup>1</sup> is

$$u^n = u^{n-1} - \tau(Au^{n-1} - b), \quad (5.1)$$

where  $\tau$  is a relaxation parameter that must be determined. Clearly, the method is consistent in the sense that if  $u^{n-1} = u$ , then  $u^n = u$  and the iterative method has converged to the exact solution. It is also clear that each iteration requires the evaluation of  $A$  on a vector, in addition to vector addition and scalar multiplication. Hence, one iteration requires the amount of  $\mathcal{O}(N)$  FLOPS and only  $\mathcal{O}(N)$  of memory. This is a dramatic improvement when compared Gaussian elimination at least if the number of iterations are few. The key to obtain few iterations is preconditioning, but let's first consider the Richardson's method without.

The standard approach to analyze iterative methods is to look at what happens with the *error*. Let the error at the  $n$ 'th iteration be  $e^n = u^n - u$ . As this is a linear system of equations, we may subtract  $u$  from both sides of (5.1) and obtain an equation for the iterative error:

$$e^n = e^{n-1} - \tau Ae^{n-1}.$$

We may therefore quantify the error in terms of the  $L^2$ -norm as

$$\|e^n\| = \|e^{n-1} - \tau Ae^{n-1}\| \leq \|I - \tau A\| \|e^{n-1}\|.$$

Clearly, if  $\|I - \tau A\| < 1$  then the iteration will be convergent.

Assuming for the moment that  $A$  is symmetric and positive definite, then the norm of  $A$  in general defined as

---

<sup>1</sup> Richardson developed his method prior to computers. In his 1910 paper, where the focus is to predict stresses in a masonry dam, he describes how he uses humans as computational resources. He writes "So far I have paid piece rates for the operation [Laplacian] of about  $n/18$  pence per coordinate point,  $n$  being the number of digits. As for the rate of working, one of the quickest boys average 2000 operations per week, for numbers of three digits, those done wrong being discounted."

$$\|A\| = \max_x \frac{\|Ax\|}{\|x\|}$$

equals the largest eigenvalue of  $A$ ,  $\lambda_{max}$ . Furthermore, if we assume that the eigenvalues are ordered with respect to increasing value, such that  $\lambda_0$  and  $\lambda_N$  are the smallest and largest eigenvalue, then the norm of  $I - \tau A$ ,

$$\|I - \tau A\| = \max_x \frac{\|(I - \tau A)x\|}{\|x\|}$$

is attained either for the smallest or largest eigenvalue as either  $(1 - \tau\lambda_0)$  or  $-(1 - \tau\lambda_N)$ . The optimal relaxation parameter  $\tau_{opt}$  can be stated in terms of the eigenvalues,  $\lambda_i$ , of  $A$ . Minimum is attained when  $(1 - \tau_{opt}\lambda_0) = -(1 - \tau_{opt}\lambda_N)$  which makes  $\tau_{opt} = \frac{2}{\lambda_0 + \lambda_N}$ .

Let the convergence factor  $\rho$  be defined as

$$\rho = \|I - \tau A\|$$

The convergence factor with an optimal relation is then

$$\rho = \|I - \tau A\| = \max_{\lambda_i} |1 - \tau\lambda_i| = 1 - \tau\lambda_0 = 1 - \frac{2\lambda_0}{\lambda_0 + \lambda_N} = \frac{\lambda_N - \lambda_0}{\lambda_N + \lambda_0} = \frac{\kappa - 1}{\kappa + 1}.$$

Here,  $\kappa = \frac{\lambda_N}{\lambda_0}$  is the condition number.

We estimate the error reduction per iteration in terms of the convergence factor as,

$$\|e^n\| = \|(I - \tau A)e^{n-1}\| \leq \rho\|e^{n-1}\|.$$

which leads to

$$\|e^n\| \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^n \|e^0\|.$$

For iterative methods, we never iterate until the true solution exactly. Instead a convergence criteria needs to be chosen such that the error obtained by the iterative method is less than or at least comparable to the approximation error of the original system. Determining an appropriate convergence criteria is problem dependent and quite often challenging.

Nevertheless, let us assume that we need to reduce the error by a factor of  $\epsilon$ , that is, we need  $\frac{\|e^n\|}{\|e^0\|} < \epsilon$ . From the iteration, we have

$$\|e^n\| \leq \rho\|e^{n-1}\| \leq \rho^n\|e^0\|. \quad (5.2)$$

An estimate for the number of iterations is then obtained by assuming equality in the equation (5.2) and  $\frac{\|e^n\|}{\|e^0\|} = \epsilon$ . Then the number of iterations needed to achieve the desired error is:

$$n = \frac{\log \epsilon}{\log \rho} = \frac{\log \epsilon}{\log(\frac{K-1}{K+1})}. \quad (5.3)$$

If  $n$  is independent of the resolution of the discretization, the computational cost of the algorithm is  $\mathcal{O}(N)$  in FLOPS and memory and the algorithm is *order-optimal*.

The current analysis of the simplest iterative method there is, the Richardson iteration, shows that the efficiency of the method is determined by the condition number of the matrix. In the literature you will find a jungle of methods of which the following are the most famous: the Conjugate Gradient method, the Minimal Residual method, the BiCGStab method, and the GMRES method. It is remarkable that in general the convergence of these methods is determined by the condition number with one exception; the Conjugate Gradient method which often can be estimated in terms of the square root of the condition number. One main advantage is however that these methods do not require the determination of a  $\tau$  to obtain convergence.

### Eigenvalues of an elliptic problem in 1D and 2D.

Let us consider an elliptic problem:

$$u - \Delta u = f, \quad \text{in } \Omega, \quad (5.4)$$

$$\frac{\partial u}{\partial n} = 0, \quad \text{on } \partial\Omega. \quad (5.5)$$

Notice that the lower order term  $u$  in front of  $-\Delta u$  makes removes the singularity associated with Neumann conditions and that in the continuous case the smallest eigenvalue is 1 (associated with the eigenfunction that is a constant throughout  $\Omega$ ). The following code computes the eigenvalues using linear Lagrangian elements and

```
from dolfin import *
from numpy import linalg

for D in [1, 2]:
    for N in [4, 8, 16, 32]:
```

```

if D == 1: mesh = UnitIntervalMesh(N)
elif D == 2: mesh = UnitSquareMesh(N, N)

V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)

a = u*v*dx + inner(grad(u), grad(v))*dx
A = assemble(a)
e = linalg.eigvals(A.array())
e.sort()
c = e[-1] / e[0]

print "D=%d, N=%3d, min eigenvalue=%5.3f, max
      eigenvalue=%5.3f, cond.
      number=%5.3f " % (D, N, e
[0], e[-1], c)

```

yields the following output:

```

D=1, N= 4, min eig=0.199, max eig=14.562, cond. number=73.041
D=1, N= 8, min eig=0.111, max eig=31.078, cond. number=279.992
D=1, N= 16, min eig=0.059, max eig=63.476, cond.
number=1079.408
D=1, N= 32, min eig=0.030, max eig=127.721, cond.
number=4215.105
D=2, N= 4, min eig=0.040, max eig=7.090, cond. number=178.444
D=2, N= 8, min eig=0.012, max eig=7.735, cond. number=627.873
D=2, N= 16, min eig=0.003, max eig=7.929, cond. number=2292.822
D=2, N= 32, min eig=0.001, max eig=7.982, cond. number=8693.355

```

The output shows that the condition number grows as  $h^{-2}$  in both 1D and 2D although the behaviour of the eigenvalues clearly are dimension dependent (see Exercise 5.2). The smallest eigenvalue decrease in both 1D and 2D as  $h \rightarrow 0$  but at different rates. To obtain eigenvalues corresponding the true eigenvalue we would need to solve a generalized eigenvalue problem as discussed in Chapter 2.

---

**The Richardson iteration applied to a 1D Poisson equation.**

The Richardson iteration on the Poisson equation in 1D, discretized with finite difference method (FDM).

$$Lu = \begin{cases} -u'' = f & \text{for } x \in (0, 1) \\ u(0) = u(1) = 0 \end{cases} \quad (5.6)$$

Eigenvalues and eigenfunctions of  $Lu$  are  $\lambda_k = (k\pi)^2$  and  $v_k = \sin(k\pi x)$  for  $k \in \mathbb{N}$ . When discretizing with FDM we get a  $Au = b$  system, where  $A$  is a tridiagonal matrix ( $A = \text{tridiagonal}(-1, 2, -1)$ ) when the Dirichlet conditions have been eliminated. The discrete and continuous eigenvectors are the same, but the eigenvalues are a little bit different:  $\lambda_k = \frac{4}{h^2} \sin^2(\frac{k\pi h}{2})$ , where  $h$  is the step length  $\Delta x$ . We find the smallest and largest discrete eigenvalues

$$\lambda_{\min}(A) = \pi^2, \quad \lambda_{\max}(A) = \frac{4}{h^2}.$$

Let  $\tau = \frac{2}{\lambda_{\max} + \lambda_{\min}}$  then from the analysis above,

$$\|e^n\| \leq \left(\frac{1-K}{1+K}\right)^n \|e^0\|.$$

The below code perform the Richardson iteration for various resolution on the 1D Poisson problem and stops when the convergence criteria  $\frac{\|r_k\|}{\|r_0\|} \leq 10^{-6}$  is obtained.

```
from numpy import *

def create_stiffness_matrix(N):
    h = 1.0/(N-1)
    A = zeros([N,N])
    for i in range(N):
        A[i,i] = 2.0/(h**2)
        if i > 0:
            A[i,i-1] = -1.0/(h**2)
        if i < N-1:
            A[i,i+1] = -1.0/(h**2)
    A = matrix(A)
    return A

Ns = [10, 20, 40, 80, 160, 320]
for N in Ns:
    A = create_stiffness_matrix(N) # creating
                                   matrix
```

```

x = arange(0, 1, 1.0/(N))
f = matrix(sin(3.14*x)).transpose()           # right hand
                                              side
u0 = matrix(random.random(N)).transpose()      # initial guess
u_prev = u0

eigenvalues = sort(linalg.eigvals(A))          # compute
                                              eigenvalues and tau
lambda_max, lambda_min = eigenvalues[-1], eigenvalues[0]
print "lambda_max ", lambda_max, " lambda_min ", lambda_min
tau = 2/(lambda_max + lambda_min)

norm_of_residual = 1.0                        # make sure the
                                              iteration starts
no_iterations = 0
while norm_of_residual > 1.0e-6:
    r = A*u_prev - f                          # compute the
                                              residual
    u = u_prev - tau*r                         # the Richardson
                                              iteration
    u_prev = u
    norm_of_residual = r.transpose()*r          # check for norm
                                              of residual
    no_iterations += 1                          # count no
                                              iterations

print "N ", N, " number of iterations ", no_iterations

```

$N$	$\lambda_{min}$	$\lambda_{max}$	no. iterations	Estimated FLOPS
10	6.6	317	277	$11 \cdot 10^3$
20	8.1	1435	1088	$87 \cdot 10^3$
40	8.9	6075	4580	$732 \cdot 10^3$
80	9.4	$25 \cdot 10^3$	$20 \cdot 10^3$	$6.4 \cdot 10^6$
160	9.6	$101 \cdot 10^3$	$84 \cdot 10^3$	$53 \cdot 10^6$
320	9.7	$407 \cdot 10^3$	$354 \cdot 10^3$	$453 \cdot 10^6$

**Table 5.1** The number of iterations of the Richardson iteration for solving a 1D Poisson problem. The FLOPS is estimated as the number of iterations times four times the number of unknowns,  $N$ , as the matrix is tridiagonal and there is both a matrix vector product ( $3N$ ) and a vector addition involved in (5.1).

We remark that in this example we have initialized the iteration with a random vector because such a vector contains errors at all frequencies. This is recommended practice when trying to establish a worst case scenario. Testing

the iterative method against a known analytical solution with a zero start vector will often only require smooth error to be removed during the iterations and will therefore underestimate the complications of a real-world problem.

---

### 5.1.1 The stopping criteria

In the Example 5.1 we considered the Richardson iteration applied to a Poisson problem in 1D. We saw that in order to stop the iteration we had to choose a stopping criteria. Ideally we would like to stop when the error was small enough. The problem is that the error is unknown. In fact, since  $e^n = u^n - u$  we would be able to compute the exact solution if the error was known at the  $n$ 'th iteration. What is computable is the *residual* at the  $n$ 'th iteration, defined by

$$r^n = Au^n - f.$$

It is straightforward to show that

$$Ae^n = r^n.$$

But computing  $e^n$  from this relation would require the inversion of  $A$  (which we try to avoid at all cost since it in general is a  $\mathcal{O}(N^3)$  procedure). For this reason, the convergence criteria is typically expressed in terms of some norm of the residual. We may bound the  $n$ 'th error as

$$\|e^n\| \leq \|A^{-1}\| \|r^n\|.$$

However, estimating  $\|A^{-1}\|$  is in general challenging or computationally demanding and therefore usually avoided. To summarize, choosing an appropriate stopping criteria is in general challenging and in practice the choice has to be tailored to concrete application at hand by trial and error.

## 5.2 The idea of preconditioning

The basic idea of preconditioning is to replace

$$Au = b$$



with

$$BAu = Bb.$$

Both systems have the same solution (if  $B$  is nonsingular). However,  $B$  should be chosen as a cheap approximation of  $A^{-1}$  or at least in such a way that  $BA$  has a smaller condition number than  $A$ . Furthermore  $Bu$  should cost  $\mathcal{O}(N)$  operations to evaluate. Obviously, the preconditioner  $B = A^{-1}$  would make the condition number of  $BA$  be one and the Richardson iteration would converge in one iteration. However,  $B = A^{-1}$  is a very computationally demanding preconditioner. We would rather seek preconditioners that are  $\mathcal{O}(N)$  in both memory consumption and evaluation.

The generalized Richardson iteration becomes

$$u^n = u^{n-1} - \tau B(Au^{n-1} - b). \quad (5.7)$$

The error in the  $n$ -th iteration is

$$e^n = e^{n-1} - \tau BAe^{n-1}$$

and the iteration is convergent if  $\|I - \tau BA\| < 1$ .

### 5.2.1 Spectral equivalence and order optimal algorithms

Previously we stated that a good preconditioner is supposed to be similar to  $A^{-1}$ . The precise (and most practical) property that is required of a preconditioner is:

- $B$  should be spectrally equivalent with  $A^{-1}$ .
- The evaluation of  $B$  on a vector,  $Bv$ , should be  $\mathcal{O}(N)$ .
- The storage of  $B$  should be  $\mathcal{O}(N)$ .

**Definition 5.1** Two linear operators or matrices  $A^{-1}$  and  $B$ , that are symmetric and positive definite are spectral equivalent if:

$$c_1(A^{-1}v, v) \leq (Bv, v) \leq c_2(A^{-1}v, v) \quad \forall v \quad (5.8)$$

If  $A^{-1}$  and  $B$  are spectral equivalent, then the condition number of the matrix  $BA$  is  $\kappa(BA) \leq \frac{c_2}{c_1}$ .

If the preconditioner  $B$  is spectrally equivalent with  $A^{-1}$  then the preconditioned Richardson iteration yields an order optimal algorithm. To see this, we note that  $e^n = (I - \tau BA)e^{n-1}$ . We can estimate the behavior of  $e^n$  by using the  $A$ -norm,  $\rho_A = \|I - \tau BA\|_A$ . Then we get

$$\|e^n\|_A \leq \rho_A \|e^{n-1}\|_A.$$

Hence, if the condition number is independent of the discretization then the number of iterations as estimated earlier in (5.3) will be bounded independently of the discretization.

In general, if  $A$  is a discretization of  $-\Delta$  on a quasi-uniform mesh then both multigrid methods and domain decomposition methods will yield preconditioners that are spectrally equivalent with the inverse and close to  $\mathcal{O}(N)$  in evaluation and storage. The gain in using a proper preconditioner may provide speed-up of several orders of magnitude, see Example 5.3.

### 5.3 Krylov methods and preconditioning

For iterative methods, any method involving linear iterations may be written as a Richardson iteration with a preconditioner. However, iterative methods like Conjugate Gradient method, GMRES, Minimal Residual method, and BiCGStab, are different. These are nonlinear iterations where for instance the relaxation parameter  $\tau$  changes during the iterations and are in fact often chosen optimally with respect to the current approximation. Avoiding the need to determine a fixed relaxation parameter prior to the iterations is of course a huge practical benefit. Still, the convergence in practice can usually be roughly estimated by the convergence analysis above for the Richardson iteration.

We will not go in detail on these methods. We only remark that also with these methods it is essential with a good preconditioning technique in order for efficient computations. Furthermore, some of them have special requirements and in some cases it is well-known what to use.

General Advice for usage of different methods:

We classify the methods according to the matrices they are used to solve.

- If a matrix is Symmetric Positive Definite (SPD), i.e.,  $A = A^T$  and  $x^T A x \geq 0 \forall x$  the *Conjugate Gradient method* (CG) is the method of choice. CG needs an SPD preconditioner, see also Exercise 5.6.
- If a matrix is Symmetric but indefinite, i.e.  $A = A^T$  but both positive and negative eigenvalues then the *Minimal Residual method* (MR) is the best choice. MR requires an SPD preconditioner, see also Exercise 5.9.
- If the matrix is positive, i.e.,  $x^T A x \geq 0 \forall x$  which is often the case for convection-diffusion problems or flow problems then *GMRES* with either ILU or AMG are often good, but you might need to experiment, see also Exercise 5.7.
- For matrices that are both nonsymmetric and indefinite there is a jungle of general purpose methods but they may be categorized in two different families. In our experience the *BiCGStab* and *GMRES* methods are the two most prominent algorithms in these families. *GMRES* is relatively robust but may stagnate. *BiCGStab* may break down. *GMRES* has a parameter 'the number of search vectors' that may be tuned.

Most linear algebra libraries for high performance computing like for instance PETSc, Trilinos, Hypr have these algorithms implemented. They are also implemented in various libraries in Python and Matlab. There is usually no need to implement these algorithms yourself.

[

CPU times of different algorithms]

In this example we will solve the problem

$$\begin{aligned} u - \Delta u &= f, & \text{in } \Omega \\ \frac{\partial u}{\partial n} &= 0, & \text{on } \partial\Omega \end{aligned}$$

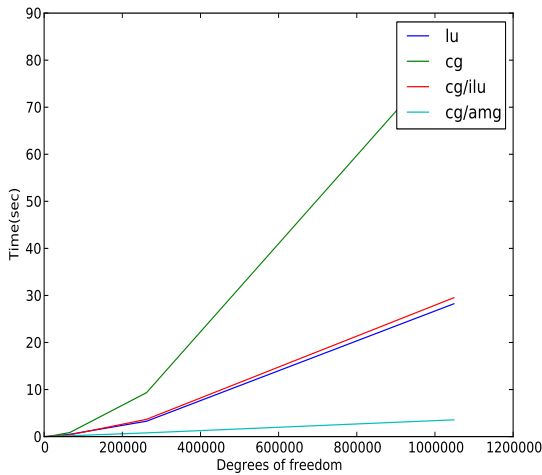
where  $\Omega$  is the unit square with first order Lagrange elements. The problem is solved with four different methods:

- a LU solver,
- Conjugate Gradient method,
- Conjugate Gradient method with an ILU preconditioner, and
- Conjugate Gradient method with an AMG preconditioner,

for  $N = 32^2, 64^2, 128^2, 256^2, 512^2, 1024^2$ , where  $N$  is the number of degrees of freedom.

Figure 5.1 shows that there is a dramatic difference between the algorithms. In

fact the Conjugate gradient (CG) with an AMG preconditioner is over 20 times faster than the slowest method, which is the CG solver without preconditioner. One might wonder why the LU solver is doing so well in this example when it costs  $\mathcal{O}(N^2) - \mathcal{O}(N^3)$ . However, if we increase the number of degrees of freedom, then the method would slow down compared to the other methods. The problem is then that it would require too much memory and the program would probably crash.



**Fig. 5.1** CPU time (in seconds) for solving a linear system of equation with  $N$  degrees of freedom (x-axis) for different solvers

```
from dolfin import *
import time
lu_time = []; cgamg_time = []
cg_time = []; cgilu_time = []
Ns = []

parameters["krylov_solver"]["relative_tolerance"] = 1.0e-8
parameters["krylov_solver"]["absolute_tolerance"] = 1.0e-8
parameters["krylov_solver"]["monitor_convergence"] = False
parameters["krylov_solver"]["report"] = False
parameters["krylov_solver"]["maximum_iterations"] = 50000
```

```

def solving_time(A,b, solver):
    U = Function(V)
    t0 = time.time()
    if len(solver) == 2:
        solve(A, U.vector(), b, solver[0], solver[1]);
    else:
        solve(A, U.vector(), b, solver[0]);
    t1 = time.time()
    return t1-t0

for N in [32, 64, 128, 256, 512, 1024]:

    Ns.append(N)

    mesh = UnitSquare(N, N)
    print " N ", N, " dofs ", mesh.num_vertices()
    V = FunctionSpace(mesh, "Lagrange", 1)
    u = TrialFunction(V)
    v = TestFunction(V)

    f = Expression("sin(x[0]*12) - x[1]")
    a = u*v*dx + inner(grad(u), grad(v))*dx
    L = f*v*dx

    A = assemble(a)
    b = assemble(L)

    t2 = solving_time(A,b, ["lu"])
    print "Time for lu ", t2
    lu_time.append(t2)

    t2 = solving_time(A, b, ["cg"])
    print "Time for cg ", t2
    cg_time.append(t2)

    t2 = solving_time(A, b, ["cg", "ilu"])
    print "Time for cg/ilu ", t2
    cgilu_time.append(t2)

    t2 = solving_time(A, b, ["cg", "amg"])
    print "Time for cg/amg ", t2
    cgamg_time.append(t2)

import pylab

pylab.plot(Ns, lu_time)

```

```

pylab.plot(Ns, cg_time)
pylab.plot(Ns, cgilu_time)
pylab.plot(Ns, cgamg_time)
pylab.xlabel('Unknowns')
pylab.ylabel('Time(sec)')
pylab.legend(["lu", "cg", "cg/ilu", "cg/amg"])
pylab.show()

pylab.loglog(Ns, lu_time)
pylab.loglog(Ns, cg_time)
pylab.loglog(Ns, cgilu_time)
pylab.loglog(Ns, cgamg_time)
pylab.legend(["lu", "cg", "cg/ilu", "cg/amg"])
pylab.savefig('tmp_cpu.pdf')
pylab.show()

```

When we employ iterative methods, we need to specify the convergence criterion. This is often not an easy task. We have the continuous solution  $u$ , the discrete solution  $u_h$ , and the appropriate discrete solution,  $u_h^n$  found by an iterative method at iteration  $n$ . Obviously, we may estimate the error as

$$\|u - u_h^n\| \leq \|u - u_h\| + \|u_h - u_h^n\|,$$

and it does make sense that the values of  $\|u - u_h\|$  and  $\|u_h - u_h^n\|$  are balanced. Still both terms may be hard to estimate in challenging applications. In practice, an appropriate convergence criterion is usually found by trial and error by choosing a stopping criterion based on the residual. Let us therefore consider a concrete example and consider  $\|u - u_h^n\|$  as a function of the mesh resolution and a varying convergence criterion.

$\epsilon \backslash N$	64	128	256	512	1024
1.0e-1	1.3e-02 (1.1e-02)	1.4e-02 (3.5e-02)	8.8e-03 (1.4e-01)	3.4e-03 (5.9e-01)	1.1e-02 (2.5e+00)
1.0e-2	1.2e-03 (1.0e-02)	2.0e-03 (3.7e-02)	1.3e-03 (1.5e-01)	3.5e-03 (5.8e-01)	3.7e-04 (2.7e+00)
1.0e-3	3.6e-04 (1.1e-02)	3.1e-04 (3.9e-02)	2.6e-04 (1.6e-01)	2.7e-04 (6.3e-01)	3.7e-04 (2.7e+00)
1.0e-4	3.4e-04 (1.2e-02)	8.5e-05 (4.5e-02)	2.4e-05 (1.8e-01)	3.4e-05 (6.7e-01)	1.4e-05 (2.9e+00)
1.0e-5	3.4e-04 (1.2e-02)	8.4e-05 (4.7e-02)	2.1e-05 (1.9e-01)	5.4e-06 (7.6e-01)	2.8e-06 (3.1e+00)
1.0e-6	3.4e-04 (1.3e-02)	8.4e-05 (5.0e-02)	2.1e-05 (2.1e-01)	5.3e-06 (8.1e-01)	1.3e-06 (3.3e+00)

**Table 5.2** The error  $\|u - u_h^n\|$  and corresponding CPU time in parenthesis when solving a Poisson problem with homogenous Dirichlet conditions.

Table 5.2 shows the error and the corresponding CPU timings when solving a Poisson problem at various resolutions and convergence criteria. Here, the convergence criteria is chosen as reducing the relative residual, i.e.,  $\frac{\|r_k\|}{\|r_0\|}$  by the factor  $\epsilon$ . This convergence criteria is very common, in particular for stationary problems. There are several things to note here. For coarse resolution,  $N=64$ , the error stagnates somewhere between  $1.0e-3$  and  $1.0e-4$  and this stagnation marks where an appropriate stopping criteria is. It is however worth noticing that solving it to a criteria that is  $1.0e-6$  is actually only about 30% more computationally demanding than  $1.0e-3$ . This is due to the fact that we have a very efficient method that reduces the error by about a factor 10 per iteration. If we consider the fine resolution,  $N=1024$ , we see that the stagnation happens later and that we may not even have reached the stagnating point even at  $\epsilon = 1.0e-6$ . We also notice that the decreasing  $\epsilon$  in this case only lead to a moderate growth in CPU time. If we look closer at the table, we find that the stagnation point follows a staircase pattern. The code used to generate the table is as follows:

```
from dolfin import *

def boundary(x, on_boundary):
    return on_boundary

parameters["krylov_solver"]["relative_tolerance"] = 1.0e-18
parameters["krylov_solver"]["absolute_tolerance"] = 1.0e-18
parameters["krylov_solver"]["monitor_convergence"] = True
parameters["krylov_solver"]["report"] = True
#parameters["krylov_solver"]["maximum_iterations"] = 50000
epss = [1.0e-1, 1.0e-2, 1.0e-3, 1.0e-4, 1.0e-5, 1.0e-6]
data = {}
Ns = [64, 128, 256, 512, 1024]
#Ns = [8, 16, 32, 64]
for N in Ns:
    for eps in epss:
        parameters["krylov_solver"]["relative_tolerance"] = eps

        mesh = UnitSquareMesh(N, N)
        V = FunctionSpace(mesh, "P", 1)
        u = TrialFunction(V)
        v = TestFunction(V)

        u_ex = Expression("sin(3.14*x[0])*sin(3.14*x[1])", degree=
                           3)
        f = Expression("2*3.14*3.14*sin(3.14*x[0])*sin(3.14*x[1])"
                        , degree=3)
        a = inner(grad(u), grad(v))*dx
```

```

L = f*v*dx

U = Function(V)

A = assemble(a)
b = assemble(L)

bc = DirichletBC(V, u_ex, boundary)
bc.apply(A)
bc.apply(b)

t0 = time()
solve(A, U.vector(), b, "gmres", "amg")
t1 = time()

cpu_time = t1-t0
error_L2 = errornorm(u_ex, U, 'L2', degree_rise=3)
data[(N, eps)] = (error_L2, cpu_time)

for eps in epss:
    for N in Ns:
        D1, D2 = data[(N, eps)]
        print " %3.1e (%3.1e) " % (D1, D2),
        print ""

```

### Eigenvalues of the preconditioned system.

It is often interesting to assess the condition number of the preconditioned system,  $BA$ . If the preconditioner is a matrix and the size of the system is moderate we may be able to estimate the condition number of  $BA$  using NumPy, Matlab or Octave. However, when our preconditioner is an algorithm representing a linear operator, such as in the case of multigrid, then this is not possible. However, as described in [12], eigenvalues may be estimated as a bi-product of the Conjugate Gradient method. Without going into the algorithmic details of the implementation, we mention that this is implemented in the FEniCS module `cbc.block`, see [8]. The following code shows the usage.

```

from dolfin import *
from block.iterative import ConjGrad
from block.algebraic.petsc import ML
from numpy import random

def boundary(x, on_boundary):
    return on_boundary

```



```

class Source(Expression):
    def eval(self, values, x):
        dx = x[0] - 0.5; dy = x[1] - 0.5
        values[0] = 500.0*exp(-(dx*dx + dy*dy)/0.02)

Ns = [8, 16, 32, 64, 128, 256, 512, 1024]
for N in Ns:
    mesh = UnitSquareMesh(N,N)
    V = FunctionSpace(mesh, "CG", 1)

    # Define variational problem
    v = TestFunction(V)
    u = TrialFunction(V)
    f = Source(degree=3)
    a = dot(grad(v), grad(u))*dx
    L = v*f*dx
    bc = DirichletBC(V, Constant(0), boundary)

    # Assemble matrix and vector, create precondition and
    # start vector
    A, b = assemble_system(a,L, bc)
    B = ML(A)
    x = b.copy()
    x[:] = random.random(x.size(0))

    # solve problem and print out eigenvalue estimates.
    Ainv = ConjGrad(A, precondition=B, initial_guess=x, tolerance=
        1e-8, show=2)

    x = Ainv*b
    e = Ainv.eigenvalue_estimates()
    print "N=%d iter=%d K=%.3g" % (N, Ainv.iterations, e[-1]/e
        [0])

```

In this example we see that the condition number increases logarithmic from 1.1 to 2.1 as the  $N$  increases from 8 to 1024. The AMG preconditioner has better performance and does not show logarithmic growth. For indefinite symmetric systems, the CGN method provides the means for estimating the condition number, c.f., the `cbc.block` documentation.

### 5.3.1 Insight from Functional Analysis

In the previous Chapters 3 and 4 we have discussed the well-posedness of the convection-diffusion equations and the Stokes problem. In both cases, the problems were well-posed - meaning that the differential operators as well as their inverse were continuous. However, when we discretize the problems we get matrices where the condition number grows to infinity as the element size goes to zero. This seem to contradict the well-posedness of our discrete problems and may potentially destroy both the accuracy and efficiency of our numerical algorithms. Functional analysis explains this apparent contradiction and explains how the problem is circumvented by preconditioning.

Let us now consider the seeming contradiction in more precise mathematical detail for the Poisson problem with homogeneous Dirichlet conditions: Find  $u$  such that

$$-\Delta u = f, \quad \text{in } \Omega, \quad (5.9)$$

$$u = 0, \quad \text{on } \partial\Omega. \quad (5.10)$$

We know from Lax-Milgram's theorem that the weak formulation of this problem: Find  $u \in H_0^1$  such that

$$a(u, v) = b(v), \quad \forall v \in H_0^1.$$

where

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (5.11)$$

$$b(v) = \int_{\Omega} f v \, dx, \quad (5.12)$$

is well-posed because

$$a(u, u) \geq \alpha |u|_1^2, \quad \forall u \in H_0^1 \quad (5.13)$$

$$a(u, v) \leq C |u|_1 |v|_{H_0^1} \quad \forall u, v \in H_0^1. \quad (5.14)$$

Here  $|\cdot|_1$  denotes the  $H^1$  semi-norm which is known to be a norm on  $H_0^1$  due to Poincare. The well-posedness is in this case stated as

$$|u|_{H_0^1} \leq \frac{1}{\alpha} \|f\|_{H^{-1}}. \quad (5.15)$$

In other words,  $-\Delta$  takes a function  $u$  in  $H_0^1$  and returns a function  $f = -\Delta u$  which is in  $H^{-1}$ . We have that  $\|f\|_{-1} = \|-\Delta u\|_{-1} \leq C\|u\|_1$ . Also,  $-\Delta^{-1}$  takes a function  $f$  in  $H^{-1}$  and returns a function  $u = (-\Delta)^{-1}f$  which is in  $H_0^1$ . We have that  $\|u\|_1 = \|(-\Delta)^{-1}f\|_1 \leq \frac{1}{\alpha}\|f\|_{-1}$ . In fact, in this case  $\alpha = C = 1$ .

This play with words and symbols may be formalized by using operator norms that are equivalent with matrix norms. Let  $B \in \mathbb{R}^{n,m}$  then

$$\|B\|_{\mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)} = \max_{x \in \mathbb{R}^m} \frac{\|Bx\|_{\mathbb{R}^n}}{\|x\|_{\mathbb{R}^m}}$$

Here  $\mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)$  denotes the space of all  $m \times n$  matrices.

Analogously, we may summarize the mapping properties of  $-\Delta$  and  $(-\Delta)^{-1}$  in terms of the conditions of Lax-Milgram's theorem as

$$\|-\Delta\|_{\mathcal{L}(H_0^1, H^{-1})} \leq C \quad \text{and} \quad \|(-\Delta)^{-1}\|_{\mathcal{L}(H^{-1}, H_0^1)} \leq \frac{1}{\alpha}. \quad (5.16)$$

where  $\mathcal{L}(X, Y)$  denotes the space of bounded linear operators mapping  $X$  to  $Y$ . In other words,  $-\Delta$  is a bounded linear map from  $H_0^1$  to  $H^{-1}$  and  $(-\Delta)^{-1}$  is a bounded linear map from  $H^{-1}$  to  $H_0^1$ . This is a crucial observation in functional analysis that, in contrast to the case of a matrix which is a bounded linear map from  $\mathbb{R}^n$  to  $\mathbb{R}^m$ , an operator may be map from one space to another.

From Chapter 2 we know that the eigenvalues and eigenvectors of  $-\Delta$  with homogeneous Dirichlet conditions on the unit interval in 1D are  $\lambda_k = (\pi k)^2$  and  $e_k = \sin(\pi k x)$ , respectively. Hence the eigenvalues of  $-\Delta$  obviously tend to  $\infty$  as  $k$  grows to  $\infty$  and similarly the eigenvalues of  $(-\Delta)^{-1}$  accumulate at zero as  $k \rightarrow \infty$ . Hence the spectrum of  $-\Delta$  is unbounded and the spectrum of  $(-\Delta)^{-1}$  has an accumulation point at zero. Still, the operator  $-\Delta$  and its inverse are bounded from a functional analysis point of view, in the sense of (5.18).

Let us for the moment assume that we have access to an operator  $B$  with mapping properties that are inverse to that of  $A = -\Delta$ , i.e.,

$$\|B\|_{\mathcal{L}(H^{-1}, H_0^1)} \quad \text{and} \quad \|B^{-1}\|_{\mathcal{L}(H_0^1, H^{-1})}. \quad (5.17)$$

Then it follows directly that

$$\|BA\|_{\mathcal{L}(H_0^1, H_0^1)} \quad \text{and} \quad \|(BA)^{-1}\|_{\mathcal{L}(H_0^1, H_0^1)}. \quad (5.18)$$

and the condition number

$$\kappa(BA) = \frac{\max_i \lambda_i(BA)}{\min_i \lambda_i(BA)} = \|BA\|_{\mathcal{L}(H_0^1, H_0^1)} \|(BA)^{-1}\|_{\mathcal{L}(H_0^1, H_0^1)}$$

would be bounded. In the discrete case, the mapping property (5.17) translates to the fact that  $B$  should be spectrally equivalent with the inverse of  $A$  when  $B$  and  $A$  are both positive.

While the above discussion is mostly just a re-iteration of the concept of spectral equivalence in the discrete case when the PDEs are elliptic, the insight from functional analysis can be powerful for systems of PDEs. Let us consider the Stokes problem from Chapter 4. The problem reads:

$$\mathcal{A} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} -\Delta & -\nabla \\ \nabla \cdot & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} u \\ p \end{bmatrix}$$

As discussed in Chapter 4

$$\mathcal{A} : H_0^1 \times L^2 \rightarrow H^{-1} \times L^2$$

was a bounded linear mapping with a bounded inverse. Therefore, a preconditioner can be constructed as

$$\mathcal{B} = \begin{bmatrix} (-\Delta)^{-1} & 0 \\ 0 & I \end{bmatrix}$$

Clearly

$$\mathcal{B} : H^{-1} \times L^2 \rightarrow H_0^1 \times L^2$$

and is therefore a suitable preconditioner. However, we also notice that  $\mathcal{A}$  and  $\mathcal{B}^{-1}$  are quite different.  $\mathcal{A}$  is indefinite and has positive and negative eigenvalues, while  $\mathcal{B}$  is clearly positive. Hence, the operators are not spectrally equivalent. Exercise 5.9 looks deeper into this construction of preconditioners for Stokes problem. A more comprehensive description of this technique can be found in [9].

## 5.4 Exercises

**Exercise 5.1** Estimate ratio of non-zeros per unknown of the stiffness matrix on the unit square with Lagrangian elements of order 1, 2, 3 and 4. Hint: the number of non-zeros can be obtained from the function 'nnz' of a matrix object.

**Exercise 5.2** Compute the smallest and largest eigenvalues of the mass matrix and the stiffness matrix in 1D, 2D and 3D. Assume that the condition number is on the form  $\kappa \approx Ch^\alpha$ , where  $C$  and  $\alpha$  may depend on the number of dimensions in space. Finally, compute the corresponding condition numbers. Does the condition number have the same dependence on the number of dimensions in space?

**Exercise 5.3** Repeat Exercise 5.2 but with Lagrange elements of order 1, 2 and 3. How does the order of the polynomial affect the eigenvalues and condition numbers.

**Exercise 5.4** Compute the eigenvalues of the discretized Stokes problem using Taylor-Hood elements. Note that the problem is indefinite and that there are both positive and negative eigenvalues. An appropriate condition number is:

$$\kappa = \frac{\max_i |\lambda_i|}{\min_i |\lambda_i|}$$

where  $\lambda_i$  are the eigenvalues of  $A$ . Compute corresponding condition numbers for the Mini and Crouzeix-Raviart elements. Are the condition numbers similar?

**Exercise 5.5** Implement the Jacobi iteration for a 1D Poisson problem with homogeneous Dirichlet conditions. Start the iteration with an initial random vector and estimate the number of iterations required to reduce the  $L_2$  norm of the residual with a factor  $10^4$ . For relevant code see Example 5.3.

**Exercise 5.6** Test CG method without preconditioner, with ILU preconditioner and with AMG preconditioner for the Poisson problem in 1D and 2D with homogeneous Dirichlet conditions, with respect to different mesh resolutions. Do some of the iterations suggest spectral equivalence?

**Exercise 5.7** Test CG, BiCGStab, GMRES with ILU, AMG, and Jacobi preconditioning for

$$\begin{aligned} -\mu \Delta u + v \nabla u &= f & \text{in } \Omega \\ u &= 0 & \text{on } \partial\Omega \end{aligned}$$

Where  $\Omega$  is the unit square,  $v = c \sin(7x)$ , and  $c$  varies as 1, 10, 100, 1000, 10000 and the mesh resolution  $h$  varies as  $1/8, 1/16, 1/32, 1/64$ . You may assume homogeneous Dirichlet conditions.

**Exercise 5.8** The following code snippet shows the assembly of the matrix and preconditioner for a Stokes problem:

```
a = inner(grad(u), grad(v))*dx + div(v)*p*dx + q*div(u)*dx
L = inner(f, v)*dx

# Form for use in constructing preconditioner matrix
b = inner(grad(u), grad(v))*dx + p*q*dx

# Assemble system
A, bb = assemble_system(a, L, bcs)

# Assemble preconditioner system
P, btmp = assemble_system(b, L, bcs)

# Create Krylov solver and AMG preconditioner
solver = KrylovSolver("tfqmr", "amg")

# Associate operator (A) and preconditioner matrix (P)
solver.set_operators(A, P)

# Solve
U = Function(W)
solver.solve(U.vector(), bb)
```

Here, "tfqmr" is a variant of the Minimal residual method and "amg" is an algebraic multigrid implementation in HYPRE. Test, by varying the mesh resolution, whether the code produces an order-optimal preconditioner. HINT: You might want to change the "parameters" as done in Example 5.3:

```
# Create Krylov solver and AMG preconditioner
solver = KrylovSolver("tfqmr", "amg")
solver.parameters["relative_tolerance"] = 1.0e-8
solver.parameters["absolute_tolerance"] = 1.0e-8
solver.parameters["monitor_convergence"] = True
solver.parameters["report"] = True
solver.parameters["maximum_iterations"] = 50000
```

**Exercise 5.9** Consider the mixed formulation of linear elasticity that is appropriate when  $\lambda$  is large compared to  $\mu$ . That is,

```
a = inner(grad(u), grad(v))*dx + div(v)*p*dx + q*div(u)*dx - 1
                                     /lam*p*q*dx
L = inner(f, v)*dx
```

Create two preconditioners:

```
b1 = inner(grad(u), grad(v))*dx + p*q*dx  
b2 = inner(grad(u), grad(v))*dx + 1/lam*p*q*dx
```

Compare the efficiency of the different preconditioners when increasing the resolution and when  $\lambda \rightarrow \infty$ . Can you explain why the first preconditioner is the best?





# Chapter 6

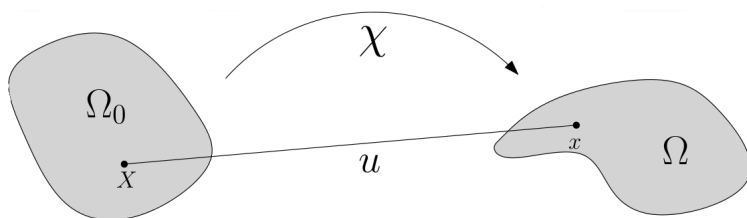
## Linear elasticity and singular problems

### 6.1 Introduction

Let us consider an elastic body  $\Omega_0$  that is being deformed under a load to become  $\Omega$ . the deformation  $\chi$  of a body in the undeformed state  $\Omega_0$  to deformed state  $\Omega$ . A point in the body has then moved

$$u = x - X, \quad (6.1)$$

by definition this is *displacement field*. An illustration is shown in Figure 6.1.



**Fig. 6.1** Deforming body and displacement vector  $u$ .

Here, the domain  $\Omega_0 \subset \mathbb{R}^3$ . From continuum mechanics, the elastic deformation is modelled by the stress tensor  $\sigma$  which is a symmetric  $3 \times 3$  tensor. In equilibrium (i.e. no acceleration terms) the Newton's second law states the balance of forces as:

$$\begin{aligned}\operatorname{div} \sigma &= f, & \text{in } \Omega, \\ \sigma \cdot n &= g, & \text{on } \partial\Omega,\end{aligned}$$

where  $f$  and  $g$  are body and surface forces, respectively and  $n$  is the outward normal vector.

For small deformations of an isotropic media, Hooke's law is a good approximation. Hooke's law states that

$$\sigma = 2\mu\epsilon(u) + \lambda \operatorname{tr}(\epsilon(u))\delta.$$

Here,  $\epsilon(u)$  is the strain tensor or the symmetric gradient:

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

$\mu$  and  $\lambda$  are the Lamé constants,  $\operatorname{tr}$  is the trace operator (the sum of the diagonal matrix entries),  $u$  is the displacement, and

$$\delta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

From Newton's second law and Hooke's law we arrive directly at the equation of linear elasticity:

$$-2\mu(\nabla \cdot \epsilon(u)) - \lambda \nabla(\nabla \cdot u) = f. \quad (6.2)$$

The equation of linear elasticity (6.2) is an elliptic equation, but there are crucial differences between this equation and a standard elliptic equation like  $-\Delta u = f$ . These differences often cause problems in a numerical setting. To explain the numerical issues we will here focus on the differences between the three operator:

1.  $-\Delta = \nabla \cdot \nabla = \operatorname{div} \operatorname{grad}$ ,
2.  $\nabla \cdot \epsilon = \nabla \cdot (\frac{1}{2}(\nabla + (\nabla^T)))$ ,
3.  $\nabla \cdot \operatorname{tr} \epsilon = \nabla \nabla \cdot = \operatorname{grad} \operatorname{div}$ .

In particular, the differences between the operators in 1. and 2. is that  $\nabla \cdot \epsilon$  has a larger kernel than  $-\Delta$ . The kernel consists of rigid motions and this leads to the usage of one of Korn's lemmas. This is the subject of Section 6.2. The kernel of the operators  $\operatorname{grad} \operatorname{div}$  and  $\operatorname{div} \operatorname{grad}$  are also different but here in fact the kernel of  $\operatorname{grad} \operatorname{div}$  is infinite dimensional and this has different

consequences for the numerical algorithms which not necessarily pick up this kernel at all. This is discussed in Section 6.3.

## 6.2 The operator $\nabla \cdot \epsilon$ and rigid motions

The challenge with the handling of the  $\nabla \cdot \epsilon$  operator is the handling of the singularity in the case of pure Neumann conditions. Let us therefore start with the simpler problem of the Poisson problem with Neumann conditions, i.e.,

$$-\Delta u = f, \quad \text{in } \Omega, \quad (6.3)$$

$$\frac{\partial u}{\partial n} = g, \quad \text{on } \partial\Omega. \quad (6.4)$$

It is easy to see that this problem is singular: Let  $u$  be a solution of the above equation, then  $u + C$  with  $C \in \mathbb{R}$  is also a solution because  $-\Delta u = \Delta(u + C) = f$  and  $\frac{\partial u}{\partial n} = \frac{\partial(u+C)}{\partial n} = g$ . Hence, the solution is only determined up to a constant. This means that the kernel is 1-dimensional.

A proper formulation of the above problem can be obtained by using the method of Lagrange multipliers to fixate the element of the 1-dimensional kernel. The following weak formulation is well-posed: Find  $u \in H^1$  and  $\lambda \in \mathbb{R}$  such that

$$a(u, v) + b(\lambda, v) = f(v) \quad \forall v \in H^1 \quad (6.5)$$

$$b(u, \gamma) = 0, \quad \forall \gamma \in \mathbb{R}. \quad (6.6)$$

Here,

$$a(u, v) = (\nabla u, \nabla v), \quad (6.7)$$

$$b(\lambda, v) = (\lambda, v), \quad (6.8)$$

$$f(v) = (f, v) + \int_{\partial\Omega} g v ds. \quad (6.9)$$

Hence, the method of Lagrange multipliers turns the original problem into a saddle problem similar that in Chapter 4. However, in this case the Brezzi conditions are easily verified. We remark however that this formulation makes the problem indefinite rather than positive definite and for this reason alternative techniques such as pin-pointing is often used instead. We will not avocate this approach as it often causes numerical problems. Instead, we include a

code example that demonstrate how this problem can be implemented with the method of Lagrange multipliers in FEniCS.

```
from dolfin import *

mesh = UnitSquareMesh(64, 64)

# Build function space with Lagrange multiplier
P1 = FiniteElement("Lagrange", mesh.ufl_cell(), 1)
R = FiniteElement("Real", mesh.ufl_cell(), 0)
W = FunctionSpace(mesh, P1 * R)

# Define variational problem
(u, c) = TrialFunction(W)
(v, d) = TestFunctions(W)
f = Expression("10*exp(-(pow(x[0] - 0.5, 2) + pow(x[1] - 0.5, 2)) / 0.02)", degree=2)
g = Expression("-sin(5*x[0])", degree=2)
a = (inner(grad(u), grad(v)) + c*v + u*d)*dx
L = f*v*dx + g*v*ds

# Compute solution
w = Function(W)
solve(a == L, w)
(u, c) = w.split()

# Plot solution
plot(u, interactive=True)
```

The kernel of the  $\epsilon$  operator is the space of rigid motions, RM. The space consists of translations and rotations. Rigid motions are on the following form in 2D and 3D:

$$\text{RM}_{2D} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} + a_2 \begin{bmatrix} -y \\ x \end{bmatrix}, \quad (6.10)$$

$$\text{RM}_{3D} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} + \begin{bmatrix} 0 & a_3 & a_4 \\ -a_3 & 0 & a_5 \\ -a_4 & -a_5 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}. \quad (6.11)$$

Hence, the kernel in 2D is three-dimensional and may be expressed as above in terms of the degrees of freedom  $(a_0, a_1, a_2)$  whereas the kernel in 3D is six-dimensional  $(a_0, \dots, a_5)$ .

The Korn's lemmas states suitable conditions for solvability. Here, we include two of the three inequalities typically listed.

- The first lemma: For all  $u \in H^1 \setminus \text{RM}$  we have that  $\|\epsilon(u)\| \geq C\|u\|_1$ .

- The second lemma: For all  $u \in H_0^1$  we have that  $\|\epsilon(u)\| \geq C\|u\|_1$ .

These lemmas should be compared with the Poincaré's lemma and the equivalence of the  $|\cdot|_1$  and  $\|\cdot\|_1$  norms. The second lemma states that when we have homogenous Dirichlet conditions we obtain a well-posed problem in a similar manner as for a standard elliptic problem. This case is often called fully-clamped conditions. For the Neumann problem, however, coersivity is not obtained unless we remove the complete set of rigid motions for the function space used for trial and test functions. Removing the rigid motions is most easily done by using the method of Lagrange multipliers.

Let us now consider a weak formulation of the linear elasticity problem and describe how to implement it in FEniCS. For now we consider the case where  $\lambda$  and  $\mu$  are of comparable magnitude. In the next section we consider the case where  $\lambda \gg \mu$ . The weak formulation of the linear elasticity problem is: Find  $u \in H^1$  and  $r \in \text{RM}$  such that

$$a(u, v) + b(r, v) = f(v), \quad \forall v \in H^1, \quad (6.12)$$

$$b(s, u) = 0, \quad \forall s \in \text{RM}. \quad (6.13)$$

Here,

$$a(u, v) = \mu(\epsilon(u), \epsilon(v)) + \lambda(\text{div } u, \text{div } v) \quad (6.14)$$

$$b(r, v) = (r, v), \quad (6.15)$$

$$f(v) = (f, v) + \int_{\partial\Omega} g v ds. \quad (6.16)$$

As we know from Chapter 4, this is a saddle point problem and we need to comply with the Brezzi conditions. Verifying these conditions are left as Exercise 6.4.

## O

ur brain and spinal cord is floating in a water like fluid called the cerebrospinal fluid. While the purpose of this fluid is not fully known, it is known that the pressure in the fluid oscillates with about 5-10 mmHg during a cardiac cycle which is approximately one second, c.f., e.g., [3]. The Youngs' modulus has been estimated 16 kPa and 1 mmHg  $\approx$  133 Pa, c.f., e.g., [13]. To compute the deformation of the brain during a cardiac cycle we consider solve the linear elasticity problem with Neumann conditons set as pressure of 1 mm Hg and ... The following code shows the implmentation in FEniCS. The mesh of the

brain was in this case obtained from a T1 magnetic resonance image and segmentation was performed by using FreeSurfer.

```

from fenics import *

mesh = Mesh('mesh/res32.xdmf') # mm

plot(mesh, interactive=True)

# Since the mesh is in mm pressure units in pascal must be
# scaled by alpha = (1e6)**(-1)
alpha = (1e6)**(-1)

# Mark boundaries
class Neumann_boundary(SubDomain):
    def inside(self, x, on_boundary):
        return on_boundary

mf = FacetFunction("size_t", mesh)
mf.set_all(0)

Neumann_boundary().mark(mf, 1)
ds = ds[mf]

# Continuum mechanics
E = 16*1e3 *alpha
nu = 0.25
mu, lambda_ = Constant(E/(2*(1 + nu))), Constant(E*nu/((1 + nu)
                                                    *(1 - 2*nu)))
epsilon = lambda_ u: sym(grad(u))

p_outside = 133 *alpha
n = FacetNormal(mesh)
f = Constant((0, 0, 0))

V = VectorFunctionSpace(mesh, "Lagrange", 1)

# ----- Handle Neumann-problem ----- #
R = FunctionSpace(mesh, 'R', 0) # space for one
                                # Lagrange multiplier
M = MixedFunctionSpace([R]*6)   # space for all
                                # multipliers
W = MixedFunctionSpace([V, M])
u, rs = TrialFunctions(W)
v, ss = TestFunctions(W)

# Establish a basis for the nullspace of RM
e0 = Constant((1, 0, 0)) # translations

```

```

e1 = Constant((0, 1, 0))
e2 = Constant((0, 0, 1))

e3 = Expression((-x[1]', 'x[0]', '0')) # rotations
e4 = Expression((-x[2]', '0', 'x[0]'))
e5 = Expression(('0', '-x[2]', 'x[1]'))
basis_vectors = [e0, e1, e2, e3, e4, e5]

a = 2*mu*inner(epsilon(u),epsilon(v))*dx + lambda_*inner(div(u
),div(v))*dx
L = inner(f, v)*dx + p_outside*inner(n,v)*ds(1)

# Lagrange multipliers contrib to a
for i, e in enumerate(basis_vectors):
    r = rs[i]
    s = ss[i]
    a += r*inner(v, e)*dx + s*inner(u, e)*dx

# ----- #

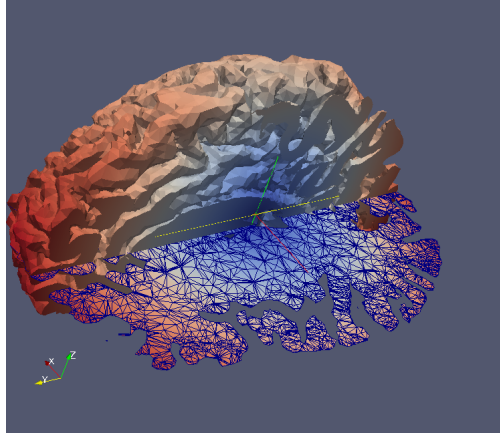
# Assemble the system
A = PETScMatrix()
b = PETScVector()
assemble_system(a, L, A_tensor=A, b_tensor=b)

# Solve
uh = Function(W)
solver = PETScLUSolver('mumps') # NOTE: we use direct solver
                                   for simplicity
solver.set_operator(A)
solver.solve(uh.vector(), b)

# Split displacement and multipliers. Plot
u, ls = uh.split(deepcopy=True)
plot(u, mode='displacement', title='Neumann_displacement',
      interactive=True)

file = File('deformed_brain.pvd')
file << u

```



**Fig. 6.2** Deformation of the human brain during a cardiac cycle.

### 6.3 Locking

The locking phenomena has nothing to do with the problem related to the rigid motions studied in the previous section. Therefore, we consider locking in the simplest case possible where we have homogenous Dirichlet conditions. In this case the elasticity equation can be reduced to

$$\begin{aligned} -\mu\Delta u - (\mu + \lambda)\nabla\nabla \cdot u &= f, & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega. \end{aligned}$$

The weak formulation of the problem then becomes: Find  $u \in H_0^1$  such that

$$a(u, v) = f(v), \quad \forall v \in H_0^1,$$

where

$$a(u, v) = \mu(\nabla u, \nabla v) + (\mu + \lambda)(\nabla \cdot u, \nabla \cdot v), \quad (6.17)$$

$$f(v) = (f, v). \quad (6.18)$$

The phenomenon locking is a purely numerical artifact that arises when  $\lambda \gg \mu$ . Roughly speaking, approximating  $\nabla$  and  $\nabla \cdot$  require different methods. While vertex based approximations work fine for  $\nabla$ , edge based methods are more



natural for  $\nabla \cdot$  since this operator relates directly to the flux through the element edges.

For smooth functions, it can be verified directly that

$$\Delta = \nabla \cdot \nabla = \nabla \nabla \cdot + \nabla \times \nabla \times$$

where  $\nabla \times$  is the curl operator. Hence in  $H_0^1$  we have

$$(\nabla u, \nabla v) = (\nabla \cdot u, \nabla \cdot v) + (\nabla \times u, \nabla \times v).$$

Furthermore, it is well known (the Helmholtz decomposition theorem) that any field in  $L^2$  or  $H^1$  can be decomposed into a the gradient of a scalar potential (irrotational, curl-free vector field) and the curl of scalar (a solenoidal, divergence-free vector field). That is,

$$u = \nabla \phi + \nabla \times \psi,$$

where  $\phi$  and  $\psi$  are scalar fields that can be determined. Furthermore,

$$\nabla \cdot \nabla \times u = 0, \tag{6.19}$$

$$\nabla \times \nabla \cdot u = 0. \tag{6.20}$$

This means that

$$\nabla \nabla \cdot u = \begin{cases} \Delta u & \text{if } u \text{ is a gradient} \\ 0 & \text{if } u \text{ is a curl} \end{cases}$$

As the material becomes incompressible, when  $\lambda \rightarrow \infty$  the gradient part is being locked and  $\phi$  tends to zero. However, the curl represented by  $\psi$  remains unaffected. Vertex based finite elements such as Lagrange are poor at distinguishing between gradients and curls and tend to lock the complete solution. Exercise 6.5 investigates this phenomena numerically.

To avoid locking it is common to introduce a the quantity solid pressure,  $p = (\mu + \lambda) \nabla \cdot u$ . Introducing this as a separate unknown into the system we obtain the equations:

$$\begin{aligned} -\mu \Delta u - \nabla p &= f, \\ \nabla \cdot u - \frac{1}{\mu + \lambda} p &= 0. \end{aligned}$$

This system of equations is similar to the Stokes problem. Hence, we may formulate a weak problems as follows. Find  $u \in H_0^1$  and  $p \in L^2$  such that

$$a(u, v) + b(p, v) = f(v) \forall v \in H^1 \quad (6.21)$$

$$b(u, q) - c(p, q) = 0, \forall q \in \mathbb{R}. \quad (6.22)$$

Here,

$$a(u, v) = (\nabla u, \nabla v), \quad (6.23)$$

$$b(p, v) = (\nabla p, v), \quad (6.24)$$

$$c(p, q) = \frac{1}{\mu + \lambda}(p, q) \quad (6.25)$$

$$f(v) = (f, v). \quad (6.26)$$

The case when  $\lambda \rightarrow \infty$  then represents the Stokes problem as  $\frac{1}{\mu + \lambda} \rightarrow 0$ . Hence, for this problem we know that stable discretizations can be obtained as long as we have Stokes-stable elements like for instance Taylor–Hood. We also remark that Stokes-stable elements handle any  $\mu, \lambda$  because the  $-c(p, q)$  is a negative term that only stabilize. In fact, this problem is identical to the proposed penalty method that was discussed for the Stokes problem.

**Exercise 6.1** Show that the inner product of a symmetric matrix  $A$  and matrix  $B$  equals the inner product of  $A$  and the symmetric part of  $B$ , i.e., that  $A : B = A : B_S$ , where  $B_S = \frac{1}{2}(B + B^T)$ .

**Exercise 6.2** Show that the term  $\operatorname{div} \epsilon(u)$  in a weak setting may be written as  $(\epsilon(u), \epsilon(v))$ . Use the result of Exercise 6.1.

**Exercise 6.3** Show that the Brezzi conditions (4.15-4.18) for the singular problem of homogenous Neumann conditions for the Poisson problem (6.5)–(6.9). Hint: use the following version of Poincaré’s lemma:

$$\|u - \bar{u}\|_0 \leq C \|\nabla u\|_0, \quad \forall u \in H^1.$$

Here,  $\bar{u} = \frac{1}{|\Omega|} \int_{\Omega} u dx$ . As always, the inf-sup condition is challenging, but notice that

$$\sup_{u \in V_h} \frac{b(u, q)}{\|u\|_{V_h}} \geq \frac{b(\bar{u}, q)}{\|\bar{u}\|_{V_h}}.$$

**Exercise 6.4** Show that three of Brezzi conditions (4.15-4.17) for problem linear elasticity problem with pure Neumann conditions (6.12)–(6.13) are valid. Hint: use Korn’s lemma for the coersivity. As always, the inf-sup condition is challenging and we refer to [6].

**Exercise 6.5** We will consider the topic 'locking'. Consider the following equation on the domain  $\Omega = (0, 1)^2$ :

$$-\mu\Delta u - \lambda\nabla\nabla \cdot u = f \text{ in } \Omega, \quad (6.27)$$

$$u = u_{\text{analytical}} \text{ on } \partial\Omega \quad (6.28)$$

where  $u_{\text{analytical}} = (\frac{\partial\phi}{\partial y}, -\frac{\partial\phi}{\partial x})$  and  $\phi = \sin(\pi xy)$ . Here, by construction,  $\nabla \cdot u_{\text{analytical}} = 0$ .

- a) Derive an expression for  $f$ . Check that the expression is independent of  $\lambda$ .
- b) Compute the numerical error for  $\lambda = 1, 100, 10000$  at  $h = 8, 16, 32, 64$  for polynomial order both 1 and 2.
- c) Compute the order of convergence for different  $\lambda$ . Is locking occurring?



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