Prof. Santiago Badia ©

Lecture Notes on

Finite Element Methods

MTH-4321, MTH-5321

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Preface

I have created these lectures notes for the unit MTH4321-MTH5321 *Methods of Computational Mathematics* at Monash University in May 2020, in order to provide students with an introduction to finite element methods. In this presentation, I have tried to provide the mathematical background of these schemes. Finite element methods rely on weak forms of partial differential equations, which are grounded on functional analysis. Likely, many students will not have much (or any) background on functional analysis. One option would be to skip these concepts and go straight to the discrete problem, without discussing why the problems are well-posed at the continuous level, but still functional spaces cannot be totally skipped, e.g., to understand the convergence properties of these methods. So, I have decided to start this presentation with a extremely short introduction to variational methods and functional analysis. I think that this chapter is accessible to Master students with a mathematical background. Next, I have introduced the Galerkin method, analyse the error of such approach, and combined it with spectral and finite element methods in one dimension. The last section extends the finite element method to multiple dimensions, showing the machinery that is needed in practical implementations of this scheme.

All this theory is combined with computational tutorials. They can be found in this `Github` repository, in the form of Jupyter notebooks on the cloud. Thus, access to a web browser is all what you need to run these tutorials. In any case, I provide instructions for a local installation of the tools being used in the tutorial. The tutorials use the `Gridap` software library developed by me and co-workers. This library provides tools for the numerical approximation of partial differential equations using mesh-based techniques (finite element methods in general). The library is written in `Julia`, a somehow recent programming language that combines the

expressiveness of dynamic languages like `Python` and the performance of static languages like `C++` or `FORTRAN`, which is an exciting new language for numerical implementations in computational and data science.

Computational mathematics is an amazing field of research that is in the core of computational science, the third pillar or science together with experiments and theory. Finite element methods (in a broad sense) are in the core of most of the state-of-the-art research on numerical partial differential equations. They have applications in almost any scientific discipline, since many mathematical models are expressed in terms of multi-dimensional differential equations on complex geometries. In 12h of lectures it is not possible to go deeper into this topic, but you will finish this unit with an idea of the field. If you want more information about these techniques or research topics on this field, please contact me.

I have compiled these notes during these four weeks of teaching. It has been a formidable task for me to select the right topics, how to present them, typesetting the equations in latex, and creating nice illustrations, together with tutorials, exercises, and computational tutorials. You will probably find typos, since you are the first cohort of students that will learn finite element methods at Monash, and the first ones that will read these recently baked lecture notes. Please, inform me of typos you find and any other feedback related to this material. It will help me to improve these notes for future students. In any case, I will go through this material, fixing and improving things, and update them at Moodle.

Santiago Badia

Melbourne, May 30, 2020

Chapter 1

Mathematical models

1.1 Introduction

In this chapter, we will start with the statement of some mathematical models in physics that can be defined as the minimisation of a potential (energy). Then, using the calculus of variations, we will end up with its corresponding variational form. Existence and uniqueness of solutions, together with the equivalence between the minimisation and variational statements will be provided. Finally, under extra regularity assumptions, we will relate these formulation with the standard *strong* partial differential equation form. We will also discuss how we can go in the opposite direction, starting from a partial differential equations, and ending up with the *weak* or variational equation or minimisation problem.

The existence issue in finite dimensional problems is straightforward. However, for infinite dimensional function spaces, it involves advanced mathematics; more specifically, it involves *functional analysis*. However, we will try to reduce the exposition to the minimum while keeping a rigorous presentation. In this sense, we will show some intuitive examples that show how important is to choose the right functional spaces in our minimisation and variational problems in order to have existence. We will introduce the concepts of Banach and Hilbert spaces, Cauchy sequences, completeness, and *maximal function space* with respect to a given norm. With this idea, we can naturally define some very useful Lebesgue and Sobolev spaces, and provide some key properties of these spaces (without proof).

As we will see in the next chapter, finite element and (some) spectral methods rely on weak formulations of partial differential equations. I consider that presenting these numerical methods without a thorough introduction to this kind of problems and their relation with partial differential equations in the classical sense is not much satisfactory for maths oriented students. This is a big difference compared to finite difference (and other collocation) methods that work with the strong form instead.

1.1.1 Minimisation problem

Let us consider a mathematical model that represents a straight bar under traction (i.e., a bar in which external forces can only be in the longitudinal directions). In this case, the physical domain that represents the bar is an interval $[a, b] \subset \mathbb{R}$ and we define the longitudinal (or tangential) displacement of the bar particles with respect to the original configuration with $u(x)$. Let us consider that the displacements of the bar particles are very small compared to the bar length $|b - a|$, i..e, the so-called *small displacement* assumption. Under these circumstances, the elastic energy stored by the bar is expressed by Hooke's law as

$$E(u) = \int_a^b \kappa(x) u'(x)^2 \mathrm{d}x, \tag{1.1}$$

where $\kappa(x)$ is the Young's modulus of the bar material, which is assumed to be in the *elastic* regime. u' represents the derivative of u with respect to x. Let us assume the following *boundary conditions*, i.e., a prescribed longitudinal displacement at the end-points:

$$u(a) = u_a, \qquad u(b) = u_b, \tag{1.2}$$

where $u_a, u_b \in \mathbb{R}$, and a *forcing* term $f : [a, b] \to \mathbb{R}$. u_a, u_b and f are *data*. Due to the *minimum energy principle*, the displacement of the bar is the function that minimises the following functional:

$$J(u) \doteq \int_a^b (\kappa(x) u'(x)^2 - f(x) u(x)) \mathrm{d}x. \tag{1.3}$$

An elastic cord with a perpendicular load $f(x)$ under the assumption of the small displacements satisfies the same problem; in this case $u(x)$ represents the displacement in the perpendicular direction. An analogous

minimisation problem is obtained when modelling the heat conduction on a bar. In this case, $u(x)$ is the temperature, $\kappa(x)$ is the heat conductivity, and $f(x)$ is the *source* term.

In any case, we have not stated yet the minimisation problem for the functional (1.3), since we have not defined yet in which set of functions we want to minimise it. Since we need to evaluate first derivatives of the function in (1.3), it is natural to consider that $u(x) \in C^1([a,b])$. Thus, the solution $u(x)$ reads as:

$$u \doteq \underset{v \in C^1([a,b]) \text{ satisfying } (1.2)}{\operatorname{argmin}} J(v). \tag{1.4}$$

Thus, using physical principles (energy minimisation), we can state mathematically physical problems as minimisation problems in *infinite dimensional* space of functions.

1.1.2 Variational formulation

In the previous subsection we have ended up with a minimisation problem on an infinite-dimensional space of functions. In particular, we are interested on *vector spaces* of functions under addition and multiplication by a real number.

Definition 1.1.1: Vector space

A vector space V of real-valued functions in a domain $\Omega \subset \mathbb{R}^d$ (where d denotes the space dimension) is such that, for any $u, v \in V$ and $\alpha \in \mathbb{R}$, it holds

$$(u+v)(x) \doteq u(x) + v(x), \quad (\alpha \cdot u)(x) \doteq \alpha u(x), \quad \forall x \in \Omega. \tag{1.5}$$

Using *calculus of variations*, we can state the minimisation problem (1.4) in a *variational* form. Assuming the existence of a global minimum $u(x)$ for (1.4), we can now consider the variation of the functional J at u with respect to a variation $v \in C_0^1([a,b])$ times $\alpha \in \mathbb{R}$. $C_0^1([a,b])$ is the subspace of functions $C^1([a,b])$ that vanish at the end-points, i.e.,

$$C_0^1([a,b]) \doteq \{v \in C^1([a,b]) \ : \ v(a) = v(b) = 0\}. \tag{1.6}$$

Without the zero boundary conditions for the perturbation, the perturbed function $u + \alpha v$ would not satisfy the boundary conditions (1.2). Since u is a global minimiser, it naturally holds

$$J(u) \leq \Phi_v(\alpha) \doteq J(u + \alpha v) \quad \forall v \in C_0^1([a,b]),\ \forall \alpha \in \mathbb{R}. \tag{1.7}$$

Thus, $\Phi_v(\alpha)$ has a global minimum at 0. If Φ_v is differentiable, $\Phi_v'(0) = 0$. It means that since u is the minimum energy configuration, any perturbation of u cannot produce a decrease of energy.

The derivative of Φ reads

$$\Phi_v'(0) = \lim_{\alpha \to 0} \frac{J(u + \alpha v) - J(u)}{\alpha}. \tag{1.8}$$

Such derivative is the so-called *directional derivative* of J at u in the direction v. Enforcing $\Phi_v'(0)$ to be zero for any perturbation $v \in C_0^1([a,b])$, we get, under simple algebraic manipulations and eliminating high order terms, that

$$\int_a^b (\kappa(x)u'(x)v(x) - f(x)v(x))\mathrm{d}x = 0 \quad \forall v \in C_0^1([a,b]). \tag{1.9}$$

This expression is the *weak or variational form* of the physical problem at hand. In the field of statics, this statement of the elastic problems above is called the *principle of virtual work*, which means that ant perturbation of the equilibrium configuration requires to supply energy to the system.

1.1.3 Differential equation

Now, we would like to relate the variational and minimisation formulations above with standard differential equations. In this process we will observe that, in order to reach this form, we will need to make some additional regularity assumptions over the solution.

Lemma 1.1.2: Fundamental lemma of calculus of variations

If a function $f \in C^0([a,b])$ is such that

$$\int_a^b f(x)v(x)\mathrm{d}x = 0,\ \forall v \in C_0^0([a,b]), \tag{1.10}$$

then $f \equiv 0$.

Let us assume that the solution u of the variational formulation (1.9) is in $C^2([a,b])$, $\kappa \in C^1([a,b])$, and $f \in C^0([a,b])$. Using integration by parts, we get for any $v \in C_1^0([a,b])$

$$\int_a^b \kappa(x)u'(x)v'(x)\mathrm{d}x - \int_a^b f(x)v(x)\mathrm{d}x = -\int_a^b ((ku')' - f(x))v(x)\mathrm{d}x. \tag{1.11}$$

Lemma 1.1.2 leads to

$$-(\kappa u')' = f \quad \text{in } [a,b], \quad u(a) = u_a,\ u(b) = u_b. \tag{1.12}$$

As a result, if the solution of (1.9) with the boundary conditions in (1.2) is in $C^2([a,b])$, it satisfies the two-point boundary value problem (1.12).

1.2 Abstract setting

In this section, we consider an abstract setting for minimisation and variational problems that includes the examples above, and (under regularity assumptions) show to find their corresponding boundary value problem. We consider minimisation problems that are related to an energy functional J on a space of functions $\Omega \subset \mathbb{R}^d \to \mathbb{R}$, where d is the space dimension, e.g., $d = 2, 3$. Ω is assumed to be bounded, i.e.,

$$\mathrm{diam}(\Omega) = \sup_{x,y\in\Omega} \|x - y\| < \infty, \tag{1.13}$$

and its boundary $\partial\Omega$ is piecewise smooth, i.e. it can be expressed as a smooth diffeomorphism from a reference polyhedron boundary.

Definition 1.2.1: (Bi)linear forms

Given a vector space V in the field of scalars $\mathbb{R}$, a form $\ell : V \to \mathbb{R}$ is linear if it satisfies:

$$\ell(u+v) = \ell(u) + \ell(v),\ u,\ v \in V,\ \ \ell(\alpha u) = \alpha\ell(u)\ \forall u \in V,\ \alpha \in \mathbb{R}. \tag{1.14}$$

A form $a : V \times V \to \mathbb{R}$ is a bilinear form if it is linear with respect to each of its two arguments separately.

1.2.1 Abstract minimisation

We are interested in an important class of minimisation problems that covers the examples introduced above.

Definition 1.2.2: Quadratic minimisation problem

Let us consider a functional $J : V \to \mathbb{R}$ on a vector space V that can be expressed as

$$J(v) \doteq \frac{1}{2}a(v,v) - \ell(v) + c \tag{1.15}$$

for a symmetric bilinear form $a : V \times V \to \mathbb{R}$, a linear form $\ell : V \to \mathbb{R}$ and $c \in \mathbb{R}$. The problem

$$u = \operatorname*{argmin}_{v \in V} J(v) \tag{1.16}$$

is called a quadratic minimisation problem *on V.*

We note that the space of functions with non-homogeneous boundary conditions is not a vector space but an affine space. The minimisation in an affine space can easily be transformed into a vector space using the *offset function* method. We consider a vector space of functions V_0 and an affine space V that can be expressed as $u_0 + V_0$, where u_0 is the so-called *offset function*. In the examples in Section 1.1, u_0 is a function in $C^1([a,b])$ that satisfies the boundary conditions (1.2) (while keeping a desired level of smoothness), whereas V_0 is a space of functions with homogeneous (zero) boundary conditions, i.e., $V_0 = C_0^1([a,b])$. Given J, V_0 and u_0, the minimisation problem in V can be expressed as follows. We have

$$J(v+u_0) = \frac{1}{2}a(v+u_0, v+u_0) - \ell(v+u_0) + c \tag{1.17}$$

$$= \frac{1}{2}a(v,v) + a(v,u_0) - \ell(v) + \frac{1}{2}a(u_0,u_0) - \ell(u_0) + c \doteq \tilde{J}(v) \tag{1.18}$$

where $\tilde{J}$ is a quadratic functional too. Thus,

$$\operatorname*{argmin}_{u \in u_0 + V_0} J(u) = u_0 + \operatorname*{argmin}_{v \in V_0} \tilde{J}(v). \tag{1.19}$$

As a result, we can restrict to quadratic minimisation problems on vector spaces without loss of generality. Now, let us consider the well-posedness of the quadratic minimisation problem.

Definition 1.2.3: Positive definiteness

A symmetric bilinear form $a : V_0 \times V_0 \to \mathbb{R}$ *on a real vector space* V_0 *is* semi-positive definite *if*

$$a(u,u) \geq 0 \quad \forall u \in V_0. \tag{1.20}$$

Moreover, it is positive definite *if*

$$a(u,u) > 0 \quad \forall u \in V_0 \setminus \{0\}. \tag{1.21}$$

Lemma 1.2.4: Necessary condition for existence of a global minimum

If the quadratic minimisation problem in Definition 1.2.2 has a solution, then its bilinear form $a : V_0 \times V_0 \to \mathbb{R}$ *must be semi-positive definite.*

Proof. If the bilinear form is not semi-positive definite, we can pick a $u \in V_0$ such that $a(u,u) < 0$. Thus, $J(\alpha u) = 1/2\alpha^2 a(u,u) - \alpha \ell(u) + c$ and $\lim_{\alpha \to \infty} J(\alpha u) = -\infty$. □

Lemma 1.2.5: Necessary condition for uniqueness of the global minimum

If the quadratic minimisation problem in Definition 1.2.2 has a solution and its bilinear form a is positive definite, then the solution is unique.

Proof. Let us assume that there exist two solutions $u,\ v \in V_0$ such that $u \neq v$. $\Phi(\alpha) \doteq J(\alpha u + (1-\alpha)v)$ has two distinct global minima at $\alpha = 0$ and $\alpha = 1$. Besides, $\Phi(\alpha) = \alpha^2/2a(u-v, u-v) +$ lower order terms and $a(u-v, u-v) > 0$. Thus, Φ is a non-degenerate parabola that opens up and can only have a minimum at its vertex. It proves the result by contradiction. □

If a is semi-positive definite, there are infinite solutions that can only differ in an element of the kernel of a, i.e., two solutions $u,\ v \in V_0$ must satisfy $a(u-v, u-v) = 0$.

Let us introduce some additional concepts that will allow us to prove more necessary conditions for existence.

Definition 1.2.6: Norm on a vector space

A norm $\|\cdot\|$ on a vector space V is a map $\|\cdot\| : V \to \mathbb{R}_+$ such that

- *Positive definiteness:* $\|v\| = 0 \iff v = 0\ \forall \in V$,
- *Absolutely homogeneous:* $\|\alpha v\| = |\alpha|\|v\|,\ \forall \alpha \in \mathbb{R},\ \forall v \in V$,
- *Triangle inequality:* $\|v + w\| \leq \|v\| + \|w\| \forall v,\ w \in V$.

Definition 1.2.7: Positive definite bilinear form

A symmetric positive definite bilinear form $a : V \times V \to \mathbb{R}$ induces the energy norm

$$\|u\|_a \doteq a(u,u)^{1/2}. \tag{1.22}$$

Definition 1.2.8: Continuity of (bi)linear forms

Given a vector space V with norm $\|\cdot\|$, a linear form $\ell : V \to \mathbb{R}$ is continuous *or* bounded *if*

$$\exists C > 0 \ : \ |\ell(v)| \leq C\|v\| \ \forall v \in V. \tag{1.23}$$

A bilinear form $a : V \times V \to \mathbb{R}$ is continuous *if*

$$\exists K > 0 \ : \ |a(u,v)| \leq K\|u\|\|v\|, \ \forall u, \ v \in V. \tag{1.24}$$

We note that continuity of the energy norm can readily be checked for $K = 1$ by using the Cauchy-Schwarz inequality.

It is essential to prove that the potential J is bounded from below to have a well-posed minimisation problem.

Lemma 1.2.9: Boundedness from below

The quadratic functional J in Definition 1.2.2 is bounded from below *in V_0 if and only if the bilinear form is positive definite and the linear form ℓ is continuous in V_0 with respect to the energy norm $\|\cdot\|_a$.*

Proof. If a is positive definite and ℓ is continuous, using the generalised Young's inequality

$$ab \leq \frac{a^2}{2\epsilon} + \frac{\epsilon b^2}{2},\ a,\ b \in \mathbb{R},\ \epsilon > 0, \tag{1.25}$$

we readily get

$$J(u) = 1/2a(u,u) - \ell(u) \geq 1/2\|u\|_a^2 - C\|u\|_a \geq -1/2C. \tag{1.26}$$

In the other direction, let us assume that J is bounded below and the conditions in the lemma do not hold. For every $n \in \mathbb{N}$, we can pick $u_n \in V_0$ such that

$$\ell(u_n) \geq n\|u_n\|_a. \tag{1.27}$$

By re-scaling $u_n \leftarrow \frac{u_n}{\|u_n\|_a}$ we can assume that $\|u_n\|_a = 1$, thus

$$J(u) \leq 1/2 - n \to -\infty,\ \text{as}\ \ n \to \infty. \tag{1.28}$$

Thus, J cannot be bounded below, leading to a contradiction. It proves the result. □

So far, we have found necessary conditions for existence and uniqueness of solutions. If we assume that the vector space V_0 is finite dimensional, existence can readily be proven. At the end of the day, the quadratic minimisation functional in finite dimension is nothing but a non-degenerate parabola opening up for which there is a unique global minimum at its vertex.

Theorem 1.2.10: Existence and uniqueness of a minimiser in finite dimension

If the vector space V_0 in the quadratic minimisation problem in Definition 1.2.2 involves a positive definite symmetric bilinear form a and a continuous functional ℓ, and V_0 has finite dimension, there exists a unique solution for this problem.

Proof. If the vector space V_0 has a finite dimension, we can define an ordered basis for it, and thus V_0 is isomorphic to $\mathbb{R}^N$. The variational form of the quadratic minimisation problem can be recast as a *square* linear system of equations with a positive-definite system matrix (thus non-singular) and right-hand side with bounded entries. Thus, the unique solution is equal to the inverse of that matrix times the right-hand side vector. □

More elaboration on the concepts of the previous proof can be found later on, when we will discuss finite dimensional discretisations of infinite dimensional problems. Unfortunately, sufficient conditions for existence in infinite dimensions are more elusive and are strongly related to the right choice of the vector space V_0. It must be *large enough* for existence but *small enough* for uniqueness.

1.2.2 Abstract variational form

In this section, we provide an abstract definition of variational forms. In the most general case, a (possibly nonlinear) variational problem ca be stated as follows.

Definition 1.2.11: Variational problem

A variational problem reads as:

$$u \in V \ : \ a(u; v) = 0, \ \forall v \in V_0 \tag{1.29}$$

where V_0 is a vector space, V is an affine space of functions, and $a : V \times V_0 \to \mathbb{R}$ is a map that is linear with respect to its second argument.

In Definition 1.2.11, the space V in which we seek the solution is the *trial space* (affine space) and the space V_0 of admissible test functions is the *test space* (vector space). Variational problems can also be stated in terms of vector spaces by using the fact that $V = u_0 + V$ for an arbitrary *offset function* $u_0 \in V$. The abstract variational problem in Definition 1.2.11 can be written as:

$$\tilde{u} \in V_0 : \ a(\tilde{u} + u_0, v) = 0 \ \ \forall v \in V_0, \ \ u = \tilde{u} + u_0. \tag{1.30}$$

Thus, we can consider variational problems for trial and test spaces without loss of generality.

Let us consider now the relationship between minimisation and variational problems. Let us restrict ourselves to quadratic minimisation problems. Let us *assume the existence* of a global minimiser u. Using the calculus of variations (as described above), we can compute the directional derivative of the functional as

$$\begin{aligned}\lim_{\alpha\to 0}\frac{J(u+\alpha v)-J(u)}{\alpha} &= \lim_{\alpha\to 0}\frac{\alpha a(u,v)+\frac{\alpha^2}{2}a(v,v)-\alpha\ell(v)}{\alpha}\\ &= a(u,v)-\ell(v),\quad \forall v\in V_0. \end{aligned} \tag{1.31}$$

Enforcing that such derivative is equal to zero because u is a minimum of the functional, we end up with a *linear* variational problem.

Definition 1.2.12: Linear variational problem

A linear variational problem reads as:

$$u\in V\ :\ a(u,v)=\ell(v),\ \forall v\in V_0 \tag{1.32}$$

where V_0 is a vector space, V is an affine space of functions, $a: V\times V_0\to\mathbb{R}$ is a bilinear form and and $\ell: V_0\to\mathbb{R}$ is a linear form.

As a result, *the global minimiser u of a quadratic function is the solution of a linear variational problem.*

1.2.3 Well-posedness

In the previous sections, we have proved some necessary conditions for existence of solutions of a quadratic minimisation problem and, in turn, its corresponding linear variational problem. Whereas existence is not complicated in finite dimensional vector spaces, the situation is far more subtle in infinite dimensions. Let us start with a necessary condition for existence. Clearly, if a global minimiser u exist for the quadratic minimisation problem, its energy norm $\|u\|_a$ must be bounded. It leads to the following necessary condition.

Corollary 1.2.13: Necessary continuity of the linear form

If there is a global minimiser for the quadratic minimisation problem in Definition 1.2.2 with a symmetric positive definite bilinear form a, then the linear form ℓ must be continuous.

Proof. Any minimiser $u \in V_0$ of the quadratic minimisation problem satisfies the variational problem in Definition 1.2.11. If the linear form in the quadratic minimisation problem is continuous and the bilinear form is symmetric positive definite, it holds:

$$|\ell(v)| = |a(u,v)| \leq \|u\|_a \|v\|_a \leq C\|v\|_a, \tag{1.33}$$

for $C \doteq \|u\|_a < \infty$, where we have used the Cauchy-Schwarz inequality for the energy norm. □

The trial space should be large enough to find a solution but if the space is *too small*, existence of solution will not hold. The following example shows the issue.

Example 1.2.14: Non-existence of positive definite quadratic minimisation problems

Let us consider the positive definite quadratic minimisation problem

$$J \doteq \int_0^1 \frac{1}{2}u^2(x) - u(x)\mathrm{d}x = \frac{1}{2}\int_0^1 (u(x)-1)^2 - 1\mathrm{d}x, \tag{1.34}$$

and seek the global minimiser in $C_0^0([0,1])$. It can be cast in the abstract linear variational form with

$$a(u,v) \doteq \int_0^1 u(x)v(x)\mathrm{d}x, \quad \ell(v) \doteq \int_0^1 v(x)\mathrm{d}x. \tag{1.35}$$

Let us assume that $u \in V_0$ is the global minimiser of J in V_0. Now, let us consider

$$\Phi_u(x) \doteq \min\{1, 2\max\{u(x), 0\}\}, \ x \in [0,1] \tag{1.36}$$

After some algebraic manipulations, taking into account that J penalises the distance between $u(x)$ and 1, one can check that $J(\Phi_u) < J(u)$ unless $u \neq 1$, which is not possible since $1 \notin C_0^0([0,1])$. Thus, u cannot be the global minimiser and we cannot get a minimum in $C_0^0([0,1])$.
We can create a sequence $\{u_n\}_{n\in\mathbb{N}}$ with $u_0 \doteq u \in V_0$ and $u_{n+1} \doteq \Phi_{u_n}$. Thus, $J(u_{n+1}) < J(u_n)$ but the sequence has no limit in $C_0^0([0,1])$. The problem strives in the boundary conditions. If we would seek a solution in $C([0,1])$, we would just take $u(x) = 1$, but we cannot.

In the next section, we will show how to *complete* functional spaces in such a way that one can prove existence of solutions for a given quadratic minimisation problem.

1.3 Functional spaces

The motivation of this section is to define functional spaces for which the variational (or minimisation) problems above have solutions. We present here some functional spaces that solve the question of existence for some simple quadratic minimisation functionals. The broad idea is to define the largest space of functions for which the bilinear form *a has sense* and

satisfies *suitable* boundary conditions.

As commented above, a minimiser $u : \Omega \to \mathbb{R}$ of the quadratic minimisation problem must have bounded energy, i.e., $a(u,u) < \infty$. Thus, we define the space V in terms of J as follows:

$$V \doteq \{v : \Omega \to \mathbb{R} \ : \ a(v,v) < \infty\}. \tag{1.37}$$

It is the so-called *maximal functional space* on which J is defined.

1.3.1 The $L^2(\Omega)$ space

Let us consider the potential

$$J_0(u) \doteq 1/2 \int_\Omega |u(x)|^2 \mathrm{d}x. \tag{1.38}$$

The *maximal functional space* with respect to J_0 leads to

$$V_0 \doteq \{v : \Omega \to \mathbb{R} : \int_\Omega |v(x)|^2 \mathrm{d}x < \infty\}. \tag{1.39}$$

Definition 1.3.1: $L^2(\Omega)$ space

The function space (1.39) *is the space of* square-integrable *functions on* Ω*, which is represented with* $L^2(\Omega)$*. It is a normed space for*

$$\|v\|_0 \doteq \|v\|_{L^2(\Omega)} \doteq (\int_\Omega |v(x)|^2 \mathrm{d}x)^{1/2}. \tag{1.40}$$

We note that boundary values of $L^2(\Omega)$ functions are ill-posed.

Example 1.3.2: Boundary conditions cannot be imposed in $L^2(\Omega)$

Let us consider a function in $u \in C^0([0,1]) \subset L^2((0,1))$ with $u_0 \doteq u(0) \neq 0$ and $u_1 \doteq u(1) \neq 0$. Now, let us consider a sequence of perturbations $\{\tilde{u}_n\}_{n\in\mathbb{N}}$ of this function where

$$\tilde{u}_n \doteq \begin{cases} u(x) + (1-nx)(u_0 - u(0)), & 0 \leq x \leq 1/n, \\ u(x), & 1/n < x < 1 - 1/n \\ u(x) - n(1-1/n-x)(u_1 - u(1)), & 1 - 1/n < x \leq 1. \end{cases} \tag{1.41}$$

Clearly $\tilde{u}_n(0) = u_0$, $\tilde{u}_n(1) = u(1)$ for any $n \in \mathbb{N}$. On the other hand, we obtain after integration $\|\tilde{u}_n - u\|^2_{L^2((0,1))} = \frac{1}{3n}(u_0 - u(0) + u_1 - u(1)) \to 0$ as $n \to \infty$.
Thus, we can find functions arbitrary close to u in the L^2-norm that satisfy whatever boundary condition on the boundary. Thus, the L^2-norm is not strong enough to feel *the boundary conditions. It means that the space $V \doteq \{u \in L^2((0,1)) \ : \ u(0) = u(1) = 0\}$ is not a* closed *subspace of $L^2((0,1))$, i.e., we can find functions that are not in V but can be arbitrarily well approximated by functions in V (as in the example above). Another way to express this situation is saying that the linear operator that takes a solution in $L^2((0,1))$ and returns its value at one of the end-points is not continuous.*

Definition 1.3.3: Cauchy sequence

Consider a normed vector space V equipped with the norm $\|\cdot\|$. A sequence $\{v_n\}_{n\in\mathbb{N}}$ of elements of V_0 is called a Cauchy sequence *if*

$$\forall \epsilon > 0 : \exists n = n(\epsilon) \in \mathbb{N} \ : \ \|v_k - v_m\| \leq \epsilon, \ \forall k, m \geq n. \tag{1.42}$$

It is obvious to check that every convergent sequence is a Cauchy sequence. However, the equivalence between Cauchy and convergent sequences is only true for a particular type of spaces of paramount importance for the statement of well-posed variational problems.

Definition 1.3.4: Banach space

A normed vector space is called complete *if every Cauchy sequence converges. A complete normed vector space is called a* Banach space.

Definition 1.3.5: Inner product

An inner product $(\cdot,\cdot) : V \times V \to \mathbb{R}$ *in a vector space V is a symmetric positive definite bilinear form in V.*

Definition 1.3.6: Hilbert space

If a Banach space is endowed with a norm that is an energy norm with respect to a symmetric positive definite bilinear form, it is called a Hilbert space.

Let us list some examples of Banach and Hilbert spaces. The set of real numbers $\mathbb{R}$ with the modulus norm is complete. Finite dimensional spaces are also complete. The space $C^0(\Omega)$ for $\Omega \subset \mathbb{R}$ bounded endowed with the supremum norm $\|\cdot\|_\infty$, where $\|u\|_\infty \doteq \sup_{x\in\Omega} u(x)$, is complete. The space $L^2(\Omega)$ is a Hilbert space.

Completeness is the essential ingredient that is needed to prove the existence of a minimiser for the quadratic minimisation problem in Definition 1.2.2 (and thus, a solution of the variational problem in Definition 1.2.11).

Theorem 1.3.7: Existence and uniqueness of solutions in Hilbert spaces

Let us consider a Hilbert space V_0 endowed with the inner product $a : V_0 \times V_0 \to \mathbb{R}$ and a linear functional $\ell : V_0 \to \mathbb{R}$. The quadratic minimisation problem

$$u = \operatorname*{argmin}_{v\in V_0} J(v),\ J(v) \doteq 1/2a(v,v) - \ell(v) \tag{1.43}$$

has a unique solution.

Proof. By Lemma 1.2.9, the quadratic functional J is bounded below. Thus, we can define a sequence $\{v_n\}_{n\in\mathbb{N}}$ such that

$$|J(v_n) - \mu| \leq 1/n, \quad \mu \doteq \inf_{v\in V_0} J(v). \tag{1.44}$$

On the other hand, due to the bilinearity of a, we obtain

$$\begin{aligned} &\frac{1}{2}(J(v) + J(w)) - J(1/2(v+w)) && (1.45)\\ &= 1/4\,(a(v,v) + a(w,w) - 2a(1/2(v+w), 1/2(v+w)) && (1.46)\\ &= 1/8\|v-w\|_a. && (1.47)\end{aligned}$$

Clearly, $J(1/2(v+w)) \geq \mu$, which combined with the previous results leads to

$$\begin{aligned} 1/8\|v_k - v_m\|_a^2 &\leq 1/2(J(v_k) + J(v_m)) - \mu && (1.48)\\ &\leq 1/2(1/k + 1/m) \leq \max\{1/k, 1/m\}. && (1.49)\end{aligned}$$

Thus, $\{v_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence and

$$u \doteq \lim_{n\to\infty} v_n \in V_0 \tag{1.50}$$

due to completeness of V_0. Since J is a continuous functional in V_0, we have that

$$J(u) = J(\lim_{n\to\infty} v_n) = \lim_{n\to\infty} J(v_n) = \mu. \tag{1.51}$$

Thus, $u \in V_0$ is a global minimiser of the problem at hand. Uniqueness is proved using Lemma 1.2.5. □

We can observe that the problem in Example 1.3.2 was ill-posed in $C^0([a,b])$ but it is well-posed in $L^2((a,b))$. The space $C^0([a,b])$ was *too small*; it did not include the limits of Cauchy sequences, i.e., not complete. In fact, a quadratic minimisation problem can always be *fixed* by *completing* the vector space, which means to augment the space by including also all the potential limits of Cauchy sequences in it.

Definition 1.3.8: Dense space

A subset $W \subset V$ is dense *in a normed vector space V if V is the union of W and all the limits of sequences in W.*

Theorem 1.3.9: Completion of a normed vector space

For every normed space V_0 there is a unique complete vector space $\tilde{V}_0$ (up to isomorphisms) that contains V_0 as a dense subspace.

These results provide a constructive way to create well-posed minimisation problems. We start with an admissible space V_0 of functions with bounded energy (see (1.37)). Next, we consider the completion $\tilde{V}$ of V with respect to the energy norm. $\tilde{V}$ is complete by definition, and thus, the problem is well-posed in $\tilde{V}$ by Theorem 1.3.7. For instance, in the case of Example 1.3.2, we should consider the completion of $C^0([0,1])$ with respect to $a(u,u) = \int_0^1 u(x)v(x)\mathrm{d}x$. On the other hand, we know that the space in which this problem is well-posed in $L^2((a,b))$. The following result give sense to these two observations.

Theorem 1.3.10: $L^2(\Omega)$ as completion of $C^0(\Omega)$

Given $\Omega \subset \mathbb{R}^d$, the completion of $C^0(\Omega)$ with respect to $\|\cdot\|_{L^2(\Omega)}$ is the space $L^2(\Omega)$.

1.3.2 The $H^1(\Omega)$ space

Definition 1.3.11: Gradient of a function

Given a function $f : \Omega \subset \mathbb{R}^d \to \mathbb{R}$, we define its gradient as $\boldsymbol{\nabla} f(x) \doteq [\partial f/\partial x_1(x), \dots, \partial f/\partial x_d(x)]^T \in \mathbb{R}^d$ for $x \in \Omega$.

We can now proceed analogously for the semi-positive definite bilinear form

$$a(u,v) \doteq \int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x)\mathrm{d}x.$$

The corresponding maximal functional set for the semi-norm endowed by this inner product reads

$$V_0 \doteq \{v : \Omega \to \mathbb{R} \ : \ v = 0 \text{ on } \partial\Omega, \ \int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x < \infty\}. \quad (1.52)$$

Definition 1.3.12: Sobolev space

A Sobolev space is a vector space of function endowed with a norm that combines L^p norms of the function itself and its derivatives up to a given order.

Definition 1.3.13: Sobolev space $H_0^1(\Omega)$

The function space (1.52) *is the space of* square integrable *functions with* square integrable *gradients on Ω that vanish on $\partial\Omega$, which is represented with $H_0^1(\Omega)$. It is a semi-normed space for*

$$|v|_{H^1(\Omega)} \doteq \left(\int_\Omega |\boldsymbol{\nabla} v(x)|^2 \mathrm{d}x \right)^{1/2}. \quad (1.53)$$

We note that we have started considering the space $H_0^1(\Omega)$, in which the zero subscripts means zero value on $\partial\Omega$. The control provided by the semi-norm $\|\cdot\|_{H^1(\Omega)}$ is enough to make boundary conditions meaningful. For instance, if we consider Example 1.3.2, we can observe that $|u - u|_{H^1((0,1))} = n(u_0 - u(0) + u_1 - u(1)) \to \infty$ as $n \to \infty$. Thus, the H^1-seminorm *feels* the boundary value, since it cannot be changed without changing the energy of the function.

Now, we want to consider more general boundary values, not just zero on $\partial\Omega$. We eliminate the boundary condition and add an additional to the semi-norm $|\cdot|_{H^1(\Omega)}$ the norm $\|\cdot\|_0$ to end up with a new norm.

Definition 1.3.14: The $H^1(\Omega)$ space

The Sobolev *space*

$$H^1(\Omega) \doteq \{v \in L^2(\Omega) \ : \int_\Omega |\boldsymbol{\nabla} v(x)|^2 \mathrm{d}x < \infty\} \tag{1.54}$$

is a normed space with

$$\|v\|^2_{H^1(\Omega)} \doteq \|v\|^2_0 + |v|^2_{H^1(\Omega).} \tag{1.55}$$

$H^1(\Omega)$ is the maximal function space with respect to the norm $\|v\|_{H^1(\Omega)}$. Analogously as $L^2(\Omega)$, the $H^1(\Omega)$ space can be defined by completion.

Theorem 1.3.15: $H^1(\Omega)$ and $H^1_0(\Omega)$ by completion

Given a piecewise smooth domain Ω, the space $H^1(\Omega)$ is the completion of $C^\infty(\Omega)$ with respect to the norm $\|\cdot\|_{H^1(\Omega)}$. For a bounded domain $\Omega \subset \mathbb{R}^d$, $H^1_0(\Omega)$ is the completion of $C^\infty_0(\Omega)$ with respect to the seminorm $|\cdot|_{H^1(\Omega)}$.

Thus, the space of smooth functions $C^\infty(\Omega)$ and $C^\infty_0(\Omega)$ are dense in $H^1(\Omega)$ and $H^1_0(\Omega)$, respectively.

We note that $|\cdot|$ is a semi-norm because $|v| = 0$ for v a non-zero constant, violating the definiteness condition. However, it is a norm in the subspace of function of V with zero mean value.

Example 1.3.16: Piecewise continuous functions in $H^1(\Omega)$

We observe that the space $H^1(\Omega)$ includes functions that do not posses classical derivatives, *i.e., they are not differentiable at all points. For instance, let us consider a* piecewise *function in* $[0,1]$

$$u(x) = \begin{cases} 2x, & 0 < x < 1/2, \\ 2(1-x), & 1/2 \leq x < 1. \end{cases} \tag{1.56}$$

This function belongs to $H^1(\Omega)$ since

$$|u|_{H^1(\Omega)} = \int_0^1 |u(x)|^2 \mathrm{d}x = 4 \leq \infty. \tag{1.57}$$

In general, it can be checked that the space $C^1_{\mathrm{pw}}(\bar{\Omega})$ of functions with piecewise continuous first derivatives is a subset of $H^1(\Omega)$.

1.4 A multidimensional problem

At this point, we are in position to consider the multi-dimensional version of the model problem in (1.4), which models the normal displacement u of a membrane under a normal external pressure f and prescribed displacement on the boundary; we consider $\kappa = 1$ and zero boundary conditions for simplicity. This problem is represented by the quadratic minimisation problem with the functional

$$J(u) = 1/2 \int_\Omega |\boldsymbol{\nabla} u(x)|^2 - f(x)u(x)\mathrm{d}x. \tag{1.58}$$

Thus, the energy norm of this problem is $\|\cdot\|_a^2 \doteq a(u,u)$ for

$$a(u,v) \doteq \int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x)\mathrm{d}x, \tag{1.59}$$

whereas the corresponding linear form reads

$$\ell(u) \doteq \int_\Omega f(x)u(x)\mathrm{d}x. \tag{1.60}$$

Thus, we consider the maximal functional space for this energy, i.e., the space of functions with bounded energy, which we know now that is $H^1(\Omega)$. The subspace of functions in $H^1(\Omega)$ that satisfy zero boundary conditions is $H_0^1(\Omega)$ and thus, this is going to be the test space.

As proved in Corollary 1.2.13, the continuity of the linear form is necessary for the existence of a global minimiser. Assuming that $f \in L^2(\Omega)$, using the Cauchy-Schwarz inequality we readily get:

$$\int_\Omega f(x)v(x)\mathrm{d}x \leq (\int_\Omega |f(x)|^2)^{1/2}(\int_\Omega |v(x)|^2)^{1/2} = \|f\|_0\|v\|_0,\ v \in H_0^1(\Omega), \tag{1.61}$$

where $\|f\|_0 < \infty$. We note that the continuity must be in terms of the energy (semi)norm $|\cdot|_{H^1(\Omega)}$ but the above result is bounded with respect to the norm $\|\cdot\|_0$. The following classical inequality solves this issue.

Theorem 1.4.1: First Poincarè-Friedrichs inequality

Given a bounded domain $\Omega \subset \mathbb{R}^d$, it holds

$$\|u\|_0 \leq \mathrm{diam}(\Omega)\|\boldsymbol{\nabla} u\|_0,\ \ \forall u \in H_0^1(\Omega). \tag{1.62}$$

Proof. We can prove this result by relying on the fact that smooth functions in $C_0^\infty(\bar{\Omega})$ are dense in $H_0^1(\Omega)$. If the result holds for these smooth functions, it readily holds for $H_0^1(\Omega)$, using the definition of density; such strategy is common in functional analysis and is called a *density argument*. We show the result for $d = 1$ for the sake of simplicity. Using the fundamental theorem of calculus, we have:

$$u(x) = u(0) + \int_0^x u'(s)\mathrm{d}s,\ 0 \leq x \leq 1, \forall u \in C^0(\bar{\Omega}). \tag{1.63}$$

Using the fact that $u(0) = 0$ for $u \in C_0^\infty(\bar{\Omega})$, we get, using the Cauchy-Schwarz inequality

$$\|u\|_0^2 = \int_0^1 \left|\int_0^1 u'(s)\mathrm{d}s\right|^2 \mathrm{d}x \leq \int_0^1 \left(\int_0^x 1\mathrm{d}s \cdot \int_0^1 |u'(s)|^2\mathrm{d}s\right)^2 \mathrm{d}x \leq \|u'\|_0^2. \tag{1.64}$$

□

It leads to the following result.

Corollary 1.4.2: Admissible forcing term

The linear functional $\int_\Omega f(x)u(x)\mathrm{d}x$ *with* $f \in L^2(\Omega)$ *is continuous in* $H_0^1(\Omega)$.

Corollary 1.4.3: $|\cdot|_{H^1(\Omega)}$ **is a norm in** $H_0^1(\Omega)$

The semi-norm $|\cdot|_{H^1(\Omega)}$ *is a norm in* $H_0^1(\Omega)$.

Proof. Due to the Poincarè-Friedrichs inequality in 1.4, we have that

$$\|u\|_{H^1(\Omega)} \leq (\mathrm{diam}(\Omega)+1)|u|_{H^1(\Omega)}. \tag{1.65}$$

□

Now, let us consider non-homogeneous boundary conditions

$$u(x) = g(\boldsymbol{x}),\ \forall x \in \partial\Omega, \tag{1.66}$$

where $g : \partial\Omega \to \mathbb{R}$ is the boundary value to be prescribed on the boundary. Let us define the trial space $H_g(\Omega) \doteq \{v \in H^1(\Omega)\ :\ v = g\ \text{ on } \partial\Omega\}$. The way we understand the equality in the boundary conditions is also weak, and the regularity assumptions over g and why this boundary conditions have sense are out of the scope of the book. The interested student can look for *trace theorems in Sobolev spaces* for more information.

Taking the directional derivatives of the quadratic functional and enforcing them to be zero, we end up with the following variational formulation:

$$u \in H_g^1(\Omega)\ :\ \int_\Omega \boldsymbol{\nabla} u(x)\cdot\boldsymbol{\nabla} v(x)\mathrm{d}x = \int_\Omega f(x)v(x),\ \forall v \in H_0^1(\Omega). \tag{1.67}$$

As commented above, this problem can also be stated using the *offset function* method. Pick a function $u_0 \in H_g(\Omega)$, and re-state the problem

as:

$$\delta u \in H_0^1(\Omega) \ : \ \int_\Omega \boldsymbol{\nabla} \delta u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x \tag{1.68}$$

$$= \int_\Omega f(x) v(x) - \int_\Omega \boldsymbol{\nabla} u_0(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x, \ \forall v \in H_0^1(\Omega), \tag{1.69}$$

and return $u = u_0 + \delta u$. It is obvious to check that the additional right-hand side term due to boundary conditions is continuous, since $u_0 \in H^1(\Omega)$.

Clearly, this problem is a linear variational problem with $V_0 \doteq H_0^1(\Omega)$,

$$a(u, v) \doteq \int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x, \tag{1.70}$$

and

$$\ell(v) \doteq \int_\Omega f(x) v(x) \mathrm{d}x - a(u_0, v) \tag{1.71}$$

for $f(x) \in L^2(\Omega)$ and $u_0 \in H_g^1(\Omega)$. It is obvious to check that ℓ is continuous in $H_0^1(\Omega)$. As a result, the energy norm of the problem is $\| \cdot \|_a \doteq | \cdot |_{H^1(\Omega)}$, which is in fact a norm in $H_0^1(\Omega)$ due to the first Poincare-Friedrichs inequality.

We note that the regularity $f(x) \in L^2(\Omega)$ is sufficient for well-posedness but not necessary. Instead, we could just consider $f : H_0^1(\Omega) \to \mathbb{R}$ to be a linear and continuous functionals, i.e., $f(v) < \infty$ for any $v \in H_0^1(\Omega)$; the application of f to v can still be symbolically represented using integration, i.e., $f(v) = \int_\Omega f(x) v(x)$. The vector space of these bounded functionals is the *dual* space of $H_0^1(\Omega)$ and is usually represented with $H^{-1}(\Omega)$. It is a Banach space (normed and complete) with norm

$$\| f \|_{H^{-1}(\Omega)} \doteq \sup_{v \in H_0^1(\Omega)} \frac{f(v)}{\| v \|_{H^1(\Omega)}} \tag{1.72}$$

We have the following very important result that shows that *primal* and dual spaces are *isometrically isomorphic*.

Theorem 1.4.4: Riesz representation theorem

For a linear continuous functional $\ell : V \to \mathbb{R}$ in a real Hilbert space V endowed with the inner product $a(\cdot,\cdot)$ and corresponding norm $\|\cdot\|_a$, there exists a unique $u \in V$ such that

$$a(u,v) = \ell(v), \qquad \|u\|_a = \sup_{v\in V} \frac{\ell(v)}{\|v\|_a} \doteq \|\ell\|_{a'}. \tag{1.73}$$

Proof. The existence and uniqueness of a solution for the linear variational problem has already been proved above. With regard to the second part, the one related to the equivalence between the primal norm of the solution and the dual norm of the linear form, we proceed as follows. First, due to the Cauchy-Schwarz inequality, we have $|\ell(v)| = |a(u,v)| \leq \|u\|_a \|v\|_a$ and thus $\sup_{v\in V} \frac{\ell(v)}{\|v\|_a} \leq \|u\|_a$ for any $v \in V$. The supremum is attained since $\ell(u) = \|u\|_a^2$. It proves the theorem. □

Corollary 1.4.5: Well-posedness of a 2nd order elliptic problem

The variational formulation (1.68) has a unique solution for $f \in H^{-1}(\Omega)$ and $u_0 \in H^1(\Omega)$.

Example 1.4.6: Load force

Let us consider the unit interval $[0,1]$. It is obvious to check that the Dirac delta $\delta_s(v) \doteq v(s)$ for $0 < s < 1$ is linear but does not belong to $L^2((0,1))$. On the other hand, it is possible to check that in 1D the functions in $H_0^1(\Omega)$ are continuous and thus, $\delta(\cdot) \in H^{-1}((0,1))$. It has some physical implications, e.g., one can consider the elastic bar problem with a point load whereas it does not have sense in the strong form of the problem.

1.5 Boundary value problem

In this section, we will go from the variational formulation to its corresponding boundary value problem and its corresponding partial differential equation. As we did in the introduction for a 1D problem, it will require some regularity assumptions. They key to transform the variational form into a partial differential equations is *integration by parts*. We need the following standard results.

Lemma 1.5.1: Product rule

For all $\boldsymbol{\psi} \in C^1(\bar{\Omega})^d$, $v \in C^1(\bar{\Omega})$, *it holds*

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\psi} v) = v \boldsymbol{\nabla} \cdot (\boldsymbol{\psi}) + \boldsymbol{\psi} \cdot \boldsymbol{\nabla} v. \tag{1.74}$$

Theorem 1.5.2: Gauss theorem

Let us represent with $\boldsymbol{n} : \partial\Omega \to \mathbb{R}^d$ *the outwards normal vector field on* $\partial\Omega$. *It holds:*

$$\int_\Omega \boldsymbol{\nabla} \cdot \boldsymbol{\psi}(x) \mathrm{d}x = \int_{\partial\Omega} \boldsymbol{\psi}(s) \cdot \boldsymbol{n}(s) \mathrm{d}s, \quad \forall \boldsymbol{\psi} \in C^1(\bar{\Omega})^d. \tag{1.75}$$

where $\mathrm{d}s$ *denotes integration with respect to the surface measure.*

Theorem 1.5.3: Green's first formula

For all $\boldsymbol{\psi} \in C^1(\bar{\Omega})^d$, $v \in C^1(\bar{\Omega})$, *it holds:*

$$\int_\Omega \boldsymbol{\psi}(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x = -\int_\Omega \boldsymbol{\nabla} \cdot (\boldsymbol{\psi}(x)) v(x) \mathrm{d}x + \int_{\partial\Omega} \boldsymbol{\psi}(s) \cdot \boldsymbol{n}(s) v(s) \mathrm{d}s. \tag{1.76}$$

At this point, if we assume that $u \in C^2(\bar{\Omega})$ and thus, $\boldsymbol{\nabla} u \in C^1(\Omega)$, we can use Green's first formula to get:

$$\int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x \tag{1.77}$$

$$= -\int_\Omega \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} u(x)) v(x) \mathrm{d}x, \quad \forall v \in C_0^1(\bar{\Omega}), \tag{1.78}$$

using the fact that the boundary terms vanish because $v = 0$ on $\partial\Omega$. As a result, using the variational formulation (since $C_0^1(\bar{\Omega}) \subset H_0^1(\Omega)$) and assuming that $f \in C^0(\Omega)$, we get

$$\int_\Omega \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x) - f(x)v(x)\mathrm{d}x = 0, \ \forall v \in C_0^1(\Omega). \tag{1.79}$$

Lemma 1.5.4: Fundamental lemma of calculus of variations

If a function $f \in C^0(\Omega)$ is such that

$$\int_a^b f(x)v(x)\mathrm{d}x = 0, \ \forall v \in C_0^\infty(\bar{\Omega}) \tag{1.80}$$

then $f(x) = 0$ for any $x \in \Omega$.

As a result, if the solution of the variational formulation is in $C^2(\Omega)$, it satisfies the following boundary value problem:

$$-\Delta u = f \quad \text{in} \ \ \Omega, \quad u = g \quad \text{on} \ \ \partial\Omega. \tag{1.81}$$

Δ defined as $\Delta v \doteq \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} v)$ is the so-called *Laplacian* operator.

Solutions of (1.81) are called *classical (or strong)* solutions. If they exist, they are also solution of the variational formulation. However, the extra regularity assumption requires additional smoothness over the data (not only over the forcing term, which has been made explicit above, but also the domain Ω and the boundary value g). Summarising, the variational formulations has been proved to be well-posed, i.e., it has a unique solution in the maximal function space. The corresponding boundary value problem (1.81) is not well-posed in general, because it requires additional smoothness assumptions over the solution that are not true in general.

The general strategy to obtain the boundary value problem out of a variational formulation is to use integration by parts to transfer all derivatives over test functions to the trial functions, as above. After this process, we end up with the following re-statement of the variational equation in the following form

$$u \in V \ : \ \int T(u)v\mathrm{d}x = 0, \ \forall v \in V. \tag{1.82}$$

We note that the integral could involve bulk and surface integration. One can ask whether it has sense to do integration by parts for the space V. In fact, it is related to the fact that we consider derivatives *in a weak (or distributional) way*, but we do not want to go further into these concepts. When we want $T(u)$ to have classical pointwise sense, we need to enforce the additional regularity over u. The equation $T(u) = 0$ is the so-called *Euler-Lagrange* equation of the underlying functional.

1.6 Boundary conditions

So far, we have always enforced the value of the unknown $u : \Omega \to \mathbb{R}$ on the whole domain boundary $\partial\Omega$: $u = g$ on $\partial\Omega$, where we can assume that $g \in C^0(\Omega)$. These are the so-called Dirichlet boundary conditions or *essential* boundary conditions. But we can consider other types of boundary conditions too. For instance, in the model for an elastic membrane above, we could instead consider that part of $\partial\Omega$ is not clamped and instead, we provide the surface load on that boundary. Analogously, the model above also represents heat conduction, and instead of just imposing the temperature on the whole boundary, we could just prescribe the heat flux in part of the boundary. Let us see how these physically relevant boundary conditions are described in our mathematical formulations above.

Let us consider $\Gamma_0 \neq \partial\Omega$, and enforce the Dirichlet boundary condition $u = g$ on Γ_0. On the other hand, let us assume that there exists an offset function $u_0 \in H^1(\Omega)$ that satisfies this boundary conditions. Using the offset function method, $u - u_0 \in V_0 \doteq \{v \in H^1(\Omega) \ : \ v = g \ \text{ on } \Gamma_0\}$; clearly, V_0 is a vector space. On the other hand, we can now define a function $h : \partial\Omega \setminus \Gamma_0 \to \mathbb{R}$ and state the following linear variational problem:

$$\delta u \in V_0 \ : \ \int_\Omega \boldsymbol{\nabla}\delta u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x \tag{1.83}$$

$$= -\int_\Omega \boldsymbol{\nabla} u_0(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x \tag{1.84}$$

$$+ \int_\Omega f(x)v(x)\mathrm{d}x + \int_{\partial\Omega\setminus\Gamma_0} h(s)v(s)\mathrm{d}s, \ \forall v \in V_0. \tag{1.85}$$

h is a prescribed flux on the Neumann boundary $\partial\Omega \setminus \Gamma_0$ (e.g., a heat flux in thermal problems or surface tension in fluid/solid mechanics), and it is data (as f).

Now, since the test functions do not vanish anymore on $\partial\Omega$, we can add boundary *loads*. In order to keep a linear continuous form, the only thing that we need is that $h(v) \doteq \int_{\partial\Gamma_0} h(s)v(s)\mathrm{d}s < \infty$ for any $v \in V_0$.

Now, we are going to use the procedure defined above to recover the boundary value problem associated to this linear variational problem. Let us assume that $u \in C^2(\bar{\Omega})$, $f \in C^0(\Omega)$, and $h \in C^0(\partial\Omega \setminus \Gamma_0)$. We also need to assume that $\partial\Omega$ is such that its outward normal vector field $\boldsymbol{n}$ is in $C^0(\partial\Omega)^d$. Using first Green's formula, now keeping (part of) the boundary terms, we obtain

$$\int_\Omega (-\Delta u(x) - f(x)v(x)\mathrm{d}x + \int_{\partial\Omega\setminus\Gamma_0} (\boldsymbol{n}\cdot\boldsymbol{\nabla}u(x) - h(s))v(s)\mathrm{d}s = 0,\ \forall v \in C^1_{\Gamma_0}(\Omega). \tag{1.86}$$

where $C^1_{\Gamma_0} \doteq \{v \in C^1(\Omega)\ :\ v = 0\ \text{ on } \Gamma_0\}$. Using the fundamental lemma of calculus of variations, we get that u satisfies the following boundary value problem:

$$-\Delta u = f\ \text{ on } \Omega, \quad \boldsymbol{n}\cdot\boldsymbol{\nabla}u = h\ \text{ in } \partial\Omega\setminus\Gamma_0, \quad u = g\ \text{ on } \Gamma_0. \tag{1.87}$$

Thus, we have seen how we can define so-called *Neumann (or natural)* boundary conditions for variational formulations, i.e., via a boundary source or load term, and how it transforms into a flux boundary condition in the corresponding boundary value problem.

1.7 Further topics

In the previous presentation, I have not considered some important concepts that are out of the scope of this course. For instance, I have not talked about Lebesgue integration, Lebesque measure, and what a measurable function is. I have also omitted the concept of weak derivative and I have not been rigorous about boundary conditions; why one can, e.g., define the trace of a function in $H^1(\Omega)$, in which sense that equality is understood, or the regularity required on the boundary data g for the problem to be well-posed. It would involve to introduce trace theorems, which were also out of the scope of this course. In any case, the interested reader can just seek these keywords on the Internet and find lots of material discussing these issues.

1.8 Tutorial

1. Let us consider the problem: find u such that $-u''(x) = \delta(0)$ (where δ is the Dirac delta) in $(-1,1)$ and $u(-1) = u(1) = 0$. Do you think that this problem has sense in a strong, classical, or pointwise form? State the weak form of the problem. Can you find the solution of this problem? Hint: Use the fact that $H_0^1((-1,1)) \subset C_0^0([-1,1])$.

2. Show that pointwise evaluations of $L^2((0,1))$ are not continuous/bounded in general. Hint: Find a counterexample in a function in $L^2((0,1))$ that is not bounded.

3. We want to solve the following problem: find u such that

$$-\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\boldsymbol{u} + \boldsymbol{u} = \boldsymbol{f} \text{ in } \Omega \subset \mathbb{R}^3, \tag{1.88}$$

   for the boundary conditions $\boldsymbol{u}\cdot\boldsymbol{n} = 0$ on $\partial\Omega$. Can you obtain the weak formulation of this problem? Which functional space would you consider as trial/test space? (Hint: Maximal functional space) Which are the natural boundary conditions for this problem? (Hint: Leave free part of the boundary)

4. We want to solve the following minimisation problem: find u that minimises the functional

$$J(u) \doteq 1/2\int_\Omega |\alpha(x)^{1/2}u(x)|^2 + 1/2\int_\Omega |\beta(x)^{1/2}\boldsymbol{\nabla}u(x)|^2 \mathrm{d}x - \int_\Omega f(x)u(x)\mathrm{d}x, \tag{1.89}$$

   with zero boundary conditions. Can you state the variational formulation? Can you provide *sufficient* conditions on α, β for the problem to be well-posed?

Chapter 2

Discretisation

In the previous section, we have presented different ways to look at mathematical models that involve partial differential equations. We have observed that, for the elliptic problems, we can state the same problem as a minimisation problem, a variational problem or a boundary value problem. We have also observed that these formulations are equivalent only under special circumstances, i.e., when we have enough regularity. We have been able to show the well-posedness of the variational (and minimisation) problems, and shown that the choice of the right functional space is essential.

We have learned that variational formulations allow one to understand the problem in a weaker (non-pointwise) sense, which allows one to solve more general problems. This problem has clear *practical* implications. As an example, the solution of a clamped elastic structure in an L-shaped domain does not have a solution in classical sense, since the stresses in the inner corner are infinite.

Even though the variational formulations have all the nice properties commented so far, it is still impossible in general to find an analytical solution for them. These problems are infinite-dimensional and cannot be mapped to computers. A computer can only perform floating point operations with finite precision. This has motivated whole fields of mathematics, namely numerical analysis and scientific computing. These fields are about the design and analysis of *approximations* of mathematical models, with applications in almost any scientific discipline. They are part of a broad scientific area called *computational science*, which has become the third pillar of science after traditional theory and experimentation.

In this course, we are especially focused on the numerical approximation of partial differential equations. The idea is simple, try to get the most accurate approximation of a partial differential solution with the minimum computational cost. The spectral and finite element methods that we will study in this course rely on the variational formulation of a mathematical model. It is a clear difference with respect to finite difference methods that work on the strong form. It also motivates *why* we have started this course with an introduction to *variational forms and functional spaces.*

We start this section with an abstract discretisation framework (the Galerkin method) that makes use of finite-dimensional approximations of our variational problem. Next, we will consider two different ways to generate *accurate* finite-dimensional spaces, namely *spectral Galerkin* methods and *finite element* methods. For the time being, we will restrict these constructions to one-dimensional problems, since its multi-dimensional generalisation require some technicalities that will be explored in the next chapter.

We will perform a numerical analysis of the Galerkin method, showing that the error does depend on the approximability properties of the discrete space. For the finite element method in one dimension, we will obtain error estimates after proving some approximability results.

2.1 Galerkin method

The idea of Galerkin methods is quite simple. Let us recall an abstract variational formulation:

$$u \in V_g \ : \quad a(u;v) = \ell(v), \quad \forall v \in V_0. \tag{2.1}$$

As commented above, this problem is infinite dimensional. In order to *solve* this problem, let us consider *finite dimensional vector subspaces* $V_{N,0} \subset V_0$ (the vector space with homogeneous boundary conditions) and $V_N \subset V$ (without any Dirichlet boundary conditions), where $N \doteq \dim(V_N)$. Let us also consider the affine space with the boundary conditions is $V_{N,g} \subset V_N$. Now, we can solve the following problem.

Definition 2.1.1: Galerkin approximation

Let us consider the variational formulation in (2.1) and subspaces $V_{N,0} \subset V_0$ and $V_N \subset V$. The Galerkin approximation of (2.1) in $V_{N,0}$ reads:

$$u \in V_{N,g} \; : \quad a(u;v) = \ell(v), \quad \forall v \in V_{N,0}. \tag{2.2}$$

We can readily check that if the variational formulation is linear and well-posed (which now we can check using the results in the previous chapter), the Galerkin approximation is also well-posed (see Theorem 1.2.10). We note that the Galerkin problem in (2.2) is also called the *Galerkin projection* of the problem. In fact, the previous problem can be understood as solving (2.1) in the subspace V_N.

Analogously, we could consider the discrete version of the quadratic minimisation problem in Definition 1.2.2. Besides, for non-homogeneous boundary conditions, we can analogously use at the discrete level the offset function method commented above.

$V_{N,0}$ and V_N are real vector space of finite dimension, for which we can pick a *basis*.

Definition 2.1.2: Basis of a finite dimensional vector space

Given a finite dimensional real vector space V_M, the set $\{b_1, \ldots, b_M\} \subset V_M$, $M \in \mathbb{N}$ is a basis of V_M if $\forall v \in V_M$ there is a unique set of coefficients $\{v_i\}_{i=1}^M \subset \mathbb{R}$ such that $v = v_1 b_1 + \ldots + v_M b_M$. M is equal to the dimension of V_M.

A finite dimensional functional space V_N of dimension N is isomorphic with respect to $\mathbb{R}^N$. Such an isomorphism can be defined by considering an *ordered* basis and mapping functions in V_N with its unique vector of coefficients $\boldsymbol{\mu} \in \mathbb{R}^N$.

In order to consider the linear system related to the Galerkin problem, let us first use the offset function method to the Galerkin formulation Definition 2.1.1. Let us also assume that the bilinear form is linear.

Definition 2.1.3: Galerkin method with offset function

Let us consider the Galerkin problem in Definition 2.1.1 for a linear bilinear form. Let us pick an offset function $u_{N,0} \in V_{N,g} \subset V_N$. The solution of the Galerkin problem reads as $u = u_{N,0} + \delta u_N$, where

$$\delta u_N \in V_{N,0} \; : \; a(\delta u_N, v_N) = \ell(v_N) - a(u_{N,0}, v_N), \;\; \forall v_N \in V_{N,0}. \tag{2.3}$$

Lemma 2.1.4: Galerkin system as linear system

We consider a basis $\mathcal{B} \doteq \left\{ b_N^1, \dots, b_N^{N_0} \right\}$ of $V_{N,0}$, where clearly $N_0 \doteq \dim(V_{N,0})$. The Galerkin problem in (2.3) is equivalent to the linear system: find $u = \sum_{i=1}^{N_0} \mu_i b_N^i$ with

$$\begin{aligned} \boldsymbol{\mu} \in \mathbb{R}^{N_0} \quad : \quad & \boldsymbol{A}\boldsymbol{\mu} = \boldsymbol{f}, \quad \text{where} \\ & \boldsymbol{A} \in \mathbb{R}^{N_0 \times N_0}, \quad \boldsymbol{A}_{ij} \doteq a(b_N^j, b_N^i), \quad i, j \in \{1, \dots, N_0\}, \\ & \boldsymbol{f} \in \mathbb{R}^{N_0}, \quad \boldsymbol{f}_i \doteq \ell(b_N^i), \quad i \in \{1, \dots, N_0\}. \end{aligned} \tag{2.4}$$

Proof. Let us consider the solution $u \in V_{N,0}$ of (2.2), and its unique expression $u = \sum_{i=1}^{N_0} \mu_i b_N^i$. Using (2.2) with this expression of u as a linear combination of elements in $\mathcal{B}$ and using as test function the elements of the basis, we get

$$a\left(\sum_{j=1}^{N_0} \mu_j b_N^j, b_N^i \right) = \boldsymbol{A}_{ij}\boldsymbol{\mu}_j = \ell(b_N^j) = \boldsymbol{f}_j, \quad \forall j \in \{1, \dots, N_0\}. \tag{2.5}$$

Thus, it solves the linear system. On the other hand, for any $v \in V_{N,0}$, we can write it as $v = \sum_{n=1}^{N_0} \nu_i b_N^i$. Multiplying (2.5) times ν_j and adding up for $j = 1, \dots, N_0$, we readily check that the variational equation (2.2) holds. □

We note that the choice of the basis $\mathcal{B}$ *does not affect* the solution u of (2.2) but it does affect the matrix $\boldsymbol{A}$, the right-hand side $\boldsymbol{f}$ and the solution vector $\boldsymbol{\mu}$. In short, it determines the isomorphism between $V_{N,0}$ and $\mathbb{R}^{N_0}$.

2.2 Spectral Galerkin methods

Spectral Galerkin methods use as approximation for the infinite-dimensional vector space V (and V_0) the complete set of polynomials up to a given order that vanish on the boundary. For simplicity, let us consider that $\Omega \subset \mathbb{R}$, even though the generalisation to d-cubes is straightforward. We choose V_N to be the set of polynomials up to order p in $\mathbb{R}$, which is represented with $\mathcal{P}_p\left(\mathbb{R}^d\right) \doteq \text{span}\{1, x, \ldots, x^p\}$. In order to enforce boundary conditions, we consider $V_{N,0} \doteq \mathcal{P}_p\left(\mathbb{R}\right) \cap C_0^0(\overline{\Omega})$. We note that the space of polynomials $\mathcal{P}_p\left(\mathbb{R}\right)$ is a vector space of dimension $p+1$. On the other hand, the imposition of the zero boundary conditions at the end-points of Ω reduces the dimension in two, since they involve two indepedent restrictions over such space. As a result $N \doteq p+1$ and $N_0 \doteq p-1$.

Example 2.2.1: Choice of the basis in finite dimension

As commented in the previous section, the choice of the basis for our finite dimensional space does not affect the solution. This assertion would be certainly true if computations were performed with exact arithmetics. However, this is not the case of computers, which can only perform floating point operations up to a finite precision. Thus, in practise, the choice of the basis can dramatically affect the solution *due to rounding errors. One example is the basis for the polynomial spaces. For instance, one can easily check that*

$$V_{N,0} = \text{span}\left\{1 - x^2, x(1-x^2), \ldots, x^{p-2}(1-x^2)\right\}.$$

However, such monomial-like basis is highly ill-conditioned and useless for high values of p. Instead, one must consider other polynomial bases like Legendre polynomials. In any case, we are not going to explore this issue here.

In practical applications, the right-hand side will have a general expression. The matrix can also involve physical parameters, e.g., a non-constant heat conductivity or Young's modulus. So, in general, we want to have a general procedure for numerical integration of functions in terms of floating point of operations that can easily be implemented in computers. Thus, we can replace integrals by an m-point quadrature for-

mula on $\Omega \doteq [a,b] \subset \mathbb{R}$, $m \in \mathbb{N}$,

$$\int_a^b f(x)\mathrm{d}x \approx Q_m^{[a,b]}(f) \doteq \sum_{j=1}^{m} \omega_j^m f(\xi_j^m),$$

where ω_j^m are the quadrature *weights* and ξ_j^m are the quadrature *points*. The optimal choice for these weights and quadratures in the domain $[-1,1]$ is the m-point Gauss quadrature, which is exact up to polynomials of degree $2m-1$. We note that the integral over a general interval $[a,b]$ can be written as

$$\int_a^b f(x)\mathrm{d}x = \frac{b-a}{2}\int_{-1}^{1} f(\xi)\mathrm{d}\xi,$$

and now apply the Gauss quadrature formula. This way, we can state the spectral Galerkin method in terms of floating point operations only, and thus, solve it using computers.

Non-homogeneous boundary conditions in the spectral Galerkin method can be applied as follows. Given the boundary condition

$$u(a) = u_a, \quad u(b) = u_b$$

on the end-points of $[a,b]$, we need to find a polynomial that *goes through* these two points, i.e., that interpolates these values. For two points, we need at least a polynomial in $\mathcal{P}_1(\mathbb{R})$. So, let us consider the *unique* first order interpolation polynomial for the data (a,u_a), (b,u_b) (thus satisfying the boundary conditions), which has the following expression

$$u_0(x) = \frac{bu_a - au_b}{b-a} + \frac{u_b - u_a}{b-a}x.$$

In the next definition, we state the spectral Galerkin method.

Definition 2.2.2: Spectral Galerkin method with offset function

Let us consider the continuous problem in (2.1) where a is a bilinear form. Let us consider the domain $\Omega \doteq [a,b] \subset \mathbb{R}$ and the boundary conditions $u(a) = u_a$ and $u(b) = u_b$. We define the Spectral Galerkin approximation u_p of order $p \in \mathbb{N}^+$ as follows. First, we define the offset function

$$u_{p,0}(x) = \frac{bu_a - au_b}{b-a} + \frac{u_b - u_a}{b-a}x, \qquad x \in [a,b].$$

Next, we compute

$$\begin{aligned} \delta u_p \in \mathcal{P}_p([a,b]) \cap C_0^0([a,b]) \ : \\ a(\delta u_p, v_p) = \ell(v_p) - a(u_{p,0}, v_p), \\ \forall v_p \in \mathcal{P}_p([a,b]) \cap C_0^0([a,b]). \end{aligned} \tag{2.6}$$

The Spectral Galerkin approximation finally reads $u_p \doteq u_{p,0} + \delta u_p$.

We note that we have not only defined a finite dimensional space but a *family* of spaces parameterised with the order p, i.e., $\{V_p\}_{p=1}^{\infty}$. In our simulations, we will certainly pick an order, but it will be very interesting to consider how the solution improves as we increase that order, i.e., to perform a *convergence* analysis of the solution.

2.3 Finite element methods

Spectral methods make use of global polynomials in the domain Ω to build the finite dimensional spaces in the Galerkin formulation. Instead, finite element methods consider a partition of the domain into pieces (*elements or cells* in a *mesh*) and globally continuous functions that are polynomials inside the cells, i.e., *piecewise* polynomial continuous functions.

The first ingredient in a finite element method is the *mesh*, i.e., a partition of the domain Ω. As for the spectral Galerkin method, we consider a 1D problem with $\Omega \doteq [a,b]$. The first ingredient that we require is the concept of *mesh*.

Definition 2.3.1: Mesh in $\Omega \subset \mathbb{R}$

Given a domain $\Omega \doteq [a, b] \subset \mathbb{R}$, $M \in \mathbb{N}$, *and a set of* nodes

$$\Xi_M \doteq \{a \doteq x_0 < x_1 < \ldots < x_{M-1} < x_M \doteq b\}, \tag{2.7}$$

we can define a mesh $\mathcal{M}_M$ *of* Ω *as*

$$\mathcal{M}_M \doteq \{(x_{j-1}, x_j), \, : \, 1 \leq j \leq M\}. \tag{2.8}$$

The open sub-intervals (x_{j-1}, x_j) *are the* cells *of* $\mathcal{M}_M$, *with cell* size $h_j \doteq |x_j - x_{j-1}|$. *The mesh* width *is* $h \doteq \max_{j \in \{1,\ldots,M\}} h_j$. *In the particular case in which all cells have the same size, i.e.,* $h_j \doteq h$ *for any* $j \in \{1, \ldots, M\}$, *the mesh is called* uniform.

On top of the 1D mesh, let us create a finite dimensional space $V_{N,0}$. In order to do that, we define the following function.

Definition 2.3.2: Hat function in 1D linear finite elements

Given a mesh $\mathcal{M}_{N+1}$, for every interior node x_j, $j = 1, \dots, N$, we define its corresponding hat function b_N^j as

$$b_N^j \doteq \begin{cases} \frac{x - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \leq x < x_j, \\ 1 - \frac{x - x_j}{x_{j+1} - x_j}, & x_j \leq x < x_{j+1}, \\ 0 & \text{otherwise}, \end{cases} \tag{2.9}$$

At the end-points, i.e., $j \in \{0, N+1\}$, we consider the hat functions as

$$b_N^0(x) \doteq \begin{cases} 1 - \frac{x-a}{h_1} & a \leq x \leq x_1 \\ 0 & \text{otherwise}, \end{cases} \tag{2.10}$$

$$b_N^{N+1}(x) \doteq \begin{cases} 1 - \frac{b-x}{h_{N+1}} & x_N \leq x \leq b, \\ 0 & \text{otherwise}. \end{cases} \tag{2.11}$$

The linear finite element space with respect to $\mathcal{M}_{N+1}$ is defined as

$$V_N \doteq \left\{ b_N^0, b_N^1, \dots, b_N^{N+1} \right\}, \qquad V_{N,0} \doteq \left\{ b_N^1, \dots, b_N^N \right\}.$$

It is obvious to check that $V_{N,0}$ vanishes at the end-points. We can also observe that the hat functions are continuous and piecewise linear polynomials. In fact, the hat function b_N^j associated to node x_j is equal to zero at all cells of the mesh $\mathcal{M}_{N+1}$ but the ones that *contain* x_j, i.e., $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$. In these two cells, the function is a first order polynomial, reason why it is called a linear finite element space. We can also re-state the global finite element spaces as

$$\begin{aligned} V_N &\doteq \left\{ v \in C^0([a,b]) \ : \ v_{[x_{j-1}, x_j]} \in \mathcal{P}_1([x_{j-1}, x_j]), \ j = 1, \dots, N \right\}, \\ V_{N,0} &\doteq V_N \cap C_0^0([a,b]). \end{aligned} \tag{2.12}$$

On the other hand, we can also check that $b_N^j(x_i) = \delta_{ij}$, i.e., hat functions take the value one in their corresponding node and zero at all other nodes. In finite element method, the basis $\mathcal{B}_N$ that satisfy this property is the basis of *shape functions*, that we will define below.

We also know from the first chapter that the hat functions are in $H^1(\Omega)$. Thus, $V_N \subset H^1((a,b))$ and $V_{N,0} \subset H^1_0((a,b))$. The derivative of the interior hat function b_N^j takes the following value

$$\frac{\mathrm{d}b_N^j}{\mathrm{d}x}(x) \doteq \begin{cases} \frac{1}{h_j}, & x_{j-1} \leq x < x_j \\ -\frac{1}{h_{j+1}}, & x_j \leq x \leq x_{j+1} \\ 0, & \text{otherwise.} \end{cases} \tag{2.13}$$

Similarly for the end-point shape functions. Let us remark that *finite element spaces could not be used if we would require a pointwise well-defined (classical) derivative*. The fact that we will only need our space to be a subset of $H^1(\Omega)$ is what allow us to use finite element spaces (for partial differential equations that involve at most second order derivatives in their strong form).

Definition 2.3.3: Finite element method with offset function

Let us consider the continuous problem in (2.1) where a is a bilinear form. Let $\Omega \doteq [a,b] \subset \mathbb{R}$ and the boundary conditions $u(a) = u_a$ and $u(b) = u_b$. Given a mesh $\mathcal{M}_{N+1}$, we build the finite element spaces V_N and $V_{N,0}$ in (2.12) . With these ingredients, we define the finite element approximation u_N as follows. First, we define the offset function

$$u_{N,0}(x) = u_a b_N^0 + u_b b_N^{N+1}.$$

Next, we compute

$$\delta u_N \in V_{N,0} \ : \ a(\delta u_N, v_N) = \ell(v_N) - a(u_{N,0}, v_N), \ \forall v_N \in V_{N,0}. \tag{2.14}$$

The finite element approximation finally reads $u_N \doteq u_{N,0} + \delta u_N$.

2.3.1 Computing the entries of the linear system

In this section, we are going to apply the finite element method to a very simple problem, and compute by hand the matrix and right-hand side of this problem.

Example 2.3.4: 1D model problem

We consider our 1D model problem introduced in the previous chapter:

$$u \in H_0^1((a,b)) : \int_a^b \kappa(x)\frac{\mathrm{d}u}{\mathrm{d}x}(x)\frac{\mathrm{d}v}{\mathrm{d}x}(x)\mathrm{d}x = \int_a^b f(x)v(x)\mathrm{d}x,$$

$\forall v \in H_0^1((a,b))$. *We consider homogeneous boundary conditions,* $f(x) = 1$ *and* $\kappa(x) = 1$ *for simplicity. We want to compute the system matrix for a uniform mesh with* $N+1$ *cells.*

Using Lemma 2.1.4, the entries of the matrix and right-hand side using the Galerkin method applied with the 1D linear finite element space in a uniform mesh read

$$\boldsymbol{A} = \int_a^b \frac{\mathrm{d}b_N^j}{\mathrm{d}x}(x)\frac{\mathrm{d}b_N^i}{\mathrm{d}x}(x)\mathrm{d}x,$$

Now, using the expression of the derivatives of the hat functions in (2.13) , we get

$$\boldsymbol{A}_{ij} \doteq \begin{cases} -\frac{1}{h_{i+1}}, & \text{if } j = i+1 \\ -\frac{1}{h_i}, & \text{if } j = i-1 \\ \frac{1}{h_i} + \frac{1}{h_{i+1}}, & \text{if } j = i \\ 0 & \text{otherwise,} \end{cases} \tag{2.15}$$

for $i,\ j = 1,\ldots,N$. An extremely important property of finite element methods is their *sparsity*; the entries $\boldsymbol{A}_{ij}$ of the matrix are equal to zero if $|i-j| \geq 2$. Thus, the system matrix will read:

$$\begin{bmatrix} \frac{1}{h_1}+\frac{1}{h_2} & -\frac{1}{h_2} & 0 & \ldots & & & 0 \\ -\frac{1}{h_2} & \frac{1}{h_2}+\frac{1}{h_3} & -\frac{1}{h_3} & 0 & \ldots & & 0 \\ 0 & \ddots & \ddots & \ddots & & & 0 \\ \vdots & & & & & & \vdots \\ 0 & \ddots & \ddots & & 0 & -\frac{1}{h_{N-1}} & \frac{1}{h_{N-1}}+\frac{1}{h_N} \end{bmatrix} \tag{2.16}$$

As commented above, we need a numerical quadrature for the integration of the right-hand side in general. For simplicity, let us consider the

trapezoidal rule to integrate at every cell of the mesh, i.e.,

$$\int_{x_{i-i}}^{x_i} j(x)\mathrm{d}x \approx \frac{1}{2}h_i(j(x_{i-1}) + j(x_i)).$$

Assuming that we have a subroutine that allows us to evaluate the forcing term at a point, we can compute the entries of the right-hand side for a unit force as follows:

$$\boldsymbol{f}_j = \int_a^b b_N^j(x)\mathrm{d}x = \frac{h_j + h_{j+1}}{2}, \qquad j = 1, \ldots, N.$$

In the particular case in which the mesh is uniform with a mesh size h, the linear system reads:

$$\begin{bmatrix} 2 & -1 & 0 & \ldots & & & 0 \\ -1 & 2 & -1 & 0 & \ldots & & 0 \\ 0 & \ddots & \ddots & \ddots & & & 0 \\ \vdots & & & & & & \vdots \\ 0 & \ddots & \ddots & & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \\ \vdots \\ \\ \mu_N \end{bmatrix} = h \begin{bmatrix} 1 \\ \\ \vdots \\ \\ 1 \end{bmatrix} \tag{2.17}$$

In the particular case of a 1D uniform mesh and a trapezoidal rule for the right-hand side integration, *the system that arises from finite element and finite difference schemes are identical*. However, this is not the case for general meshes and it is never the case for $d > 1$, as we will see.

Now, let us consider the non-homogeneous boundary conditions $u(a) = u_a$ and $u(b) = u_b$. Let us note that the end-point hat functions are not being used for solving the problem with homogeneous boundary conditions, they are essential to pick a suitable offset function. As commented above, we take $u_0 \doteq u_a b_N^0 + u_b b_N^{N+1}$. It is obvious to check that u_0 satisfies the right boundary conditions. The main reason why we use such technique for finite element methods is to keep *sparsity*. With this expression, the additional term to be added to the right hand side is

$$-\int_a^b \frac{\mathrm{d}b_N^j}{\mathrm{d}x}\frac{\mathrm{d}u_0}{\mathrm{d}x}\mathrm{d}x = -\int_a^b \frac{\mathrm{d}b_N^j}{\mathrm{d}x}\frac{\mathrm{d}b_N^0}{\mathrm{d}x}\mathrm{d}x - \int_a^b \frac{\mathrm{d}b_N^j}{\mathrm{d}x}\frac{\mathrm{d}b_N^{N+1}}{\mathrm{d}x}\mathrm{d}x \tag{2.18}$$

$$\doteq \begin{cases} \frac{u_a}{h_1} & j = 1 \\ \frac{u_b}{h_{N+1}} & j = N \\ 0 & j \in \{2, \ldots, N-1\}. \end{cases} \tag{2.19}$$

On the contrary, if we chose the offset function in the spectral Galerkin method, all the entries in the right hand side would be different from zero. It would imply computation of terms in all the cells of the mesh, which is a computational cost that we can avoid. On the other hand, as we will see, the finite element approach is a practical way to impose Dirichlet boundary conditions for general geometries in 2D and 3D, while it is not possible to do this with global polynomials.

2.4 Error analysis of the Galerkin method

Let us consider our linear variational problem

$$u \in V_0 \ : \ a(u,v) = \ell(v), \qquad \forall v \in V_0,$$

where we recall that V_0 is a real vector space of functions from a physical domain Ω to $\mathbb{R}$.

Assumption 2.4.1: Requirements for a well-posed linear variational problem

We assume $a : V_0 \times V_0 \to \mathbb{R}$ to be a bilinear symmetric and positive definite form and $\ell : V_0 \to \mathbb{R}$ a continuous linear form with respect to the energy norm $\|\cdot\|_a$. Furthermore, V_0 endowed with the inner product provided by a is a Hilbert space (it is complete).

Under these assumptions, we already know from Theorem 1.3.7 that there exists a unique solution $u_N \in V_0$ to Theorem 1.3.7. Now, let us consider the Galerkin discretisation of this problem, using as trial and test space the vector space $V_{N,0} \subset V_0$, $\dim V_{N,0} < \infty$. The Galerkin approximation reads:

$$u \in V_{N,0} \ : \ a(u,v) = \ell(v), \qquad \forall v \in V_{N,0}.$$

Existence and uniqueness of the discrete problem is a direct consequence of the continuous couterpart since the discrete problem inherits the requirements in Assumption 2.4.1 above (even though we already observed that the proof for the discrete case is much simpler). The remaining point in the Galerkin formulations is the definition of the discrete space $V_{N,0}$; we have learned two ways to define such space in 1D, using either the spectral Galerkin method or the finite element method.

Now, the essential questions that arise are: Which is the error we are committing with our discrete scheme? How does this error change with N?. In the following, we will analyse bounds for the error for the abstract Galerkin problem above. As we will see, the dependence of the error with respect to N does (naturally) depend on the particular construction of the discrete space $V_{N,0}$, e.g., whether we are using a spectral Galerkin or a finite element method, etc.

2.4.1 Errors in the energy norm

We want to analyse the error commited by the Galerkin method. A natural way to look at this problem is to find bounds for the norm of the error function $u - u_N$. The easiest choice for the error norm is to pick the energy norm. First, let us state what we know about u and u_N. These functions are solution of the continuous and Galerkin problems:

$$a(u, v) = \ell(v), \qquad \forall v \in V_0, \tag{2.20}$$
$$a(u_N, v_N) = \ell(v_N), \qquad \forall v \in V_{N,0}. \tag{2.21}$$

Thus, using the linearity of the bilinear form and the fact that $V_{N,0} \subset V_0$, we can also pick $v_N \in V_{N,0}$ as test function in the continuous problem. Choosing the same test function in both problems and subtracting, we readily get:

$$a(u - u_N, v_N) = 0, \qquad \forall v \in V_{N,0}. \tag{2.22}$$

This result is called *Galerkin orthogonality*; the error function is orthogonal to the discrete space $V_{N,0}$ with respect to the a-inner product.

It tells us that the Galerkin solution is the best possible solution in $V_{N,0}$ with respect to the energy norm. For any $v_N \in V_{N,0}$ we have

$$\|u - v_N\|_a^2 = \|u - u_N\|_a^2 + \|u_N - v_N\|_a^2 - 2a(u - u_N, u_N - v_N) \tag{2.23}$$
$$= \|u - u_N\|_a^2 + \|u_N - v_N\|_a^2. \tag{2.24}$$

Theorem 2.4.2: Cea's lemma

Let us assume that the boundary conditions on the Dirichlet boundary $u = g$ on Γ_0 can be exactly imposed with the discrete finite element space V_N, i.e., we can pick $u_{N,g} \in V_N$ such that $u_{N,g} = g$ on Γ_0. The Galerkin discretisation in Definition 2.1.3 under Assumption 2.4.1 satisfies

$$\|u - u_N\|_a = \inf_{v_N \in V_{N,0}} \|u - v_N\|_a.$$

Proof. First, we note that due to the assumtions in the theorem, we can pick the same offset function for both the continuous and discrete problem, thus having exactly the same right-hand side. As a result, we can use the orthogonality in (2.22). Using the bilinearity of a, we readily get

$$\|u - u_N\|_a^2 = a(u - u_N, u - u_N) = a(u - v_N, u - u_N) + a(v_N - u_N, u - u_N)$$

for any $v_N \in V_{N,0}$. The last term in this expression vanishes due to the orthogonality of the Galerkin projection. Thus, using the Cauchy-Schwarz inequality we readily get

$$\|u - u_N\|_a^2 \leq \|u - v_N\|_a \cdot \|u - u_N\|_a.$$

Dividing this expression by $\|u - u_N\|_a$, and taking the infimum with respect to v_N, we prove the result. □

This result gives us a very important piece of information. The Galerkin solution is the best possible solution in the trial space in terms of the energy norm error. As a result, the only thing that we need to check is how well functions in $V_{N,0}$ can approximate the continuous solution.

Cea's lemma also tells us that if we consider two discrete spaces $V_{N,0}$ and $V_{M,0}$ such that $V_{N,0} \subset V_{M,0}$, then the error $\|u - u_N\|$ is smaller than $\|u - u_M\|$, since

$$\inf_{v_N \in V_{N,0}} \|u - v_N\|_a \leq \inf_{v_M \in V_{M,0}} \|u - v_M\|_a.$$

For spectral Galerkin methods, the solution is reduced as we increase the order, since $V_{p+1} \subset V_p$. For finite element methods, it also holds when

refining the mesh $\mathcal{M}_{N+1}$; in 1D, it implies to split every cell into two cells, in order to get $\mathcal{M}_{2N+2}$. Thus, $V_{2N+2,0} \subset V_{N+1,0}$. As a result, we can obtain more accurate approximations of our problem by enlarging the discrete space in the Galerkin method. In any case, we still do not know how this reduction is in terms of N.

2.5 Approximation theory

As we have commented above, the question about how good is the Galerkin approximation can be determined if we can obtain information about how well functions in the discrete space approximate functions in the continuous space. This question can be answered using approximation theory. First, we are going to introduce the concept of *interpolator operator*, which takes continuous functions and provide discrete functions. We will use this interpolation operator to determine the *interpolation error* when using piecewise polynomial (finite element) spaces. This will provide a bound for the error of the Galerkin solution by the results in the previous section, i.e., Cea's lemma.

Definition 2.5.1: Interpolation operator for 1D finite elements

Given the linear 1D finite element space

$$V_{N,0} = \left\{ v \in C^0([a,b]) \ : \ v_{[x_{i-1},x_i]} \in \mathcal{P}_1([x_{i-1},x_i]) \right\},$$

we define the interpolation operator $\pi : V \to V_N$ as follows:

$$\pi(v) \doteq \sum_{i=0}^{N+1} v(x_i) b_N^i,$$

where b_N^i stands for the hat functions in Definition 2.3.2.

We can see that this operator is an interpolation operator. It has sense in 1D for $V = H^1((a,b))$ because $C^0([a,b]) \subset H^1((a,b))$ and thus, the functions have pointwise sense. Thus, given a function $v \in V$, to compute its interpolant $\pi(v) \in V_N$, we must evaluate v at the mesh nodes. These functionals (pointwise evaluations $v \mapsto v(x_i)$ for $i = 0, \ldots, N+1$) are the so-called *degrees of freedom* of the finite element space V_N.

Definition 2.5.2: Degrees of freedom

Let us consider a set of $\{\sigma_i\}_{i=0}^{N+1}$ *linear functionals in* V_N. *We say that* $\{\sigma_i\}_{i=0}^{N+1}$ *is an admissible basis of* degrees of freedom *if the operator* $I : V_N \to \mathbb{R}^{N+1}$ *such that*

$$I(v) \doteq [\sigma_0(v), \sigma_1(v), \ldots, \sigma_{N+1}(v)]^T$$

is a bijection.

Definition 2.5.3: Shape functions

Given a basis of degrees of freedom, we say that a basis $\left\{b_N^0, \ldots, b_N^{N+1}\right\}$ *of* V_N *is the basis of* shape functions *if* $\sigma_N^i(b_N^j) = \delta_{ij}$ *for* $i, j = 1, \ldots, N+1$.

It is obvious to check from the properties of the basis of degrees of freedom that there is a unique basis of shape functions. Furthermore, the definition of the shape functions in Definition 2.3.2 are the basis of shape functions for the finite element space V_N.

Now, let us prove some key interpolation theory results. First, we prove stability and next error bounds.

Lemma 2.5.4: Continuity of the 1D interpolant

The map $\pi : H^1(\Omega) \to V_{N+1} \subset H^1(\Omega)$ *is continuous (bounded) uniformly with respect to the mesh width* h *for a bounded* $\Omega \subset \mathbb{R}$.

Proof. First, let us note that $V_N \subset H^1(\omega)$ is a consequence of the fact that hat functions are in $H^1(\omega)$. Besides, functions in $H^1(\omega)$ for a bounded $\omega \subset \mathbb{R}$ are continuous in one dimension. Thus, for any $v \in H^1(\omega)$ and $x,\ y \in \overline{\omega}$, we have:

$$|v(y) - v(x)| \leq \int_x^y |v'(s)| \mathrm{d}s \leq |y - x|^{\frac{1}{2}} |v|_{H^1(\omega)}, \tag{2.25}$$

where we have used the Cauchy-Schwarz inequality. Let us pick x as the point in which $|v|$ reaches its minimum on $\overline{\omega}$. We readily have that $|v(x)| \leq |\omega|^{-\frac{1}{2}} \|v\|_{L^2(\Omega)}$; $|\omega|$ denotes the size (length) of the domain. Thus, we have, by the triangle inequality:

$$\|v\|_{\infty,\omega} \doteq \sup_{y \in \omega} |v(y)| \leq |\omega|^{-\frac{1}{2}} \|v\|_{L^2(\omega)} + |\omega|^{\frac{1}{2}} |v|_{H^1(\omega)}. \tag{2.26}$$

Therefore, pointwise evaluations are bounded in $H^1(\omega)$. As a result, $\pi : H^1(\omega) \to H^1(\omega)$ is a bounded operator in $H^1(\omega)$. Now, we can easily check that $\pi(v)'|_{[x_{i-1},x_i]} = \frac{v(x_i) - v(x_{i-1})}{h_i}$. Using the result (2.25) for $\omega \doteq [x_{i-1}, x_i]$, we get

$$|\pi(v)|_{H^1([x_{i-1},x_i])} = h_i^{-\frac{1}{2}} |v(x_i) - v(x_{i-1})| \leq |v|_{H^1([x_{i-1},x_i])}.$$

Adding up for all cells, we get

$$|\pi(v)|_{H^1(\Omega)} \leq |v|_{H^1(\Omega)}.$$

On the other hand,

$$\|\pi(v)\|_{L^2(\Omega)} \leq |b - a|^{\frac{1}{2}} \|\pi(v)\|_{\infty,\Omega}, \qquad \|\pi(v)\|_{\infty,\Omega} \leq \|v\|_{\infty,\Omega}$$

Using these expressions in (2.26) for the domain Ω, we get:

$$\|\pi(v)\|_{L^2(\Omega)} \leq \|v\|_{L^2(\Omega)} + |b - a||v|_{H^1(\Omega)} \leq c\|v\|_{H^1(\Omega)}.$$

As a result, $\|\pi(v)\|_{H^1(\Omega)} \leq c\|v\|_{H^1(\Omega)}$, and thus a continuous (bounded) operator with a constant that is independent of the mesh size h. □

The error estimates below require some regularity over the solution.

Definition 2.5.5: The $H^2(\Omega)$ space

The space $H^2(\Omega)$ is the subspace of functions in $H^1(\Omega)$ such that its second derivatives are in $L^2(\Omega)$. The corresponding norm reads:

$$\|v\|_{H^2(\Omega)} \doteq \|v\|_{H^1(\Omega)} + |\boldsymbol{\nabla} v|_{H^1(\Omega)}, \qquad |v|_{H^2(\Omega)} \doteq |\boldsymbol{\nabla} v|_{H^1(\Omega)}.$$

Lemma 2.5.6: Error bounds for the 1D interpolant

For all $v \in H^2(\Omega)$, the interpolant π in a mesh with mesh width h holds:

$$\|v - \pi(v)\|_{L^2(\Omega)} \leq h^2 |v|_{H^2(\Omega)}, \qquad |v - \pi(v)|_{H^1(\Omega)} \leq h |v|_{H^2(\Omega)}.$$

Proof. Let us consider the cell $[x_{i-1}, x_i]$ and $w_i \doteq (v - \pi(v))|_{[x_{i-1}, x_i]}$. Using the fact that $v - \pi(v)$ vanishes at the end-points of the interval, using (2.26), we prove that

$$\|v - \pi(v)\|_{L^2((x_{i-1}, x_i))} \leq h_i \|v - \pi(v)\|_{H^1((x_{i-1}, x_i))}. \tag{2.27}$$

Now, let us consider the function $v' - \pi(v)'$. We know that this function vanishes at some point of the cell, due to the mean-value theorem. On the other hand, $\pi(v)'' = 0$ on the cell, since it is a first order polynomial. Thus, we can use the previous bound also for the derivative, and obtain

$$\|v - \pi(v)\|_{H^1((x_{i-1}, x_i))} \leq h_i \|v\|_{H^2((x_{i-1}, x_i))}.$$

Combining these results and adding up for all cells in the mesh, we prove the results in the lemma. □

The following corollary is a direct consequence of the previous approximation error estimates and Cea's lemma.

Corollary 2.5.7: Error estimates for the finite element solution in 1D

Under the conditions in Cea's lemma and assuming that $\Omega \subset \mathbb{R}$ *for a linear finite element space* V_N *for a mesh with mesh width* h*, the following* a priori *error bound holds:*

$$\|u - u_N\|_{H^1(\Omega)} \leq h|u|_{H^2(\Omega)}$$

Results with respect to the $L^2(\Omega)$ norm also hold:

$$\|u - u_N\|_{L^2(\Omega)} \leq h^2\|u\|_{H^1(\Omega)}, \tag{2.28}$$

where we have weakened the norm of the error estimate and in turn improved the convergence order. We are not going to prove this result, since it involves *duality* arguments that are out of the scope of this course.

2.5.1 Higher order methods

Now that we have learned how to construct and analyse linear finite element methods, we can go one step further. We can now consider at every cell of the mesh a polynomial of an arbitrary order p. Given a $p \in \mathbb{N}$ and a mesh $\mathcal{M}_{N+1}$ of the domain $\Omega \doteq [a, b]$, we define the p-th order finite element space as:

$$V_N^p \doteq \left\{ v \in C^0([a,b]) \ : \ v_{\text{-}}[x_{i-1}, x_i] \in \mathcal{P}^p([x_{i-1}, x_i]) \right\}.$$

Now, we must define its corresponding set of degrees of freedom and its associated dual space of shape functions. It is clear that using only the mesh nodes of the *linear* mesh $\mathcal{M}_{N+1}$ is not enough to uniquely define elements of V_{n+1}^p. We need to add more degrees of freedom. We know that a function

In order to do that, let us consider the following set of DOFs

$$\begin{aligned} &\sigma_i^1 \doteq v(x_i), && i = 0, \ldots, N+1, \\ &\sigma_i^k \doteq v\left(x_{i-1} + \frac{(x_i - x_{i-1})k}{p}\right), && i = 1, \ldots, N+1, \ k = 1, \ldots, p-1 \end{aligned} \tag{2.29}$$

Clearly, for linear finite elements ($p = 1$) we recover the previous definition. For *quadratic* elements ($p = 2$), we have to add one additional node at the mid-point of each cell. For an element of order p, we add $p - 1$ equidistant nodes at each cell of the mesh. It is easy to check that this set of degrees of freedom define a bijective map between V_{N+1}^p and $\mathbb{R}^{N_p}$, with $N_p = N + (N - 1) \cdot (P - 1)$.

With respect to the shape functions, we still keep locality properties. The shape functions associated to *interior* degrees of freedom (the high order ones) σ_i^k vanish in all cells but the cell $[x_{i-1}, x_i]$. At such cell, shape functions are zero on the cell boundary and all interior nodes, i.e., $\frac{x_{i-1}-x_i}{p}, \ldots, \frac{(x_{i-1}-x_i)(p-1)}{p}$, but one. E.g., in the case of quadratic elements, there is only one interior node, one interior degree of freedom, and its corresponding shape function is a parabola that vanishes on the end-points of the cell and takes value on the mid-point. The shape functions associated to interior *linear* nodes have support on two cells, e.g., σ_i^1 for $i = 1, \ldots, N$ has support in cells $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$.It takes the value one in such nodes and vanishes in the other end-points and interior nodes of these two cells.

High-order polynomials pay the price (in fact, they are much better than mesh refinement in terms of accuracy vs. number of degrees of freedom) as soon as the solution of the problem at hand is regular enough. We can now extend the definition of the interpolant π^p to arbitrary order by simply using the set of degrees of freedom in (2.29). The following error estimates provides us very important information.

Lemma 2.5.8: Error bounds for the 1D interpolant

Given a finite element space of order p, i.e., V_N^p, on a mesh with mesh width h, the interpolant π^p holds:

$$\|v - \pi^p(v)\|_{L^2(\Omega)} \leq h^{p+1}|v|_{H^{p+1}(\Omega)}, \qquad |v - \pi^p(v)|_{H^1(\Omega)} \leq h^p|v|_{H^{p+1}(\Omega)},$$

for any $v \in H^{p+1}(\Omega)$.

Proof. The proof of this result is analogous to the one of the linear case. The idea is to obtain a similar result as (2.27) for all derivates up to order p of the error function $v - \pi^p(v)$. Next, we use the same result for its $p+1$ derivative and observe that the $p+1$ derivative of the interpolant vanishes at each cell. □

We can readily combine these interpolation errors with Cea's lemma to get the following result.

Corollary 2.5.9: Error estimates for the finite element solution in 1D

Under the conditions in Cea's lemma and assuming that $\Omega \subset \mathbb{R}$ *for a finite element space* V_N^p *of order* p *in a mesh with mesh width* h *and* $u \in H^{q+1}(\Omega)$ *for* $0 < q < p$ *, the following* a priori *error bound holds:*

$$\|u - u_N\|_{H^1(\Omega)} \leq h^q |u|_{H^{q+1}(\Omega)}.$$

2.6 Tutorial

1. We want to use a third order finite element method in 1D and integrate the matrix corresponding to the following bilinear form

$$a(u,v) \doteq \int_a^b u(x)v(x) + \boldsymbol{\nabla} u(x) \cdot \boldsymbol{\nabla} v(x) \mathrm{d}x$$

exactly. Let us consider a Gauss quadrature for the integration in every cell of the mesh. How many points would be needed in the Gauss quadrature at every cell?

2. Can you compute the system matrix of the bilinear form

$$a(u,v) \doteq \int_a^b \kappa(x) u'(x) v'(x) \mathrm{d}x,$$

in a 1D mesh, in terms of the cell mesh sizes h_i. Do a diagram as in the finite element matrix above, providing all the information needed to completely determine the matrix. Use the trapezoidal rule for the integration in each cell.

3. In a finite element code, students are told to show the error between the exact and the finite element solution (using the Galerkin method) in terms of the square of the energy norm, i.e., $\|u - u_N\|_a^2$. One student has implemented instead $\|u\|_a^2 - \|u_N\|_a^2$. Can you tell me which error is s/he committing doing that? In other words, what is the value of $\|u - u_N\|_a^2 - \|u\|_a^2 + \|u_N\|_a^2$.

4. Let us consider a linear finite element approximation of a problem with an analytical solution in $C^\infty(\Omega)$, with uniform mesh with N elements. We want a more accurate solution. We can consider to refine the mesh using *bisection*, i.e., split every cell into two cells, to get a $2N$ mesh or to consider a second order finite element space on the same mesh. What is going to be more effective in terms of error reduction? Quantify it.

Convergence plots

In the tutorials for the unit, that can be found in this Github repos, we evaluate how the error decreases when refining the mesh (h-refinement) and increasing the order (p-refinement). The main motivation is to observe how the error behaves in terms of degrees of freedom, i.e., the size of the corresponding linear system of equations, which is a measure of the computational cost.

Let us start with linear finite elements on a 1D uniform mesh with N cells. As a result, the mesh width is $\frac{1}{N}$. In this case, the number of degrees of freedom $\sharp \doteq N - 1$. Thus, using the results in Corollary 2.5.9, if our solution is in $H^2(\Omega)$, we have:

$$e_N \doteq \|u - u_N\|_a \leq \frac{C_1}{N},$$

for some constant $C > 0$, or using Landau notation, $e_N \lesssim \mathcal{O}\left(N^{-1}\right)$. We can now apply the log function on both sides of this inequality. We readily get

$$\log e_N \leq \log C_2 - \log N = C_3 - \log N.$$

If we consider now finite elements of order p on the same mesh, we can readily check that $\sharp \doteq pN - 1$, whereas $h = \frac{1}{N}$. Using the error

bounds in Corollary 2.5.9, and *assuming that* $u \in H^{p+1}(\Omega)$, we obtain

$$e_{N,p} \doteq \|u - u_N\|_a \leq \frac{C_4}{N^p}.$$

Again, if we compute the log function at both sides of the inequality, we get

$$\log e_{N,p} \leq \log C_5 - p \log N = C_6 - p \log N, \qquad \sharp = pN + 1. \tag{2.30}$$

With these bounds, we can consider the following refinements strategies:

- h-refinement: This refinement involves increasing the cells in our mesh (e.g., using bisection) keeping fixed the polynomial order p. E.g., using uniform refinement we multiply the number of degrees of freedom $\sharp$ by 2 and reduce the error by a factor $\frac{1}{2}$.

  In this situation, we have $\sharp \approx pN$ and

  $$\log e_{N,p} \leq C_6 - p \log \sharp + p \log p = C_7 - p \log \sharp.$$

  Thus, $\log e_{N,p}$ must be reduced at least linearly with slope $-p$ in terms of $\log \sharp$. As an example, using bisection, increasing $\sharp$ by two, we reduce the error by two. This is the so-called *algebraic* convergence.

- p-refinement: This refinement consists in fixing the mesh and increasing the polynomial order in the finite element method. Using the fact that $\sharp \approx pN$, we have that

  $$\log e_{N,p} \leq C_6 - p \log N = C_6 - \frac{\log N}{N} \sharp.$$

  Thus, $\log e_{N,p}$ is reduced at least linearly in terms of $\sharp$.

As a result, *if the solution is smooth enough*, p-refinement is much more effective than h-convergence. Whereas p-refinement reduces $\log e_{N,p}$ linearly with the number of degrees of freedom $\sharp$, h-refinement does it with respect to $\log \sharp$. The difference is huge!

Chapter 3

n-dimensional finite elements

At this point, we have already introduced the Galerkin method for the numerical approximation of partial differential equations. The Galerkin method requires finite dimensional subspaces of the (infinite dimensional) functional spaces in which our weak formulation is well-posed. In order to do that, we have built finite element methods for 1D problems. In this chapter we are going to extend to arbitrary dimensions the definition of finite element spaces.

3.1 The boundary value problem in weak form

We are interested in problems governed by partial differential equations (PDEs) posed in a physical domain $\Omega \subset \mathbb{R}^d$ with boundary $\Gamma \doteq \partial\Omega$. In practice $d = 2, 3$ but we are also interested in $d > 3$ for some particular applications. Let us consider a differential operator A, e.g., the Laplace operator $-\Delta$, and a force term $f : \Omega \to \mathbb{R}$. Let us also consider a partition of Γ into a Dirichlet boundary Γ_{D} and a Neumann boundary Γ_{N}, and the corresponding boundary data $u_{\mathrm{D}} : \Gamma_{\mathrm{D}} \to \mathbb{R}$ and $g_{\mathrm{N}} : \Gamma_{\mathrm{N}} \to \mathbb{R}$. The boundary value problem reads as follows: find $u(\boldsymbol{x})$ such that

$$Au(\boldsymbol{x}) = f(\boldsymbol{x}) \quad \text{in } \Omega, \tag{3.1}$$

$$B_{\mathrm{D}}u(\boldsymbol{x}) = u_{\mathrm{D}}(\boldsymbol{x}) \quad \text{on } \Gamma_{\mathrm{D}}, \tag{3.2}$$

$$B_{\mathrm{N}}u(\boldsymbol{x}) = g_{\mathrm{N}}(\boldsymbol{x}) \quad \text{on } \Gamma_{\mathrm{N}}. \tag{3.3}$$

The operator B_{D} is a trace operator[1] and B_{N} is the flux operator.[2] Other boundary conditions, e.g., Robin (mixed) conditions can also be considered. We assume that the unknown $u(\boldsymbol{x})$ in (3.1) can be a scalar, vector, or tensor field. (The case of multi-field problems is considered in Sect. 3.11.)

For finite element analysis, (3.1) must be understood in a weak sense. The weak formulation can be stated in an abstract setting. Let us consider an abstract problem determined by a Hibert space $\mathcal{X}$ (*trial space*), a continuous bilinear form $a : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and a continuous linear form $\ell : \mathcal{X} \to \mathbb{R}$. The abstract problem is stated as: find $u \in \mathcal{X}$ such that

$$a(u, v) = \ell(v), \qquad \text{for any } v \in \mathcal{X}. \tag{3.4}$$

The link between the weak and strong formulations has already been described in the previous sections. Without mathematical rigor, one can simply consider integration by parts (assuming continuous functions) to transfer derivatives from the trial to the test function. E.g., for the Laplace operator, the bilinear form reads $a(u, v) \doteq \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v \mathrm{d}\Omega$. Furthermore, homogeneous Dirichlet boundary conditions, i.e., $u = 0$ on Γ_{D}, are usually enforced in a strong way; the functions in $\mathcal{X}$ satisfy these boundary conditions. The extension to non-homogeneous boundary conditions is straightforward, using the offset function method. One can define an arbitrary extension Eu_{D} of the Dirichlet data, i.e., $Eu_{\mathrm{D}} = u_{\mathrm{D}}$ on Γ_{D}. Next, we define the function $u_0 \doteq u - Eu_{\mathrm{D}}$ with zero trace on Γ_{D} and solve (3.4) for u_0 with the right-hand side

$$\ell(v) - a(Eu_{\mathrm{D}}, v). \tag{3.5}$$

Let us consider one classical example.

[1] The trace operator tells us which are the right boundary conditions to be imposed on the boundary and in which sense do they have sense. E.g., for $H^1(\Omega)$ we can impose the full unknown in the space of traces $H^{\frac{1}{2}}(\partial\Omega)$.

[2] We have already seen how we can infer the Neumann or natural boundary conditions, e.g., using integration by parts assuming smooth trial and test functions. E.g., for problems posed in $H^1(\Omega)$, the fluxes are to be understood in $H^{-\frac{1}{2}}(\Gamma_{\mathrm{N}})$, the dual of the trace space.

Example 3.1.1: Heat equation

Let us consider the Poisson problem $-\boldsymbol{\nabla}\cdot\boldsymbol{\kappa}\boldsymbol{\nabla}u = f$ *with* $u = u_{\mathrm{D}}$ *on* Γ_{D} *and* $\boldsymbol{n}\cdot\boldsymbol{\kappa}\boldsymbol{\nabla}u = g_{\mathrm{N}}$*;* $\boldsymbol{n}$ *is the outward normal. Let us assume that* $\boldsymbol{\kappa} \in L^{\infty}(\Omega)^{d\times d}$*,* $f \in H^{-1}(\Omega)$*,* $g_{\mathrm{N}} \in H^{-\frac{1}{2}}(\Gamma_{\mathrm{N}})$*, and* $u_{\mathrm{D}} \in H^{\frac{1}{2}}(\Gamma_{\mathrm{D}})$*. Let us also consider an extension* $Eu_{\mathrm{D}} \in H^1(\Omega)$ *such that* $Eu_{\mathrm{D}} = u_{\mathrm{D}}$ *on* Γ_{D}*. The weak form of the problem reads as: find* $u_0 \in H^1_{\Gamma_{\mathrm{D}}}(\Omega)$ *(the subspace of functions in* $H^1(\Omega)$ *that vanishes on* Γ_{D}*) such that*

$$\int_{\Omega}\boldsymbol{\kappa}\boldsymbol{\nabla}u_0\cdot\boldsymbol{\nabla}v\mathrm{d}\Omega = \int_{\Omega}fv\mathrm{d}\Omega + \int_{\Gamma_{\mathrm{N}}}gv\mathrm{d}\Gamma - \int_{\Omega}\boldsymbol{\kappa}\boldsymbol{\nabla}Eu_{\mathrm{D}}\cdot\boldsymbol{\nabla}v\mathrm{d}\Omega,$$

for any $v \in H^1_{\Gamma_{\mathrm{D}}}(\Omega)$*. The solution is* $u \doteq u_0 + Eu_{\mathrm{D}}$*.*

3.2 Space discretization with finite elements

Problem (3.4) is an infinite-dimensional problem. In order to end up with a computable one, we must introduce finite-dimensional subspaces with some approximability properties. We restrict ourselves to *conforming* finite element schemes, which hold $\mathcal{X}_h \subset \mathcal{X}$, the discrete problem reads as: find $u_h \in \mathcal{X}_h$ such that

$$a(u_h, v_h) = \ell(v_h), \qquad \text{for any } v_h \in \mathcal{X}_h. \tag{3.6}$$

This is the *Galerkin* problem. One can also define the affine operator

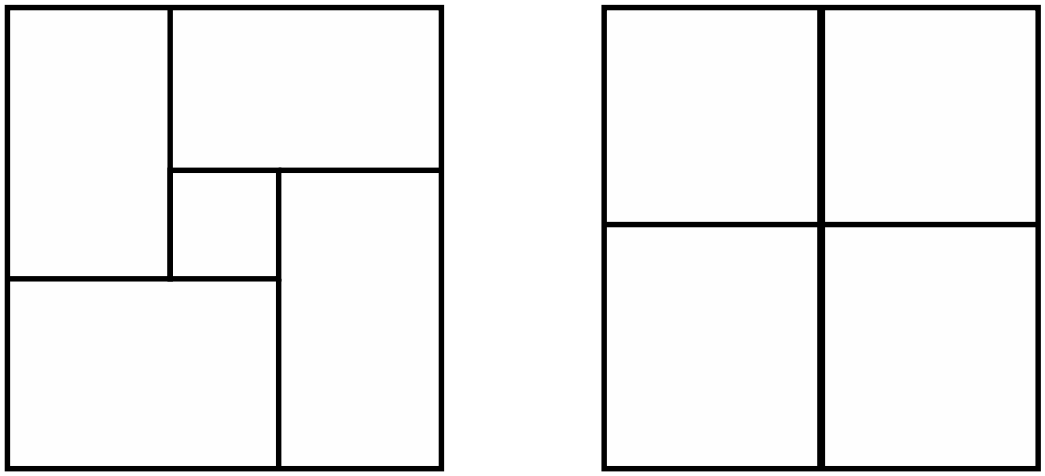
$$\mathcal{F}_h(u_h) = a_h(u_h, \cdot) - \ell_h(\cdot) \in \mathcal{X}_h'. \tag{3.7}$$

We note that for a given u_h this is a bounded linear functional that takes test functions in $\mathcal{X}_h$ and return real values, thus in its dual space $\mathcal{X}_h'$. Thus, we can state (3.6) as: find $u_h \in \mathcal{X}_h$ such that $\mathcal{F}_h(u_h) = 0$.

In order to define finite element spaces, we require a triangulation $\mathcal{T}_h$ of the domain Ω into a set $\{K\}$ of *cells*. This triangulation is assumed to be conforming, i.e., for two neighbour cells K^+, $K^- \in \mathcal{T}_h$, its intersection $K^+ \cap K^-$ is a *whole* k-face ($k < d$) of both cell[3] Thus, for every element

[3]We note that k-face refers to a geometrical entity for a *polytope*. For a three-

$K \in \mathcal{T}_h$, we assume that there is a reference cell $\hat{K}_K$ and a diffeomorphism (smooth bijective map) $\mathbf{\Phi}_K : \hat{K} \to K$. In what follows, we usually use the notation $\hat{\boldsymbol{x}} \doteq \mathbf{\Phi}_K^{-1}(\boldsymbol{x})$ (see Figure 3.2 for a conforming mesh and the geometrical map definition).



Non-conforming Conforming

Figure 3.1: A non-conforming mesh on the left-hand side; the intersection of the closure of cells is not always the closure of a vertex or edge in all cells. The mesh on the right-hand side is conforming.

Next, we will see the standard procedure for building finite element functional spaces. They rely on a *reference cell* functional space as follows:

1. We define a functional space in the reference cell $\hat{K}$;
2. We define a set of functions in the physical cell K via function and geometrical maps;
3. We define the global space as the assemble of cell-based spaces plus continuity constraints between cells.

dimensional polytope (e.g., a hexahedron or tetrahedron) the celll itself is a 3-face, the faces are 2-faces, the edges are 1-faces and vertices are 0-faces. In finite element methods, the cells can be mapped to a particular type of mapping over a set of admissible geometries (polytopes).

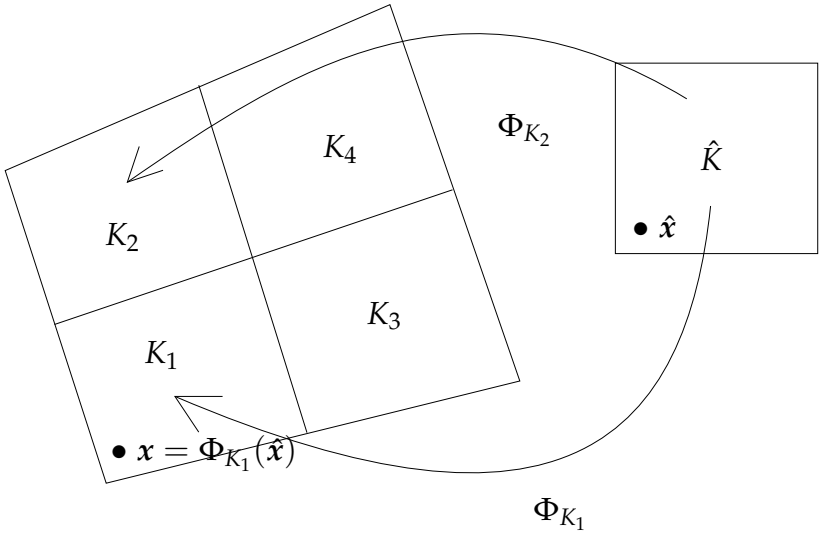


Figure 3.2: In this plot, we show a finite element mesh of 4 quadrilateral cells in the physical space on the left, and the corresponding reference squared cell $\hat{K}$ on the right. For every cell in the physical space K_i , we have a map that takes points $\hat{\boldsymbol{x}} \in \hat{K}$ and returns points $\boldsymbol{x} \in K_i$. These maps are assumed to be smooth and bijective, otherwise the mesh is not suitable for finite element analysis.

In order to present this process, we introduce the concept of reference finite element, finite element, and finite element space, respectively.

3.3 The finite element in reference and physical space

Using the abstract definition of *Ciarlet*, a finite element is represented by the triplet $\{K, \mathcal{V}, \Sigma\}$, where:

1. K is a compact, connected, Lipschitz subset of $\mathbb{R}^d$,
2. $\mathcal{V}$ is a vector space of functions,
3. and Σ is a set of linear functionals that form a basis for the dual space $\mathcal{V}'$.

The elements of Σ are the so-called degrees of freedom (DOFs) of the finite element. We denote the number of DOFs as n_Σ. The DOFs can be written as σ_a for $a \in \mathcal{N}_\Sigma \doteq \{1, \dots, n_\Sigma\}$. We can also define a basis $\left\{b^1, \dots, b^{n_\Sigma}\right\}$ for $\mathcal{V}$. In particular, we are interested in the basis $\{\phi^a\}_{a \in \mathcal{N}_\Sigma}$ for $\mathcal{V}$ such that $\sigma_a(\phi^b) = \delta_{ab}$ for $a, b \in \mathcal{N}_\Sigma$. These functions are the so-called *shape functions* of the finite element, and there is a one-to-one mapping between shape functions and DOFs.

3.3.1 The reference finite element

In the reference space, we build *reference* finite elements $(\hat{K}, \hat{\mathcal{V}}, \hat{\Sigma})$ as follows. First, we consider a bounded set of possible cell geometries, denoted by $\hat{K}$.[4] On $\hat{K}$, we build a functional space $\hat{\mathcal{V}}$ and a set of DOFs $\hat{\Sigma}$. In this chapter, we will use polynomials spaces for $\hat{\mathcal{V}}$ and the degrees of freedom will be the evaluation of the functions at a set of nodes (points). We consider some examples of reference finite elements in Sect. **??**.

In Figure 3.3 we can see on the left a bilinear squared reference finite element. The reference cell $\hat{K} \doteq (0,1)^2$. We define as a basis the so-called bilinear polynomials spanned by $\hat{\mathcal{V}} \doteq \text{span}\{1, \hat{x}, \hat{y}, \hat{x}\hat{y}\}$. If we represent

[4] Admissible geometries are a segment in one-dimension, triangles and quadrilaterals in two-dimensions, and tetrahedra and hexahedra in three-dimensions.

the four vertices of $\hat{K}$ with $\{\hat{\boldsymbol{x}}_1, \hat{\boldsymbol{x}}_2, \hat{\boldsymbol{x}}_3, \hat{\boldsymbol{x}}_4\}$, the space of degrees of freedom $\Sigma \doteq \{\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3, \hat{\sigma}_4\}$ are the node evaluations, i.e., $\hat{\sigma}_i(\hat{v}) \doteq \hat{v}(\hat{\boldsymbol{x}}_i)$.

As stated above one can easily check that Σ is a basis of $\mathcal{V}'$ (the dual space of $\mathcal{V}$, which is the space of linear functionals from $\mathcal{V}$ to $\mathbb{R}$). It can be proved by checking that two bilinear polynomials that have the same nodal values are the same, thus it has the maximum dimension of four and thus a bijection.

3.3.2 From reference to physical spaces

In the physical space, the finite element triplet $(K, \mathcal{V}, \Sigma)$ on a mesh cell $K \in \mathcal{T}_h$ relies on:

1. a reference finite element $(\hat{K}, \hat{\mathcal{V}}, \hat{\Sigma})$;
2. a geometrical mapping $\boldsymbol{\Phi}_K$ such that $K \doteq \boldsymbol{\Phi}_K(\hat{K})$;
3. a linear bijective function mapping $\hat{\Psi}_K : \hat{\mathcal{V}} \to \hat{\mathcal{V}}$.[5]

With these ingredients, we construct the physical finite element $(K, \mathcal{V}, \Sigma)$ as follows.

1. The geometry is $K \doteq \boldsymbol{\Phi}_K(\hat{K})$;
2. The functional space in the physical space is defined as

$$\mathcal{V} \doteq \{\Psi_K(\hat{v}) \doteq \hat{\Psi}_K(\hat{v}) \circ \boldsymbol{\Phi}_K^{-1} : \hat{v} \in \hat{\mathcal{V}}\};$$

where $\Psi_K : \hat{\mathcal{V}} \to \mathcal{V}$ is defined as

$$\Psi_K \doteq \hat{\Psi}_K(\hat{v}) \circ \boldsymbol{\Phi}_K^{-1}.$$

Again, in the case of the Lagrangian elements it is just $\Psi_K(\hat{v}) \doteq \hat{v} \circ \boldsymbol{\Phi}_K^{-1}$. In Figure 3.3 we show this construction for grad-conforming finite elements, in which $\Psi_K(\hat{v}) = \hat{v} \circ \boldsymbol{\Phi}_K^{-1}$.

[5]This is the general definition for a finite element in the physical space, but the last ingredient is not required for the finite element spaces to be considered herein, Lagrangian finite element spaces for problems in $H^1(\Omega)$, a.k.a. *grad-conforming*[6] finite elements. As a result, you can think that is operator $\hat{\Psi}_K$ is just the identity.

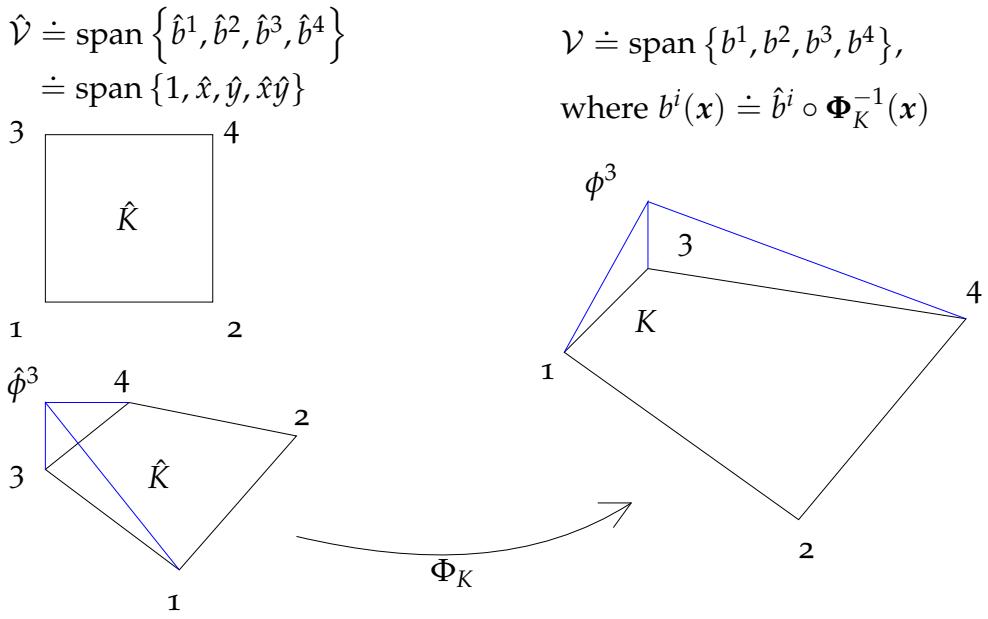


Figure 3.3: In this plot, we show the map from the reference cell $\hat{K}$ to a physical cell K. We consider a linear finite element, and show the indexing for its vertices/nodes. We have a basis for the Lagrangian reference finite element space $\hat{\mathcal{V}} \doteq \{1, \hat{x}, \hat{y}, \hat{x}\hat{y}\}$ and define the one in the reference finite element space from this one and the geometrical map $\mathcal{V}$. For node 3, we plot the shape function associated to the node both in the reference space $\hat{\phi}^3(\hat{\boldsymbol{x}}$ and the physical space $\phi^3(\boldsymbol{x}) = \hat{\phi}^3 \circ \boldsymbol{\Phi}_K^{-1}(\boldsymbol{x})$.

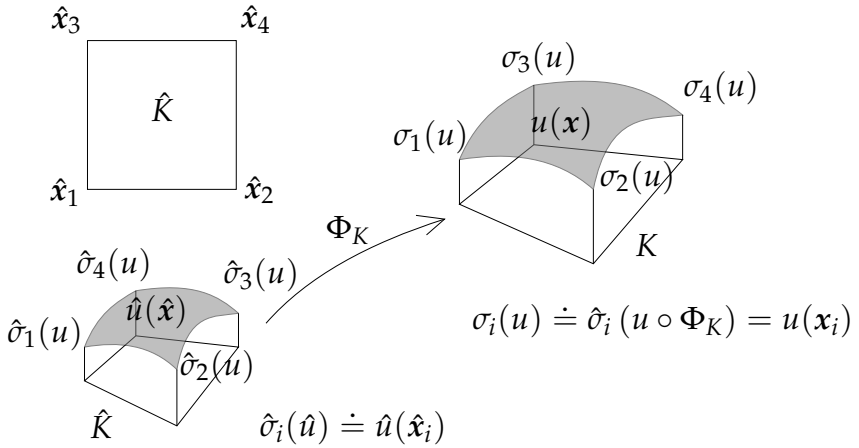


Figure 3.4: In this plot, we show the degrees of freedom for a linear finite element in two-dimensions. In Lagrangian finite elements, all degrees of freedom have a geometrical interpretation, i.e., they are linked to a node (point). For linear elements, the nodes are the vertices of the quadrilateral (idem for triangles). In the reference cell $\hat{K}$, given a function $u \in \mathcal{C}^0(\overline{\hat{K}})$, the degrees of freedom are just the evaluations of the function in the corresponding nodes, i.e., $\hat{\sigma}_i(\hat{u}) \doteq \hat{u}(\hat{x}_i)$. In the physical space, we compose the solution in $\mathcal{C}^0(\overline{K})$, compose it with Φ_K^{-1} and now we can apply the reference degree of freedom, i.e., $\sigma_i(u) \doteq \hat{\sigma}_i\,(u \circ \Phi_K) = u(x_i)$.

3. The set of DOFs in the physical space is defined as

$$\Sigma \doteq \{\hat{\sigma} \circ \Psi_K^{-1} \,:\, \hat{\sigma} \in \hat{\Sigma}\}.$$

In Figure 3.4 we show this idea for grad-conforming finite elements. The idea is to take a function defined in the physical space $u(\hat{x})$ and transform it to the reference space $\hat{u}(\hat{x}) \doteq \Psi_K^{-1}(u)(\hat{x}) = u \circ \boldsymbol{\Phi}_K^{-1}(\hat{\boldsymbol{x}})$. Now we can apply the degrees on freedom on the resulting function

$$\hat{\sigma}_i\,(u \circ \boldsymbol{\Phi}_K) = u \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_i) = u(\boldsymbol{x}_i).$$

The reference finite element space $\hat{\mathcal{V}}$ is usually a polynomial space. Thus, the first ingredient is to define bases of polynomials, e.g., monomial

bases; see Sect. 3.4. In Sect. 3.5, we show how to compute the basis of shape functions out of whatever basis $\hat{\mathcal{V}}$ in the reference space. Given the set of shape functions $\{\hat{\phi}^a : a \in \mathcal{N}_{\hat{\Sigma}}\}$ in the reference finite element, it is easy to check that $\{\phi^a_K \doteq \Psi_K(\hat{\phi}^a) : a \in \mathcal{N}_{\hat{\Sigma}}\}$ are the set of shape functions of the finite element in the physical space.

The definition of degrees of freedom in the physical space is essential to project functions in an infinite dimensional space, e.g., $\mathcal{C}^0\left(\overline{K}\right)$, into $\mathcal{V}$. Given a function v, we define the *local interpolator* for the finite element at hand as

$$\pi_K(v) \doteq \sum_{a \in \mathcal{N}_\Sigma} \sigma_a(v)\phi^a. \tag{3.8}$$

It is straightforward to check that the interpolation operator is in fact a projection. This operation is, e.g., used to project Dirichlet boundary conditions into the finite element space using the offset function method.

3.4 Construction of polynomial spaces

Local finite element spaces are usually polynomial spaces. Given an order $k \in \mathbb{N}$ and a set $\mathcal{N}_k$ of distinct points (nodes) in $\mathbb{R}$ (we will indistinctly represent nodes by their index i or position x_i), we define the corresponding set of Lagrangian polynomials $\{\ell^k_0, \ldots, \ell^k_k\}$ as:

$$\ell^k_m(x) \doteq \frac{\Pi_{n \in \mathcal{N}_k \setminus \{m\}}(x - x_n)}{\Pi_{n \in \mathcal{N}_k \setminus \{m\}}(x_m - x_n)}. \tag{3.9}$$

We can also define the Lagrangian basis $\mathcal{L}^k = \{\ell^k_i : 0 \leq i \leq k\}$. This set of polynomials are a basis for k-th order polynomials. We note that $\ell^k_m(x_l) = \delta_{ml}$, for $0 \leq m, l \leq k$.

For multi-dimensional spaces, we can define the set of nodes as the tensor product of 1D nodes. Given a d-tuple order $\boldsymbol{k}$, we define the corresponding set of nodes for n-cubes as: $\mathcal{N}^{\boldsymbol{k}} \doteq \mathcal{N}^{k_1} \times \cdots \times \mathcal{N}^{k_d}$ (see Figure 3.5).

Analogously, we define the multi-dimensional Lagrange basis

$$\mathcal{L}^{\boldsymbol{k}} = \{\ell^{\boldsymbol{k}}_{\boldsymbol{m}} : \boldsymbol{m} \in \mathcal{N}^{\boldsymbol{k}}\}, \qquad \text{where} \quad \ell^{\boldsymbol{k}}_{\boldsymbol{m}}(\boldsymbol{x}) \doteq \Pi^d_{i=1}\ell^{k_i}_{m_i}(x_i). \tag{3.10}$$

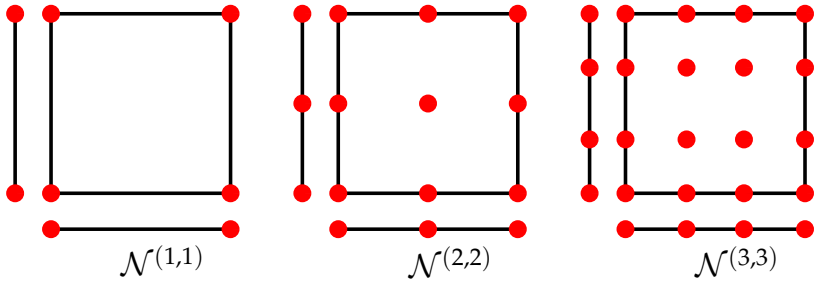


Figure 3.5: Equidistant nodes for two-dimensional Lagrangian polynomial spaces $\mathcal{Q}_{(1,1)}$, $\mathcal{Q}_{(2,2)}$ and $\mathcal{Q}_{(3,3)}$ obtained as tensor product of their one-dimensional counterparts. In short, these isotropic order spaces are expressed as $\mathcal{Q}_1$, $\mathcal{Q}_2$ and $\mathcal{Q}_3$, resp.

Clearly, $\ell_{\boldsymbol{t}}^{\boldsymbol{k}}(\boldsymbol{x}_{\boldsymbol{s}}) = \delta_{\boldsymbol{st}}$, for $\boldsymbol{s}, \boldsymbol{t} \in \mathcal{N}^{\boldsymbol{k}}$. [7]

This tensor product construction leads to a basis for the space of polynomials that are of degree less or equal to k with respect to each variable $x_1, \ldots, x_d$. We can define monomials by a d-tuple $\boldsymbol{\alpha}$ as $p_{\boldsymbol{\alpha}}(\boldsymbol{x}) \doteq \Pi_{i=1}^{d} x_i^{\alpha_i}$, and the polynomial space of order $\boldsymbol{k}$ as $\mathcal{Q}_{\boldsymbol{k}} = \text{span}\{p_{\boldsymbol{\alpha}}(\boldsymbol{x}) : 0 \leq \alpha_i \leq k_i, i = 1, \ldots, d\}$. This space is also spanned by the Lagrangian basis $\mathcal{Q}_{\boldsymbol{k}} = \text{span}\{\ell : \ell \in \mathcal{L}^{\boldsymbol{k}}\}$. For isotropic spaces in which the same order $p \in \mathbb{N}$ is used in all dimensions we simply write $\mathcal{Q}_p$.

3.4.1 Local finite element space in cubes

Let us consider the same order for all components, i.e., $k\mathbf{1} \doteq (k, \ldots, k)$. When the reference geometry $\hat{K}$ is an n-cube, we define the reference finite element space as $\mathcal{V}_k \doteq \mathcal{Q}_{k\mathbf{1}}$. The set of nodes $\mathcal{N}^{k\mathbf{1}}$ can be generated, e.g., from the equidistant Lagrangian nodes. Let us define the bijective mapping $\mathtt{i}(\cdot)$ from the set of nodes $\mathcal{N}^{k\mathbf{1}}$ to $\{1, \ldots, |\mathcal{N}^{k\mathbf{1}}|\} \equiv \mathcal{N}_\Sigma$, i.e., the local node numbering. The set of local DOFs $\mathcal{N}_{\Sigma_K}$ are the nodal values, i.e., $\sigma_{\mathtt{i}(\boldsymbol{s})} \doteq v(\boldsymbol{x}_{\boldsymbol{s}})$, for $\boldsymbol{s} \in \mathcal{N}^{\boldsymbol{k}}$. Clearly, the reference finite element shape

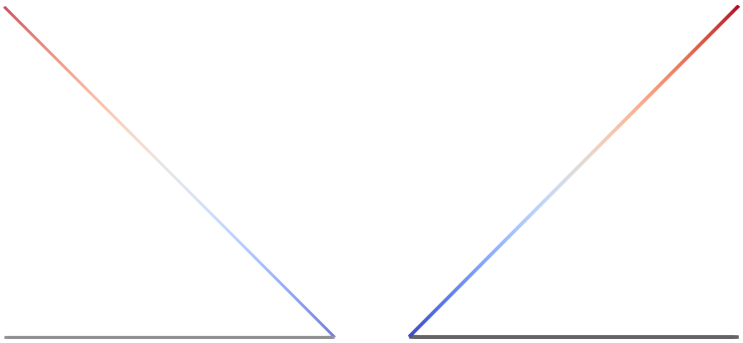
[7] The use of a different order polynomial order in each space dimension (anisotropic spaces) is required when building some finite element spaces. However, for the case we want to consider in this text, i.e., grad-conforming finite elements, we will use the same order in all dimensions (isotropic spaces). E.g., $\boldsymbol{k} \doteq (p, p)$ in two-dimensions and $\boldsymbol{k} \doteq (p, p, p)$ in three-dimensions, for $p \in \mathbb{N}$.

functions related to these DOFs are $\phi^{\mathrm{i}(s)} \doteq \ell_s^{k\mathbf{1}}$. On the other hand, we simply take $\hat{\Psi}(v) \doteq v$.

Let us start with the one-dimensional spaces (see Figure 3.6 for linear and Figure 3.7 for quadratic shape functions, resp.). These Lagrangian bases span $\mathcal{Q}_1 \doteq \{1, x\}$ and $\mathcal{Q}_2 \doteq \{1, x, x^2\}$. Using the tensor product definition we can readily construct higher-dimensional shape functions. The isotropic space obtained as tensor product of linear polynomials in two-dimensions is the bilinear space $\mathcal{Q}_1 = \text{span}\{1, x, y, xy\}$. The one for second order polynomials is

$$\mathcal{Q}_2 = \text{span}\left\{1, x, y, xy, x^2, y^2, x^2y, xy^2, x^2y^2\right\}.$$

The corresponding Lagrangian bases (of shape functions) are collected in Figure 3.8 for linear and Figure 3.9 for quadratic shape functions, resp.).

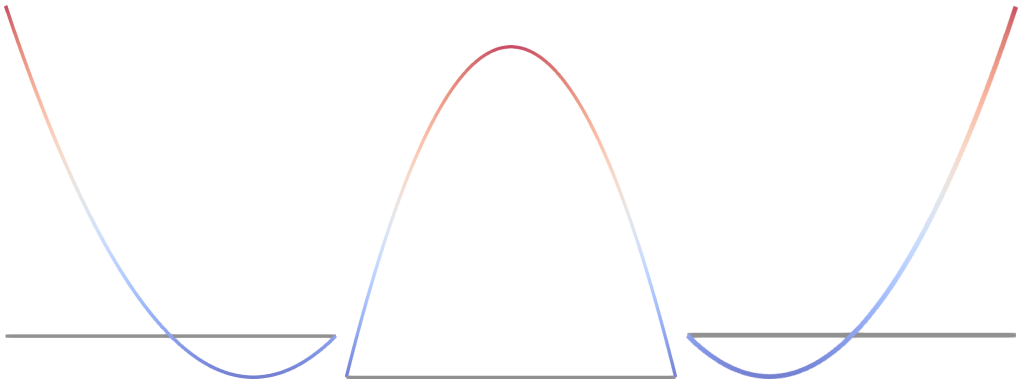


(a) 1 (b) 2

Figure 3.6: Shape functions for the one-dimensional linear finite element space $\mathcal{P}_1 = \mathcal{Q}_1$ in the reference segment. The label says which is the related Lagrangian node in $\mathcal{N}_1$.

3.4.2 Local finite element space in simplices

The definition of polynomial spaces on n-simplices is slightly different. It requires the definition of the space of polynomials of degree equal or less than k in the variables $x_1, \ldots, x_d$. It does not involve a full tensor product of 1D Lagrange polynomials (or monomials) but a truncated space, i.e.,



(a) 1 (b) 2 (c) 3

Figure 3.7: Shape functions for the one-dimensional quadratic finite element space $\mathcal{P}_2 = \mathcal{Q}_2$ in the reference segment. The label says which is the related Lagrangian node in $\mathcal{N}_2$.

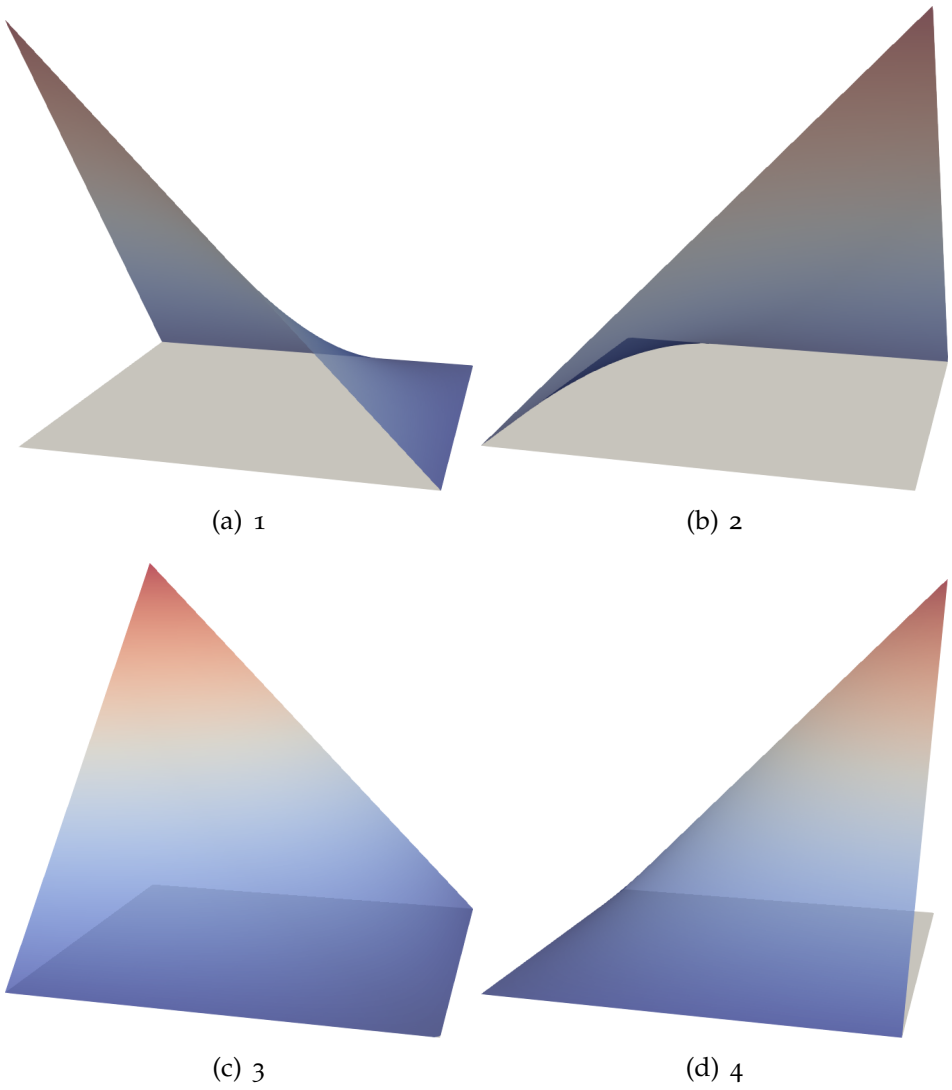
the corresponding polynomial space of polynomials up to order k, which is $\mathcal{P}_k = \text{span}\{p_{\boldsymbol{\alpha}}(\boldsymbol{x}) : |\boldsymbol{\alpha}| \leq k\}$, with $|\boldsymbol{\alpha}| \doteq \sum_{i=1}^{d} \alpha_i$.

As an example, in two-dimensions, the linear space $\mathcal{P}_1 \doteq \{1, x, y\}$ whereas the quadratic space $\mathcal{P}_2 \doteq \{1, x, y, x^2, xy, y^2\}$.

Analogously as for n-cubes, we can define a basis of the dual space, i.e., the degrees of freedom as nodal evaluations. A basis for the dual space of $\mathcal{P}_k$ are the values at the set of nodes $\tilde{\mathcal{N}}^k \doteq \{\boldsymbol{s} \in \mathcal{N}^{k\mathbf{1}} : |\boldsymbol{s}| \leq k\}$ (see Figure 3.10. It generates the typical grad-conforming finite elements on n-simplices. Whereas the construction of the shape functions bases is somehow easy for quad meshes, using the tensor product of Lagrangian basis, the situation is more complicated for tet meshes. In the following section, we show an easy method to transform a monomial basis into the shape functions basis in a general way. The shape functions for linear and quadratic elements can be found in Figures 3.11 and 3.12, resp.

3.4.3 Shape functions in the physical space

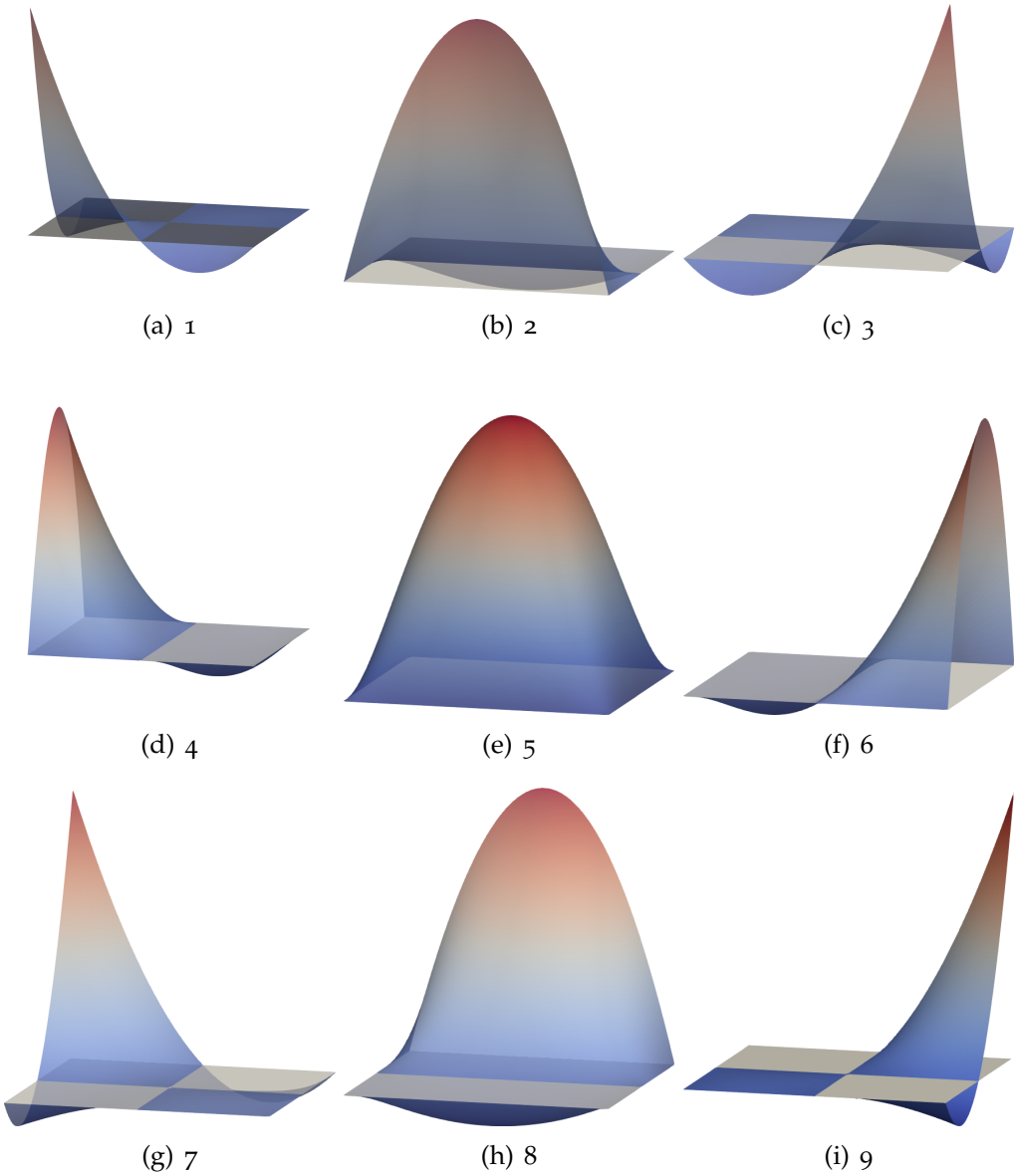
Let us consider quadrilateral finite elements. For the computation of the geometrical map Φ_K we can consider a d-linear approximation determined by the position of the vertices in the physical domain. Thus, we can use all the finite element machinery so far for the computation of this



(a) 1 (b) 2

(c) 3 (d) 4

Figure 3.8: Shape functions for the two-dimensional bilinear finite element space $\mathcal{Q}_1$ in the reference square. The label says which is the related Lagrangian node in the set $\mathcal{N}^{(1,1)}$ (see Figure 3.5).



(a) 1 (b) 2 (c) 3

(d) 4 (e) 5 (f) 6

(g) 7 (h) 8 (i) 9

Figure 3.9: Shape functions for the two-dimensional biquadratic finite element space $\mathcal{Q}_2$ in the reference square. The label says which is the related Lagrangian node in the set $\mathcal{N}^{(2,2)}$ (see Figure 3.5).

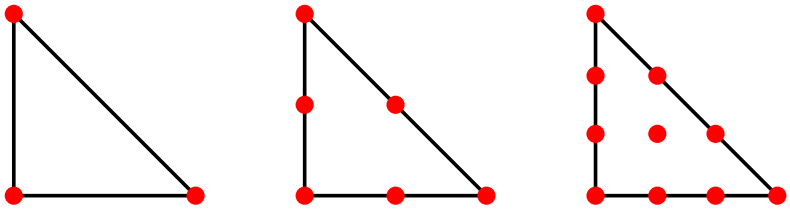


Figure 3.10: Equidistant nodes for two-dimensional Lagrangian polynomial spaces $\mathcal{P}_1$, $\mathcal{P}_2$ and $\mathcal{P}_3$ obtained as tensor product of their one-dimensional counterparts.

geometrical map. Given the nodal values, i.e., the position of the vertices $\boldsymbol{x}^a$ in the physical space, we create the map as follows:

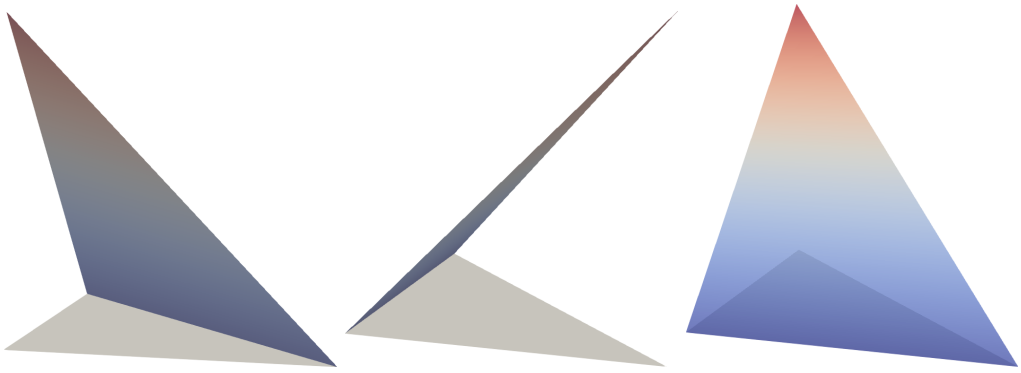
$$\boldsymbol{x} = \Phi_K(\hat{\boldsymbol{x}}) \doteq \sum_{a=1}^{n_\Sigma} \hat{\phi}_1^a(\hat{\boldsymbol{x}})\boldsymbol{x}^a,$$

where $\{\hat{\phi}_1^a\}$ are the shape functions for $\hat{\mathcal{Q}}_1$. It is easy to check from the definition of shape functions and degrees of freedom for Lagrangian elements that Φ_K maps every vertex $\hat{\boldsymbol{x}}_a$ in the reference cell $\hat{K}$ to the corresponding vertex $\boldsymbol{x}_a$ in the physical cell K.

Using what we already know for quadrilateral finite elements, $\boldsymbol{x} \in \hat{\mathcal{Q}}_1$; e.g., in two-dimensions the physical coordinates can be expressed as a bilinear polynomial in terms of the reference coordinates. As a result the map is nonlinear (due to the $\hat{x}\hat{y}$ term).[8]

Thus, the space spanned by $\{\phi^a\}$ is not the space $\mathcal{Q}_1$ in general. This is only true when the cell K can be expressed as a stretching in each direction plus a rotation of the reference cell $\hat{K}$. In this case, one can easily check that the geometrical map Φ_K is in fact linear and so its inverse, which can be expressed as $\Phi_K^{-1}(\boldsymbol{x}) = \mathbf{A}\boldsymbol{x} + \mathbf{b}$. Given the shape functions

[8] In general, the cell K will not have flat faces in three-dimensions because we cannot find a plane that contains four points unless they are aligned. In two-dimensions, the edges will be straight because two distinct points define a line.



(a) 1 (b) 2 (c) 3

Figure 3.11: Shape functions for the two-dimensional linear finite element space $\mathcal{P}_1$ in the reference triangle. The label says which is the related Lagrangian node in $\tilde{\mathcal{N}}^1$ (see Figure 3.10).

$\left\{\hat{\phi}_p^a\right\}$ of $\hat{\mathcal{Q}}_p$, it is easy to check that the physical shape functions

$$\{\phi^a(\boldsymbol{x})\} \doteq \left\{\hat{\phi}^a \circ \Phi_K^{-1}(\boldsymbol{x})\right\} = \{\hat{\phi}^a(\mathbf{A}\boldsymbol{x} + \mathbf{b})\}$$

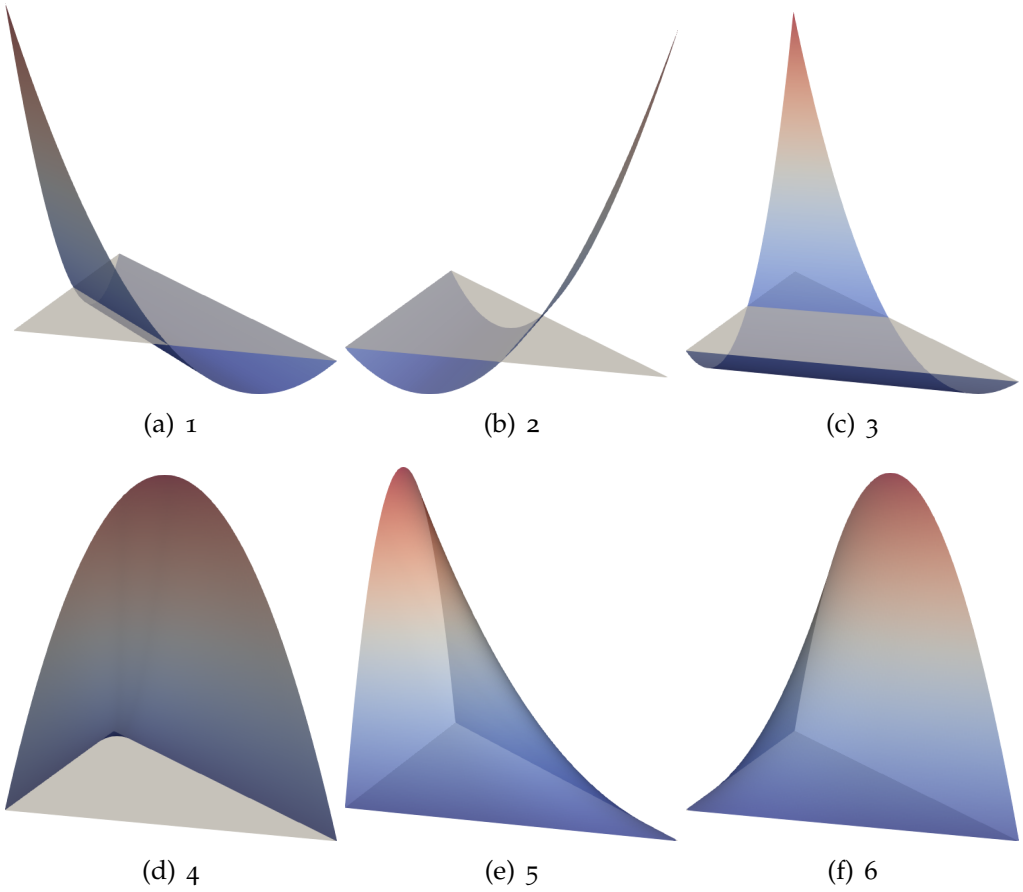
spans $\mathcal{Q}_p$.

3.5 Construction of the shape functions basis

The analytical expression of shape functions can become very complicated for high order finite elements and non-trivial definitions of DOFs, e.g., for electromagnetic applications (see below). Furthermore, to have a code that provides a basis for an arbitrary high order, an automatic generator of shape functions must be implemented. When the explicit construction of the shape functions is not obvious, we proceed as follows.

Let us consider a finite element defined by $\{K, \mathcal{V}, \Sigma\}$.[9] First, we generate a *pre-basis* $\{\psi^b\}_{b\in\mathcal{N}_\Sigma}$ that spans the local finite element space $\mathcal{V}$, e.g., a Lagrangian polynomial basis (see Sect. 3.4). On the other hand, given the

[9]In this section, we do not make difference between reference and physical spaces, e.g., using the $\hat{}$ symbol. In any case, all the following developments are usually performed at the reference finite element level.



(a) 1 (b) 2 (c) 3

(d) 4 (e) 5 (f) 6

Figure 3.12: Shape functions for the two-dimensional quadratic finite element space $\mathcal{P}_2$ in the reference triangle. The label says which is the related Lagrangian node in the set $\tilde{\mathcal{N}}^2$ (see Figure 3.10).

set of local DOFs, we proceed as follows. The shape functions can be written as $\phi^a = \sum_{b \in \mathcal{N}_\Sigma} \Xi_{ab} \psi^b$, where ψ^b are the elements of the pre-basis. By definition, the shape functions must satisfy $\sigma_a(\phi^b) = \delta_{ab}$ for a, $b \in \mathcal{N}_\Sigma$. As a result, let us define $\mathbf{C}_{ab} \doteq \sigma_a(\psi^b)$. We have (using Einstein's notation):

$$\sigma_a(\phi^b) = \sigma_a(\Xi_{bc}\psi^c) = \sigma_a(\psi^c)\Xi_{bc} = \delta_{ab},$$

or in compact form, $\mathbf{C}\Xi^T = I$, and thus $\Xi^T = \mathbf{C}^{-1}$. As a result, $\Xi_{ab} = \mathbf{C}^{-1}_{ba}$. The shape functions are computed as a linear combination of the pre-basis functions.

3.6 Global finite element space and conformity

Now that we have defined the finite element spaces at the local level, we have to glue together these pieces keeping $\mathcal{C}^0$ continuity. In this section we will consider how to build global (and conforming) finite element spaces. Next, we will learn how to integrate the bilinear forms in the corresponding weak formulation in Sect. 3.9.

Let us define the *global* finite element space. Conforming finite element spaces are defined as: $\mathcal{X}_h \doteq \{v \in \mathcal{X} : v|_K \in \mathcal{V}\}$. The main complication in this definition is to enforce the conformity of the finite element space, i.e., $\mathcal{X}_h \subset \mathcal{X}$. Since we want a conforming finite element space $\mathcal{X}_h \subset \mathcal{X}$, we must keep some continuity across inter-cell boundaries. E.g., for problems posed in $H^1(\Omega)$, it implies full continuity ($\mathcal{C}^0(\Omega)$ piecewise polynomials are in $H^1(\Omega)$).

In fact, the conformity constraint is the one that motivates the choice of $\hat{\Sigma}$ and Ψ, and as a consequence, Σ. In practice, the conformity constraint must be re-stated as a continuity constraint over finite element DOFs. For conforming meshes, these constraints are implicitly enforced via a global DOF numbering, even though it is not possible in general for adaptive schemes with non-conforming meshes and/or variable order cells (different finite element orders at different cells), which require more involved constraints.

The idea of global DOF numbering is the following. We start with the cell-local finite element spaces that we already know how to define. At every cell, we have a set of local DOFs. At the discrete level, we want to express that continuity in terms of DOFs, gluing together (enforcing

the same values) on pairs of DOFs at different cells. Before providing the abstract definition, let us think what it means in one-dimension. In one dimension, let us consider two consecutive cell (segments) $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$. At every cell, we can define a local Lagrangian basis of order p and its corresponding local $p+1$ nodes. In both cells, there is a node geometrically located at x_i. If we do not enforce any continuity, functions could have a jump at x_i. In order to enforce continuity, we must enforce these two local nodes to have the same value. Conceptually, they represent the same *global* DOFs.

This idea can be stated in an abstract way. Let us define by $\mathcal{M}_h \doteq \{(b, K) : b \in \mathcal{N}_{\Sigma_K}, K \in \mathcal{T}_h\}$ the Cartesian product of local DOFs for all cells. We define the global DOFs as the quotient space of $\mathcal{M}_h$ by an equivalence relation $\sim$. Using standard notation, given $\sim$, the equivalence class of $a \in \mathcal{M}_h$ with respect to $\sim$ is represented with $[a] \doteq \{b \in \mathcal{M}_h : a \sim b\}$, and the corresponding quotient set is $\mathcal{N}_h \doteq \{[a] : a \in \mathcal{M}_h\}$. The set $\mathcal{N}_h$ is the set of global DOF and $[\cdot]$ represents the *local-to-global* DOF map. Using the one-to-one mapping between DOFs and shape functions, the same operator allows one to define global shape functions $\phi^a = \sum_{(b,K)\sim a} \phi^b_K$. This construction should lead to conformity, i.e., $\mathcal{X}_h = \text{span}\{\phi^a\}_{a \in \mathcal{N}_h} \subset \mathcal{X}$.

For grad-conforming finite elements, the global finite element space is determined by the following equivalence relation. The set of local DOFs for n-cubes is $\mathcal{M}_h \doteq \{(\boldsymbol{s}, K) : \boldsymbol{s} \in \mathcal{N}^{k\mathbf{1}}, K \in \mathcal{T}_h\}$ due to the one-to-one mapping between DOFs and nodes; we replace the set of nodes by $\tilde{\mathcal{N}}^k$ for n-simplices. Furthermore, we say that $(\boldsymbol{s}, K) \sim (\boldsymbol{s}', K')$ iff $\boldsymbol{x}_{\boldsymbol{s}} = \boldsymbol{x}_{\boldsymbol{s}'}$, i.e., *two local degrees of freedom in two different cells are the same degree of freedom in the global space if their corresponding nodes are in the same spatial point in* Ω. The implementation of this equivalence relation, and thus, the global numbering, relies on the ownership relation between n-faces and DOFs. An illustration of the local-to-global map for grad-conforming finite elements in two-dimensions is provided in Figure 3.13. In one-dimension, we recover the *hat function* definition in the previous section.

With such global DOF definition, it is easy to check that the global finite element space is grad-conforming, i.e., $\mathcal{V} \subset \mathcal{C}^0(\overline{\Omega}) \subset H^1(\Omega)$. The idea is to check that at any n-face (edge in two dimensions or face in two dimensions), the restriction of the finite element function to that n-face is a polynomial of the same order in that n-face that is uniquely determined by the nodes on the closure of the n-face, which have the same value for

all cells, thus continuous.

3.7 Interpolant

Let us consider an infinite-dimensional space $\tilde{\mathcal{X}}$ such that 1) $\mathcal{X}_h \subset \tilde{\mathcal{X}} \subset \mathcal{X}$ and 2) for every function $v \in \tilde{\mathcal{X}}$ and global DOF $a \in \mathcal{N}_h$, all the local DOFs b, $b' \in [a]$ are such that $\sigma_b(v) = \sigma_{b'}(v)$, i.e., local DOFs related to the same global DOF are continuous among cells. The *global interpolator* is defined as:

$$\pi_{\mathcal{X}_h}(v) \doteq \sum_{K \in \mathcal{T}_h} \pi_K(v) = \sum_{K \in \mathcal{T}_h} \sum_{b \in \mathcal{N}_{\Sigma_K}} \sigma_b(v) \phi_K^b, \qquad \text{for } v \in \tilde{\mathcal{X}}. \tag{3.11}$$

Figure 3.4 shows this process at one physical cell, which for grad-conforming Lagrangian finite elements simply implies to compute at each cell the nodal values (local degrees of freedom) and use the local-to-global map. It is easy to check that it is in fact a projector (using the definition of shape function). In any case, we use *projection operator* to refer to other projectors that involve the solution of a global finite element system, e.g., based on the minimization of the L^2 or H^1 norm.

Since Lagrangian DOFs involve point-wise evaluations of functions and $H_0^1(\Omega) \not\subset \mathcal{C}^0(\Omega)$ for $d > 1$, the interpolator (3.11) is not defined in such space. This is only true in one-dimension, the case considered in the previous section. Instead, we consider that functions to be interpolated belong, e.g., to the space $\tilde{\mathcal{X}} \doteq \mathcal{C}^0(\Omega)$. There are slightly more involved interpolators for grad-conforming finite element spaces that are bounded in $H^1(\Omega)$ for any space dimension but we do not consider them here for simplicity.

3.8 Assembly and linear system

Once we have defined a basis for the finite element space $\mathcal{X}_h$ using the finite element machinery presented above, every finite element function u_h can be uniquely represented by a vector $\mathbf{u} \in \mathbb{R}^{|\mathcal{N}_h|}$ as $u_h = \sum_{b \in \mathcal{N}_h} \phi^b \mathbf{u}_b$. In fact, problem (3.6) can be re-stated as: find $\mathbf{u} \in \mathbb{R}^{|\mathcal{N}_h|}$ such that

$$a(\phi^j, \phi^i)\mathbf{u}_j = \ell_h(\phi^i), \qquad \text{for any } i \in \mathcal{N}_h.$$

We have ended up with a finite-dimensional linear problem, i.e., a linear system. In matrix form, the problem can be stated as:

$$\text{Solve} \quad \mathbf{Au} = \mathbf{f}, \qquad \text{with} \quad \mathbf{A}_{ij} \doteq a(\phi^j, \phi^i), \quad \mathbf{f}_i \doteq \ell_h(\phi^i). \tag{3.12}$$

Assuming that the bilinear form can be split into cell contributions as $a(\cdot,\cdot) = \sum_{K\in\mathcal{T}_h} a_K(\cdot,\cdot)$, e.g., by replacing $\int_\Omega$ by $\sum_{K\in\mathcal{T}_h}\int_K$, the construction of the matrix is implemented through a *cell-wise assembly process*[10], as follows:

$$\mathbf{A}_{[i][j]} = \sum_{K\in\mathcal{T}_h}\sum_{i,j\in\mathcal{N}_{\Sigma_K}} \mathbf{A}^K_{ij} \doteq \sum_{K\in\mathcal{T}_h}\sum_{i,j\in\mathcal{N}_{\Sigma_K}} a_K(\phi^j_K, \phi^i_K). \tag{3.13}$$

We remind that $[i]$ represents the global index for the local (cell) index i. The finite element affine operator (3.7) can be represented as $\mathcal{F}_h(u_h) \doteq \mathbf{Au} - \mathbf{f}$, i.e., it can be represented with a matrix and a vector of size $|\mathcal{N}_h|$.

Let us consider a practical example of this process. Let us assume that we are integrating the entries for cell K_2 in Figure 3.13. Thus, the element-local matrix reads:

$$\mathbf{A}^K \doteq \begin{bmatrix} a(\phi^1_{K_2},\phi^1_{K_2}) & a(\phi^1_{K_2},\phi^2_{K_2}) & a(\phi^1_{K_2},\phi^3_{K_2}) & a(\phi^1_{K_2},\phi^4_{K_2}) \\ a(\phi^2_{K_2},\phi^1_{K_2}) & a(\phi^2_{K_2},\phi^2_{K_2}) & a(\phi^2_{K_2},\phi^3_{K_2}) & a(\phi^2_{K_2},\phi^4_{K_2}) \\ a(\phi^3_{K_2},\phi^1_{K_2}) & a(\phi^3_{K_2},\phi^2_{K_2}) & a(\phi^3_{K_2},\phi^3_{K_2}) & a(\phi^3_{K_2},\phi^4_{K_2}) \\ a(\phi^4_{K_2},\phi^1_{K_2}) & a(\phi^4_{K_2},\phi^2_{K_2}) & a(\phi^4_{K_2},\phi^3_{K_2}) & a(\phi^4_{K_2},\phi^4_{K_2}) \end{bmatrix} \tag{3.14}$$

Now, we have to assemble the local matrix in the global one using the local to global map. The local degrees of freedom 1, 2, 3 and 4 correspond to the global ones 2, 3, 5 and 6. Thus, these entries will be added to the

[10] The implementation of finite element methods is cell-based, i.e., all the computations are at the cell level, and then, using the local-to-global map (the equivalence class) assembled in the global linear system. This is different from finite difference methods, that do not share the concept of cell and are nodal-based.

corresponding entries (in red) of the global matrix

$$\mathbf{A}+= \left[\begin{array}{ccccccccc} \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bullet & \bullet & \bigcirc & \bullet & \bullet & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bullet & \bullet & \bigcirc & \bullet & \bullet & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bullet & \bullet & \bigcirc & \bullet & \bullet & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bullet & \bullet & \bigcirc & \bullet & \bullet & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \end{array}\right]. \tag{3.15}$$

The operator $+=$ means add the object on the right to the one on the left.

3.9 Numerical integration

In general, the local bilinear form can be stated as:

$$a_K(\phi_K^b, \phi_K^a) \doteq \int_K \mathcal{I}(\boldsymbol{x}) \mathrm{d}\Omega,$$

for some integrand $\mathcal{I}(x)$, where the evaluation of $\mathcal{I}(\boldsymbol{x})$ involves the evaluation of shape function derivatives. Let us represent the Jacobian of the geometrical mapping with $\boldsymbol{J}_K \doteq \frac{\partial \boldsymbol{\Phi}_K}{\partial \boldsymbol{x}}$. We can rewrite the cell integration in the reference cell, and next consider a quadrature rule Q defined by a set of points/weights $(\hat{\boldsymbol{x}}_{\mathrm{gp}}, \mathrm{w}_{\mathrm{gp}})$, as follows:

$$\int_K \mathcal{I}(\boldsymbol{x}) \mathrm{d}\Omega = \int_{\hat{K}} \mathcal{I} \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}) |\boldsymbol{J}_K| \mathrm{d}\hat{\Omega} = \sum_{\hat{\boldsymbol{x}}_{\mathrm{gp}} \in \mathrm{Q}} \mathcal{I} \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\mathrm{gp}}) \mathrm{w}(\hat{\boldsymbol{x}}_{\mathrm{gp}}) |\boldsymbol{J}_K(\hat{\boldsymbol{x}}_{\mathrm{gp}})|. \tag{3.16}$$

Here, the main complication is the evaluation of $\mathcal{I} \circ \boldsymbol{\Phi}_k(\hat{\boldsymbol{x}}_{\mathrm{gp}})$. The evaluation of this functional requires the evaluation of $\partial_{\boldsymbol{\alpha}} \phi_K^b \circ \boldsymbol{\Phi}_k(\hat{\boldsymbol{x}}_{\mathrm{gp}})$ for some values of the multi-index $\boldsymbol{\alpha}$ (idem for the test functions). Usually, $|\boldsymbol{\alpha}| \leq 1$ in $\mathcal{C}^0$ finite elements, since higher-order derivatives would require higher inter-cell continuity.[11]

[11] There exist $\mathcal{C}^1$ finite element methods that can approximate fourth order problems, e.g., the bi-harmonic problen, but we are not going to consider them here.

Let us consider the case of zero and first derivatives, i.e., the evaluation of $\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}})$ and $\boldsymbol{\nabla}\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}})$. $\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}$ represents the gradient in the reference space. The values of the shape functions (times the geometrical mapping) on the quadrature points is determined as follows:

$$\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}}) = \hat{\Psi}(\hat{\phi}^b)(\hat{\boldsymbol{x}}_{\text{gp}}), \tag{3.17}$$

whereas shape function gradients are computed as:

$$\begin{aligned} \boldsymbol{\nabla}\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}}) &= \boldsymbol{\nabla}(\hat{\Psi}(\hat{\phi}^b) \circ \boldsymbol{\Phi}_K^{-1}) \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}}) && (3.18)\\ &= \boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\Psi}(\hat{\phi}^b)(\hat{\boldsymbol{x}}_{\text{gp}}) \cdot \boldsymbol{J}_K^{-1}(\hat{\boldsymbol{x}}_{\text{gp}}), && (3.19) \end{aligned}$$

where we have used some elementary differentiation rules and the inverse function theorem in the last equality:

$$\boldsymbol{\nabla} f(x) = \boldsymbol{\nabla}\left(\hat{f} \circ \Phi_K^{-1}\right) = \boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{f} \cdot \boldsymbol{\nabla}\Phi_K^{-1} = \boldsymbol{\nabla}_{\hat{\boldsymbol{x}}} f \cdot \boldsymbol{J}_K^{-1}$$

Using matrix notation, the term $\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}} f \cdot \boldsymbol{J}_K^{-1}$ is usually written as $\boldsymbol{J}_K^{-T}\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}} f$ Thus, one only needs to provide the values of the Jacobian matrix, its inverse, and its determinant, from one side, and the value of the shape functions $\Psi(\hat{\phi}^b)$ and their gradients $\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\Psi(\hat{\phi}^b)$ in the reference space, on the other side, at all quadrature points, to compute all the entries of the finite element matrices; second order derivatives can be treated analogously.

Once again, for grad-conforming Lagrangian finite elements, $\hat{\Psi}$ is the identity and these expressions simply read

$$\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}}) = \hat{\phi}^b(\hat{\boldsymbol{x}}_{\text{gp}}), \qquad \boldsymbol{\nabla}\phi_K^b \circ \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}_{\text{gp}}) = \boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\phi}^b(\hat{\boldsymbol{x}}_{\text{gp}}) \cdot \boldsymbol{J}_K^{-1}(\hat{\boldsymbol{x}}_{\text{gp}}),$$

As an example, a mass matrix[12] would be computed as

$$\begin{aligned} \int_K \phi^a(\boldsymbol{x})\,\phi^b(\boldsymbol{x})\,\mathrm{d}\Omega &= \int_{\hat{K}} \hat{\phi}^a(\hat{\boldsymbol{x}})\,\hat{\phi}^b(\hat{\boldsymbol{x}})\,|\boldsymbol{J}_K(\hat{\boldsymbol{x}}_{\text{gp}})|\mathrm{d}\hat{\Omega} && (3.20)\\ &= \sum_{\hat{\boldsymbol{x}}_{\text{gp}}\in \mathrm{Q}} \hat{\phi}^a(\hat{\boldsymbol{x}}_{\text{gp}})\,\hat{\phi}^b(\hat{\boldsymbol{x}}_{\text{gp}})\,\mathrm{w}(\hat{\boldsymbol{x}}_{\text{gp}})|\boldsymbol{J}_K(\hat{\boldsymbol{x}}_{\text{gp}})|. \end{aligned}$$

[12] The mass matrix is the one that arises from a zero-order (a.k.a. reaction) term, e.g., the first term in $u - \Delta u = 0$. In weak form, it leads to a term $\int_\Omega uv\mathrm{d}\Omega$. The origin of the name comes from the fact that this term arises after the finite difference discretisation of a time derivative, and the time derivative term is the so-called inertia term.

On the other hand, the Laplacian matrix would be computed as

$$\begin{aligned}
&\int_K \boldsymbol{\nabla}\phi^a(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi^b(\boldsymbol{x})\,\mathrm{d}\Omega \\
&= \int_{\hat{K}} [\boldsymbol{J}_K^{-T}\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\phi}^a](\hat{\boldsymbol{x}})\cdot[\boldsymbol{J}_K^{-T}\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\phi}^b](\hat{\boldsymbol{x}})\,|\boldsymbol{J}_K(\hat{\boldsymbol{x}})|\,\mathrm{d}\hat{\Omega} \\
&= \sum_{\hat{\boldsymbol{x}}_{\mathrm{gp}}\in\mathrm{Q}} [\boldsymbol{J}_K^{-T}\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\phi}^a](\hat{\boldsymbol{x}}_{\mathrm{gp}})\cdot[\boldsymbol{J}_K^{-T}\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\hat{\phi}^b](\hat{\boldsymbol{x}}_{\mathrm{gp}})\mathrm{w}(\hat{\boldsymbol{x}}_{\mathrm{gp}})|\boldsymbol{J}_K(\hat{\boldsymbol{x}}_{\mathrm{gp}})|.
\end{aligned} \tag{3.21}$$

Quadrature rules for $\hat{K}$ being an n-cube can readily be obtained as a tensor product of a 1D quadrature rule, e.g., the Gauss-Legendre quadrature. As it is well known, considering n-cube topologies for $\hat{K}$, Gauss quadratures with n points per direction can integrate *exactly* $2n-1$ order polynomials. E.g., for a Lagrangian reference finite element of order p and an affine geometrical map, we choose $n = p + \mathrm{ceiling}(1/2) = p+1$ per direction to integrate exactly a mass matrix.

Symmetric quadrature rules on triangles and tetrahedra for different orders can also be constructed. In any case, to create arbitrarily large quadrature rules for n-simplices, one can consider the so-called Duffy transformation. The latter is a change of variables that transform our n-simplex integration domain into an n-cube, and integrate on the n-cube using tensor product quadratures.

Let us finally mention that in some instances, e.g., for integration Neumann boundary condition terms of the type $\int_{\Gamma_{\mathrm{N}}} h(x)v(x)\mathrm{d}F$ we can use the same ideas above. Instead of integrating over the cell, we would integrate on the faces. We can consider a reference facet $\hat{F}$, and a mapping $\boldsymbol{\Phi}_F : \hat{F} \to F$ from the reference to the physical space. Let us represent the Jacobian of the geometrical mapping with $\boldsymbol{J}_F \doteq \frac{\partial \boldsymbol{\Phi}_F}{\partial \boldsymbol{x}}$, which has values in $\mathbb{R}^{(d-1)\times d}$. We can rewrite the facet integral in the reference facet, and next consider a quadrature rule Q on $\hat{F}$ defined by a set of points/weights $(\hat{\boldsymbol{x}}_{\mathrm{gp}}, \mathrm{w}_{\mathrm{gp}})$, as follows:

$$\int_F \boldsymbol{\mathcal{I}}(\boldsymbol{x})\mathrm{d}\Omega = \int_{\hat{F}} \boldsymbol{\mathcal{I}}\circ\boldsymbol{\Phi}_F(\boldsymbol{x})|\boldsymbol{J}_F|\mathrm{d}F = \sum_{\hat{\boldsymbol{x}}_{\mathrm{gp}}\in\mathrm{Q}} \boldsymbol{\mathcal{I}}\circ\boldsymbol{\Phi}_F(\hat{\boldsymbol{x}}_{\mathrm{gp}})\mathrm{w}(\hat{\boldsymbol{x}}_{\mathrm{gp}})|\boldsymbol{J}_F(\hat{\boldsymbol{x}}_{\mathrm{gp}})|. \tag{3.22}$$

$|\boldsymbol{J}_F|$ is defined as:

$$|\boldsymbol{J}_F| = \left\| \frac{\mathrm{d}\boldsymbol{\Phi}_F}{\mathrm{d}\hat{\boldsymbol{x}}} \right\|_2 \quad \text{and} \quad |\boldsymbol{J}_F| = \left\| \frac{\partial \boldsymbol{\Phi}_F^1}{\partial \hat{\boldsymbol{x}}} \times \frac{\partial \boldsymbol{\Phi}_F^2}{\partial \hat{\boldsymbol{x}}} \right\|_2, \tag{3.23}$$

for $d = 2, 3$, respectively. The facet map can easily be computed using similar ideas as in Sect. 3.4.3. The idea is to consider the shape functions related to the nodes on the closure of $\hat{F}$ their position in the physical space:

$$\boldsymbol{\Phi}_F(\hat{\boldsymbol{x}}) \doteq \sum_{a \in \bar{\hat{F}}} \hat{\phi}_1^a \boldsymbol{x}^a,$$

where $\{\hat{\phi}_1^a\}$ are the shape functions for $\hat{\mathcal{Q}}_1$.

3.10 Grad-conforming finite elements for vector fields

When one has to deal with vector or tensor fields, we can generate them as a Cartesian product of scalar spaces as follows. We define the local finite element space $\boldsymbol{\mathcal{V}}_k \doteq [\mathcal{Q}_k]^d$ (or $[\mathcal{P}_k]^d$). The local degrees of freedom are nodal values for a given component, i.e.,

$$\sigma_a^\alpha(\boldsymbol{u}) = \boldsymbol{u}_\alpha(\boldsymbol{x}_a) \qquad \text{for } a = 1, \dots, n_\Sigma, \;\; \alpha = 1, \dots, d.$$

The equivalence class for the local-to-global map is such that two local degrees of freedom represent the same global one if the nodes are at the same point in the physical space and they are related to the same component. Analogously, shape functions are computed as $\phi^a \doteq \sum_{(i,\boldsymbol{s},K)\sim a} \ell_{\boldsymbol{s}}^{k\mathbf{1}} \vec{\boldsymbol{e}}_i$; $\vec{\boldsymbol{e}}_i$ represents the i-th canonical basis vector of $\mathbb{R}^d$. E.g., for a two-dimensional vector field, the bi-linear local finite element space reads

$$\boldsymbol{\mathcal{V}} \doteq \left\{ \left(\phi^1, 0\right)^T, \dots, \left(\phi^4, 0\right)^T, \left(0, \phi^1, \right)^T \dots, \left(0, \phi^4\right)^T \right\}$$

We proceed analogously for n-simplices.

3.11 Cartesian product of finite elements for multi-field problems

Many problems governed by PDEs involve more than one field, e.g., the Navier-Stokes equations or any multi-physics problem. Let us consider a PDE that involves a set of unknown fields $(\boldsymbol{u}_1, \dots, \boldsymbol{u}_n) \in \mathcal{X}^1 \times \dots \times \mathcal{X}^n$,

defined as the Cartesian product of functional spaces. We can proceed as above, and define a finite element space for every field space separately, leading to a global finite element space $\mathcal{X}_h^1 \times \ldots \times \mathcal{X}_h^n$ defined by composition of finite element spaces. To define the global numbering of DOFs in the multi-field case, we consider that two DOFs are equivalent if they are related to the same field and satisfy the equivalence relation of the finite element space of this field.

The Cartesian product of finite element spaces is enough to define volume-coupling multi-physics problems governed on the same physical domain, i.e., the different physics are defined on the whole domain and coupled through volume terms in the formulation. However, many multi-physics problems are interface-based, i.e., the coupling between different physics that are defined on different subdomains is through transmission conditions on the interface. This is the case, e.g., of fluid-structure problems. In these cases, different finite element spaces could be defined on different parts of the global mesh, i.e., one must describe the set of subdomains $(\Omega_1, \ldots, \Omega_n)$ of the whole domain Ω in which the corresponding finite element spaces are defined and enforce the *transmission* conditions on the interface (usually, continuity of the unknown and its flux).

3.12 Approximation properties

The same error estimates that we have already proven for one-dimensional spaces hold in the multi-dimensional case. The proof is more technical and it is out of the scope of this course. With these results about the approximability properties of the polynomial spaces considered so far, we can readily obtain bounds for the error commited by the finite element method by recalling Cea's lemma in the previous section.

Before showing error estimates, we need some properties for the family of meshes being used in the h-refinement process. As in the previous chapter, let us consider a parameter N that determines the level of refinement in our mesh; e.g., N can represent the number of uniform refinements through bisection for a given initial mesh $\mathcal{T}_0$.

Definition 3.12.1: Shape regular and quasi-uniform mesh

A family of meshes (a.k.a. triangulations) $\{\mathcal{T}_N\}$ is shape regular if there exists a positive constant $c > 0$ independent of N such that

$$\max_{\tau \in \mathcal{T}_N} \frac{\operatorname{diam}(\tau)^d}{|\tau|} \leq c, \qquad \forall N.$$

We can define the cell size $h_\tau = |\tau|^{\frac{1}{d}}$ for $\tau \in \mathcal{T}_N$. The family is also quasi-uniform if

$$\frac{\max_{\tau \in \mathcal{T}_N} |\tau|}{\min_{\tau \in \mathcal{T}_N} |\tau|} \leq \rho, \qquad \forall N.$$

For quasi-uniform families, we can define a mesh width $h_N \doteq \max_{\tau \in \mathcal{T}_N} h_\tau$.

Shape regularity means that cells cannot be arbitrarily anisotropic as we increase refinement. E.g., Let us consider $\mathcal{T}_0$ to be a rectangle. At each level of refinement rectangles are split into two rectangles by a horizontal cut. This way, we can keep conforming meshes at all levels, but as $N \to \infty$ the vertical dimension of the cell goes to zero whereas the horizontal remains constant. Thus, such family of meshes is not shape-regular. Shape regularity prevents *flat* elements as $N \to \infty$ and permits the definition of a meaningful length size. Meshes constructed by uniform refinement in all directions, e.g., split the rectangle into 4 scaled rectangles makes the shape regularity coefficient constant with respect to N.

Quasi-uniformity means that the size of all the cells in a mesh must be *similar*. We cannot refine some cells while keeping others untouched. This allows us to have a meaningful definition of meshwidth in the multidimensional case. This is an essential ingredient for the statement of the multi-dimensional interpolation error estimates.

Lemma 3.12.2: Error bounds for the interpolant

Given a finite element space of order p $\mathcal{Q}^p$ (for quad meshes) or $\mathcal{P}^p$ (for tet meshes) on a family of quasi-uniform meshes with mesh width h, the interpolant π^p holds:

$$\|v - \pi^p(v)\|_{L^2(\Omega)} \leq h^{p+1}|v|_{H^{p+1}(\Omega)}, \qquad |v - \pi(v)|_{H^1(\Omega)} \leq h^p|v|_{H^{p+1}(\Omega)},$$

for any $v \in H^{p+1}(\Omega)$.

3.13 Tutorials

1. Consider a linear reference finite element $[-1,1]^2$, use as prebasis of the local space the space of monomials that span $\mathcal{Q}_1$, and apply the change of basis to get the expression of the shape functions.

2. Let us consider the problem $-\Delta u = f$ on $\Omega \subset (0,1)^2$. Can you compute the shape function gradients at the reference finite element $[-1,1]^2$ space for a linear finite element (using the result from the previous exercise)? Can you compute the corresponding Jacobian in element $(0.0, 0.5)^2$? Can you compute the linear system matrix in that element? Let us consider the element with vertices $(0.0, 0.0)$, $(0.5, 0.0)$, $(0.0, 0.5)$ and $(0.6, 0.5)$. Can you compute the Jacobian in this case?

3. Consider a structured 2×2 uniform mesh of a unit square with 4 bilinear finite elements. Can you compute the global system matrix using this local-to-global numbering and the matrix in the previous exercise? Now consider biquadratic finite elements on the same mesh, i.e., $\mathcal{Q}_2$. Provide a local and global numbering using a drawing.

4. Can you prove why grad-conforming Lagrangian finite elements lead to continuous solutions across cells after *gluing* DOFs?

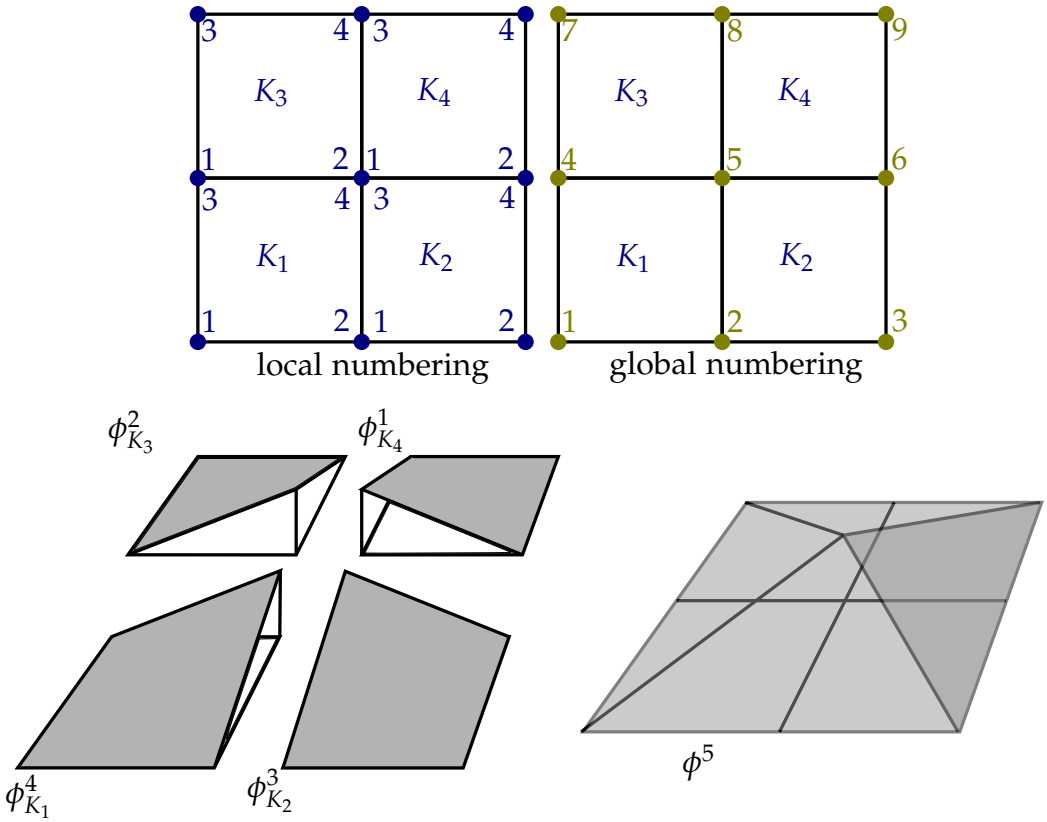


Figure 3.13: In the top-left corner we show the local numbering for each cell in a mesh. The top-right corner shows the global numbering for the same mesh. We can observe, e.g., that the local degrees of freedom (nodes) $\sigma^4_{K_1}$, $\sigma^3_{K_2}$, $\sigma^2_{K_3}$ and $\sigma^1_{K_4}$ correspond to the same global degree of freedom (node) σ_5. In the bottom-left part we show the corresponding local shape functions for these local degrees of freedom and the global shape function corresponding to the global degree of freedom.