# Chapter 1
# Introduction

The numerical solution of boundary value problems on polygonal and polyhedral discretizations is an emerging topic, and the interest on it increased continuously during the last few years. This work presents a self-contained and systematic introduction, study and application of the BEM-based FEM with high-order approximation spaces on general polytopal meshes in two and three space dimensions. This approach makes use of local boundary integral formulations that will also be discussed in more detail. The study of interpolation and approximation properties over isotropic and anisoptropic polytopal discretizations build fundamental concepts for the analysis and the development. The BEM-based FEM is applied to adaptive FEM strategies, yielding locally refined meshes with naturally included hanging nodes, and to convection-diffusion-reaction problems, showing stabilizing effects while incorporating the differential equation into the approximation space. All theoretical considerations are substantiated with several numerical tests and examples.

## 1.1 Overview

Computer simulations play a crucial role in modern research institutes and development departments of all areas. The simulations rely on physical models which describe the underlying principles and the interplay of all components. Such properties are often modelled by differential equations and in particular by boundary value problems in the mathematical framework. In order to realise these formulations on a computer, discretizations have to be introduced such that the unknown quantities of interest can be approximated accurately and efficiently. The probably most accepted and most successful discretization strategy for boundary value problems in science and engineering is the finite element method (FEM). Furthermore, there are the discontinuous Galerkin (DG), the finite volume (FV) and the boundary element methods (BEM), which all have their advantages in certain application areas.



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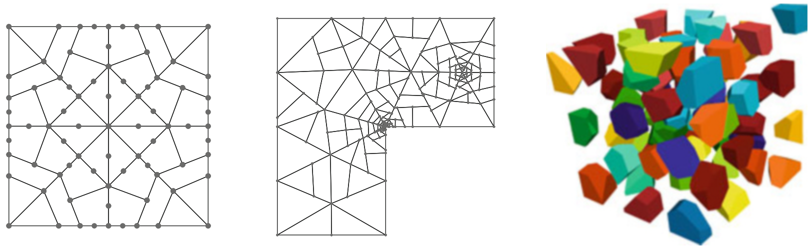

**Fig. 1.1** Polygonal and polyhedral meshes

Most of these approaches, and in particular the finite element method, rely on the decomposition of the computational domain into simplicial elements, which include triangles as well as quadrangles in two-dimensions and tetrahedra as well as hexahedra in three-dimensions. These elements form the mesh of the domain that is utilized in the discretization of the corresponding function spaces containing the sought quantities. In high-performance computing and in applications needing accurate and efficient results, the use of problem adapted meshes is essential. Such meshes might be constructed using a priori knowledge or adaptive finite element strategies, which successively and automatically refine the meshes in appropriate regions. But in all these cases the meshes have to be admissible and satisfy some regularity properties. Nowadays, there are efficient approaches, which deal with these mesh requirements. Nevertheless, they still have to be considered in the implementations. Such issues appear in contact problems and when some parts of the computational domain are meshed independently. Obviously, the restrictive nature is caused by the small variety of supported element shapes. This also results in difficulties, when meshing complex geometries.

An enormous gain on flexibility is achieved by the use of polygonal (2D) and polyhedral (3D) meshes in the discretizations, cf. Fig. 1.1. General polygonal and polyhedral element shapes adapt more easily to complex situations. They naturally include so called hanging nodes, for example, which cause additional effort in classical meshes when dealing with adaptivity or non-matching meshes. Already in 1975, Wachspress [172] proposed the construction of conforming rational basis functions on convex polygons with any number of sides for the finite element method. In that time, however, the construction was not attractive for the realization in efficient computer codes, since the processing power was too low. The advent of mean value coordinates [75] in 2003 was a turning point in the sustained interest and further development of finite element methods on polygonal meshes. Only recently, these meshes received a lot of attentions. Several improved basis functions on polygonal elements have been introduced and applied in linear elasticity for example, see [164, 165]. They are often referred to generalized barycentric coordinates and polygonal finite elements. Beside of mean value coordinates [75, 101], there are maximum entropy coordinates [12, 102, 163] and several others as described in the book *Generalized Barycentric Coordinates in Computer Graphics and Computational Mechanics*, see [103]. These coordinates are applied in computer graphics for character articulation [112, 126], for instance. A mathematical discussion of properties and applications as well as an error analysis can be found in [77, 84]. An up-to-date survey of barycentric coordinates is given in [76, 103].

Beside of the polygonal finite element methods, the finite volume methods are successfully applied on polygonal and polyhedral meshes [57]. These methods produce non-conforming approximations and they are popular in computational fluid dynamics (CFD), where polyhedral meshes often yield more accurate results as structured grids. Due to this advantage, the polyhedral meshes for CFD simulations with finite volume approximations were integrated in software packages like OpenFOAM, ANSYS Fluent and STAR-CD from CD-adapco. The mimetic finite difference methods [124] are a related methodology, which have been initially stated on orthogonal meshes and have then be transferred to general polyhedral discretizations. A mathematical analysis on general meshes has been performed in [46] and only a few years ago new insights enabled conforming and arbitrary order approximations within mimetic discretizations [24]. A detailed discussion and introduction can be found in the monograph [27]. The newly derived concept gave rise to the development of the virtual element method (VEM), see [25]. The analysis of VEM is performed in the finite element framework, which offers a rich set of tools. Since 2013, the development of VEM spread fast into several areas including linear elasticity [26, 81], the Helmholtz [138] and the Navier–Stokes problem [32], mixed formulations [42], stabilizations for convection problems [33], adaptivity [23, 31, 35, 50] and many more. Further non-conforming discretization techniques, that are applied and analysed on polygonal and polyhedral meshes, are the discontinuous Galerkin [66] and the recently introduced hybrid higher-order [65] and weak Galerkin [173] methods.

Another conforming approximation scheme came up in parallel to VEM when D. Copeland, U. Langer and D. Pusch proposed to study the boundary element domain decomposition methods [106] in the framework of finite element methods in [60]. This class of discretization methods uses PDE-harmonic shape functions in every element of a polytopal mesh. Therefore, these methods can be considered as local Trefftz FEM following the early work [168]. In order to generate the local stiffness matrices efficiently, boundary element techniques are employed locally. This is the reason why these non-standard finite element methods are called BEM-based FEM. The papers [95] and [93] provide the a priori discretization error analysis with respect to the energy and $L_2$ norms, respectively, where homogeneous diffusion problems serve as model problems. Fast FETI-type solvers for solving the large linear systems arising from the BEM-based FEM discretization of diffusion problems are studied in [97, 98]. Residual-type a posteriori discretization error estimates are derived in a sequence of papers for adaptive versions of the BEM-based FEM [174, 178–180, 182] and anisotropic polytopal elements are studied in [181]. Additionally, high-order trial functions are introduced in [145, 146, 175, 177], which open the development towards fully $hp$-adaptive strategies. Furthermore, the ideas of BEM-based FEM are transferred into several other application areas. There are, for instance, first results on vector valued, $H(\mathrm{div})$-conforming approximations [73] and on time dependent problems [176]. Additionally, the notion of anisotropic polytopal elements has been applied to VEM [9]. The construction of PDE-harmonic trial functions seems to be especially appropriate for convection-diffusion-reaction problems. First results are presented in [96] and extended in [99] utilizing the hierarchical construction discussed in [147].

One of the probably most attractive features of polygonal and polyhedral meshes is their enormous flexibility, which has not been fully exploited in the literature so far. In modern high-performance computations the use of problem adapted meshes is one of the key ingredients for their success. The finite element method is often combined with an adaptive strategy, where the mesh is successively adapted to the problem. Error indicators gauge the approximation quality and steer a local mesh refinement procedure. Refining classical elements like triangles and tetrahedra affect their neighbouring elements in the mesh. After subdividing several elements, the neighbours are not correctly aligned any more. Therefore, some kind of post-processing is mandatory in order to maintain the mesh admissibility. When polygonal and polyhedral elements are used, local refinements might affect the neighbouring elements, but these elements are still polygonal and polyhedral and are thus naturally supported. This effect solves the handling of so called hanging nodes and it has been demonstrated in [174]. Although this is a fruitful topic, there are only few results available on a posteriori error analysis and adaptivity for conforming approximation methods on polygonal and polyhedral meshes. For the virtual element method see [23, 31, 35, 50] and for the mimetic discretization technique there are also only several references which are limited to low order methods, compare the recent work [7]. Further analysis on quasi-interpolation operators, residual-based error estimates and local mesh refinement for polygonal elements has been performed in [174, 178] with applications to the BEM-based FEM. Additionally, an extension to non-convex elements and high-order approximations with upper and lower bounds for the residual-based error estimator is derived in [180]. Beside of the classical residual-based error estimation techniques, there exist goal-oriented error estimation [22]. Instead of considering the energy error, goal-oriented strategies allow for adaptive refinement steered by some quantity of interest. Thus, these methods are practical in engineering simulations. First results on polygonal meshes have been obtained in [182].

Problem adapted meshes are also utilized in computations, where sharp layers in the solution are expected. This appears in convection-dominated problems, for instance. If the unknown solution changes rapidly in one direction but rather slowly orthogonal to it, anisotropic meshes are beneficial in finite element computations. These meshes contain anisotropic tetrahedral and hexahedral elements which are stretched in one or two directions but thin in the others. In contrast to the usual, isotropic meshes these stretched elements need special care in their analysis. The anisotropy of the mesh has to be aligned with the anisotropy of the approximated function in order to obtain satisfactory results [10]. The quality of the alignment is reflected in a posteriori error estimates [119]. Such estimates can be used to steer an adaptive refinement strategy with anisotropic elements [11, 79]. In comparison to adaptive, isotropic mesh refinement, less elements are required and the efficiency is increased. Simplicial meshes with triangles and tetrahedra or rectangles and hexahedra have often restrictions on their possible anisotropic refinements. Therefore, the initial mesh should be aligned already with the sought function. The use of polygonal and polyhedral elements simplifies the anisotropic refinement, since they do not rely on any restricted direction for subdividing the elements. These new opportunities have been exploited in [9, 181].

The BEM-based FEM has its advantageous not only in the treatment of general meshes. It can be considered a local Trefftz method. This means that the shape functions in the approximation space are build with accordance to the differential equation in the underlying problem. These shape functions satisfy the homogeneous differential equation locally and thus build in some features of the problem into the approximation space. This behaviour has been studied numerically for convection-dominated diffusion problems in [96]. Where conventional approaches without any stabilization lead to oscillations in the solution, the BEM-based FEM remains stable for increased Péclet numbers, i.e., in the convection-dominated regime. The results have been improved in [99], where the idea of Trefftz approximations has been build in on the level of polyhedral elements, their polygonal faces and on the edges of the discretization. Comparisons with a stabilized FEM, the Streamline Upwind/Petrov-Galerkin (SUPG) method [48], have shown an improved resolution of exponential layers at outflow boundaries.

The use of local Trefftz-type approximation spaces is also studied in other areas. One example is the plane wave approximation for the Helmholtz equation [91] or the Trefftz-DG method for time-harmonic Maxwell equations [92]. The combination and coupling of such innovative approaches is quite appealing in order to combine the flexibility of polygonal and polyhedral meshes with problem adapted approximation spaces. Just recently, plane waves have been combined with the virtual element method [138]. All these quite new developments have a great potential and might benefit from each other. Their interplay has been studied rarely and opens opportunities for future developments.

## 1.2 Outline

The aim of this book is to give a systematic introduction, study and application of the BEM-based FEM. The topics range from high-order approximation spaces on isotropic as well as anisotropic polytopal meshes over a posteriori error estimation and adaptive mesh refinement to specialized adaptations of approximation spaces and interpolation operators. The chapters are organized as follows.

Chapter 2 contains a discussion of polygonal as well as polyhedral meshes including regularity properties and their treatment in mesh refinement. Furthermore, the construction of basis functions is carried out for an approximation space over these general meshes. They are applied in the formulation of the BEM-based FEM, which is obtained by means of a Galerkin formulation. Its convergence and approximation properties are analysed with the help of introduced interpolation operators.

In Chap. 3, best approximation results and trace inequalities are given for polytopal elements. By their application, quasi-interpolation operators for non-smooth functions over polytopal meshes are introduced and analysed. In particular, operators of Clément- and Scott–Zhang-type are studied. Furthermore, the notion of anisotropic meshes is established for polytopal discretizations. These meshes do not satisfy the classical regularity properties introduced in Chap. 2. Consequently, they have to be treated in a special way.

The local problems in the definition of basis functions for the BEM-based FEM are handled by means of boundary integral equations. Chapter 4 gives a short introduction into this topic with a special emphasis on its application in the BEM-based FEM. Therefore, the boundary integral operators for the Laplace problem are reviewed in two- and three-dimensions and corresponding boundary integral equations are derived. Their discretization is realized by a Galerkin boundary element method and by an alternative approach that relies on the Nyström method.

In Chap. 5, adaptive mesh refinement strategies are applied to polytopal meshes in the presence of singularities. In particular, a posteriori error estimates are derived which are used to drive the adaptive procedure. For the error estimation, the classical residual based error estimator as well as goal-oriented techniques are covered on general polytopal meshes. Whereas, the reliability and efficiency estimates for the first mentioned estimator are proved, the benefits and potentials of the second one are discussed for general meshes.

In Chap. 6, some further developments and extensions are taken up. The introduction of $H(\mathrm{div})$-conforming approximation spaces in the sense of the BEM-based FEM is highlighted. Additionally, a hierarchical construction of basis functions in three-dimensions is discussed and applied to convection-diffusion-reaction problems. The presented strategy integrates the underlying differential equation into the approximation space and yields therefore stabilizing properties.

Throughout the book, there are numerical examples, tests and experiments that illustrate and substantiate the theoretical findings.

## 1.3 Mathematical Preliminaries

In the following, we summarize some mathematical preliminaries on variational formulations and we give the definition of certain function spaces. For the precise definitions, however, we refer to the specialized literature. The classical results on Sobolev spaces can be found in Adams [1], and for Sobolev spaces of rational exponent we refer to Grisvard [87]. A detailed discussion on Sobolev spaces on manifolds and their application to boundary integral equations is given in

McLean [128]. The experienced reader might skip the following sections and come back to them if needed. This section serves as reference only and does not contain all mathematical details.

### 1.3.1 Function Spaces and Trace Operators

In the study of boundary value problems, the solutions have to be specified in proper function spaces. In the following, we give definitions of several spaces. For this reason, let $\Omega$ be any measurable subset of $\mathbb{R}^d$, $d \in \mathbb{N}$ with strictly positive Lebesgue measure. The Banach spaces $L_1(\Omega)$ and $L_2(\Omega)$ are defined in the usual way with the corresponding norms

$$\|u\|_{L_1(\Omega)} = \int_\Omega |u(\mathbf{x})| \,\mathrm{d}\mathbf{x} \quad \text{and} \quad \|u\|_{L_2(\Omega)} = \left( \int_\Omega |u(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \right)^{1/2} ,$$

respectively. Here, the symbol $|\cdot|$ denotes the absolute value. But in other contexts, it might denote the Euclidean norm, the $d$ or $d-1$ dimensional measure or even the cardinality of a discrete set. Furthermore, let the space of locally integrable functions be labeled by

$$L_1^{loc}(\Omega) = \{u : u \in L_1(K) \text{ for any compact } K \subset \Omega\} .$$

The space $L_2(\Omega)$ together with the inner product

$$(u, v)_{L_2(\Omega)} = \int_\Omega u(\mathbf{x}) v(\mathbf{x}) \,\mathrm{d}\mathbf{x}$$

becomes a Hilbert space. Additionally, we denote by $L_\infty(\Omega)$ the space of measurable and almost everywhere bounded functions. It is equipped with the norm

$$\|u\|_{L_\infty(\Omega)} = \operatorname*{ess\,sup}_{\mathbf{x}\in\Omega} |u(\mathbf{x})| = \inf_{K\subset\Omega, |K|=0} \sup_{\mathbf{x}\in\Omega\setminus K} |u(\mathbf{x})| ,$$

where $|K|$ is the $d$ dimensional Lebesgue measure of $K$. For a $d-1$ dimensional manifold $\Gamma$, the space $L_2(\Gamma)$ is defined in an analog way. Here, the surface measure is used instead of the volume measure.

The space of continuous functions over $\Omega$ is denoted by $C^0(\Omega)$ and equipped with the supremum norm

$$\|u\|_{C^0(\Omega)} = \sup_{\mathbf{x}\in\Omega} |u(\mathbf{x})| .$$

Let $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ be a multi-index, i.e., a $d$-tuple with non-negative entries, and set

$$|\alpha| = \alpha_1 + \cdots + \alpha_d \quad \text{as well as} \quad \partial^\alpha = \left(\frac{\partial}{\partial x_1}\right)^{\alpha_1} \cdots \left(\frac{\partial}{\partial x_d}\right)^{\alpha_d} .$$

The order of the partial derivative $\partial^\alpha$ is the number $|\alpha|$. For any integer $k \geq 0$ and $\Omega$ open, we define

$$C^k(\Omega) = \{u : \partial^\alpha u \text{ exists and is continuous on } \Omega \text{ for } |\alpha| \leq k\} .$$

In the special case that $k = 0$, the space of continuous functions over $\Omega$ is recovered. Furthermore, we define

$$C_0^k(\Omega) = \{u \in C^k(\Omega) : \operatorname{supp} u \subset \Omega\} ,$$

where

$$\operatorname{supp} u = \overline{\{\mathbf{x} \in \Omega : u(\mathbf{x}) \neq 0\}} ,$$

and set

$$C^\infty(\Omega) = \bigcap_{k \geq 0} C^k(\Omega) \quad \text{as well as} \quad C_0^\infty(\Omega) = \bigcap_{k \geq 0} C_0^k(\Omega) .$$

Finally, we review the space of Lipschitz functions

$$C^{0,1}(\Omega) = \{u \in C^0(\Omega) : \exists\, L > 0 : |u(\mathbf{x}) - u(\mathbf{y})| \leq L|\mathbf{x} - \mathbf{y}| \text{ for } \mathbf{x}, \mathbf{y} \in \Omega\}$$

and

$$C^{k,1}(\Omega) = \{u \in C^k(\Omega) : \partial^\alpha u \in C^{0,1}(\Omega) \text{ for } |\alpha| = k\}$$

for $k \in \mathbb{N}$. The space of Hölder continuous functions is a straightforward generalization. For $\kappa \in (0, 1]$, it is

$$C^{0,\kappa}(\Omega) = \{u \in C^0(\Omega) : \exists\, C > 0 : |u(\mathbf{x}) - u(\mathbf{y})| \leq C|\mathbf{x} - \mathbf{y}|^\kappa \text{ for } \mathbf{x}, \mathbf{y} \in \Omega\}$$

and

$$C^{k,\kappa}(\Omega) = \{u \in C^k(\Omega) : \partial^\alpha u \in C^{0,\kappa}(\Omega) \text{ for } |\alpha| = k\}$$

for $k \in \mathbb{N}$.

#### 1.3.1.1 Sobolev Spaces

Let $\Omega$ be a non-empty open subset of $\mathbb{R}^d$, $d \in \mathbb{N}$. The Sobolev space $H^k(\Omega)$ of order $k \in \mathbb{N}_0$ is defined by

$$H^k(\Omega) = \{u \in L_2(\Omega) : \partial^\alpha u \in L_2(\Omega) \text{ for } |\alpha| \leq k\} \tag{1.1}$$

with the norm $\|\cdot\|_{H^k(\Omega)}$ and the semi-norm $|\cdot|_{H^k(\Omega)}$, where

$$\|u\|_{H^k(\Omega)} = \left(\sum_{|\alpha|\leq k} \|\partial^\alpha u\|^2_{L_2(\Omega)}\right)^{1/2} \quad \text{and} \quad |u|_{H^k(\Omega)} = \left(\sum_{|\alpha|=k} \|\partial^\alpha u\|^2_{L_2(\Omega)}\right)^{1/2}.$$

Here, the partial derivative $\partial^\alpha u$ has to be understood in the weak sense. More precisely, let the functional $g_\alpha : C_0^\infty(\Omega) \to \mathbb{R}$ be the distributional derivative of $u$ with index $\alpha$, i.e., $g_\alpha$ satisfies

$$(u, \partial^\alpha \varphi)_{L_2(\Omega)} = (-1)^{|\alpha|} g_\alpha(\varphi)$$

for all $\varphi \in C_0^\infty(\Omega)$. Furthermore, let $g_\alpha$ have the representation

$$g_\alpha(\varphi) = \int_\Omega \varphi(\mathbf{x})\, \partial^\alpha u(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

for all $\varphi \in C_0^\infty(\Omega)$ with some function $\partial^\alpha u \in L_1^{loc}(\Omega)$ which is defined uniquely up to an equivalence class. In this case, $\partial^\alpha u$ is called the weak derivative of $u$ with index $\alpha$. The additional condition $\partial^\alpha u \in L_2(\Omega)$ in (1.1) ensures that the weak derivative can be chosen such that it is square integrable.

For the definition of Sobolev spaces with fractional order $s \geq 0$, let $s = k + \mu$ with $k \in \mathbb{N}_0$ and $\mu \in [0, 1)$. The Sobolev–Slobodekij norm is given by

$$\|u\|_{H^s(\Omega)} = \left(\|u\|^2_{H^k(\Omega)} + \sum_{|\alpha|=k} |\partial^\alpha u|^2_{H^\mu(\Omega)}\right)^{1/2},$$

where

$$|u|_{H^\mu(\Omega)} = \left(\int_\Omega \int_\Omega \frac{|u(\mathbf{x}) - u(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|^{d+2\mu}}\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{y}\right)^{1/2}.$$

Therefore, we define

$$H^s(\Omega) = \{u \in H^k(\Omega) : |\partial^\alpha u|_{H^\mu(\Omega)} < \infty \text{ for } |\alpha| = k\}.$$

The Sobolev norm $\|\cdot\|_{H^s(\Omega)}$ for arbitrary real $s \geq 0$ is induced by the inner product

$$(u, v)_{H^s(\Omega)} = (u, v)_{H^k(\Omega)} + \sum_{|\alpha|=k} (\partial^\alpha u, \partial^\alpha v)_{H^\mu(\Omega)}$$

with

$$(u, v)_{H^k(\Omega)} = \sum_{|\alpha|\leq k} (\partial^\alpha u, \partial^\alpha v)_{L_2(\Omega)}$$

and

$$(u, v)_{H^\mu(\Omega)} = \int_\Omega \int_\Omega \frac{\big(u(\mathbf{x}) - u(\mathbf{y})\big)\big(v(\mathbf{x}) - v(\mathbf{y})\big)}{|\mathbf{x} - \mathbf{y}|^{d+2\mu}} \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{y} \, .$$

Hence, $H^s(\Omega)$ is a Hilbert space for all $s \geq 0$.

#### 1.3.1.2 Sobolev Spaces on the Boundary

For the definition of Sobolev spaces on the boundary of a domain, we have to restrict the class of admitted domains. Therefore, let $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$ be a bounded open set with boundary $\Gamma$. Additionally, we assume that $\Gamma$ is non-empty and has an overlapping cover that can be parametrized in the way

$$\Gamma = \bigcup_{i=1}^{p} \Gamma_i \, , \quad \Gamma_i = \left\{ \mathbf{x} \in \mathbb{R}^d : \mathbf{x} = \chi_i(\xi) \text{ for } \xi \in K_i \subset \mathbb{R}^{d-1} \right\} \, . \tag{1.2}$$

With regard to the decomposition of $\Gamma$, let $\{\varphi_i\}_{i=1}^p$ be a partition of unity with non-negative cut off functions $\varphi_i \in C_0^\infty(\mathbb{R}^d)$ such that

$$\sum_{i=1}^{p} \varphi_i(\mathbf{x}) = 1 \quad \text{for } \mathbf{x} \in \Gamma \, , \qquad \varphi_i(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \Gamma \setminus \Gamma_i \, .$$

For a function $u$ defined on $\Gamma$, we write

$$u(\mathbf{x}) = \sum_{i=1}^{p} u(\mathbf{x})\varphi_i(\mathbf{x}) = \sum_{i=1}^{p} u_i(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Gamma \, ,$$

where $u_i(\mathbf{x}) = u(\mathbf{x})\varphi_i(\mathbf{x})$. In the next step, $\mathbf{x}$ is replaced by the parametrisation from (1.2) and we obtain

$$u_i(\mathbf{x}) = u(\mathbf{x})\varphi_i(\mathbf{x}) = u(\chi_i(\xi))\varphi_i(\chi_i(\xi)) \quad \text{for } \xi \in K_i \subset \mathbb{R}^{d-1}, \; i = 1, \ldots, p \, .$$

The last expression is abbreviated to $\widetilde{u}_i(\xi)$. These functions are defined on bounded subsets of $\mathbb{R}^{d-1}$, and thus the Sobolev spaces from Sect. 1.3.1.1 can be used. To satisfy $u_i \in H^s(K_i)$ for $s > 0$, the corresponding derivatives of the parametrisation $\chi_i$ have to exist. For the definition of these derivatives of order up to $s \leq k$, we have to assume $\chi_i \in C^{k-1,1}(K_i)$.

For $0 \leq s \leq k$, the Sobolev norm

$$\|u\|_{H^s(\Gamma),\chi} = \left( \sum_{i=1}^{p} \|u_i\|^2_{H^s(K_i)} \right)^{1/2} ,$$

which depends on the parametrisation of $\Gamma$, is defined. By the use of this norm the Sobolev spaces $H^s(\Gamma)$ can be introduced. For a Lipschitz domain $\Omega$ and $s \in (0,1)$, the Sobolev–Slobodekij norm

$$\|u\|_{H^s(\Gamma)} = \left( \|u\|^2_{L_2(\Gamma)} + \int_\Gamma \int_\Gamma \frac{|u(\mathbf{x}) - u(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|^{d-1+2s}} \, \mathrm{d}s_{\mathbf{x}} \, \mathrm{d}s_{\mathbf{y}} \right)^{1/2}$$

is equivalent to $\|\cdot\|_{H^s(\Gamma),\chi}$, and thus, the space $H^s(\Gamma)$ is independent of the parametrisation chosen in (1.2). For $s < 0$, we define $H^s(\Gamma)$ as the dual space of $H^{-s}(\Gamma)$ and equip it with the norm

$$\|u\|_{H^s(\Gamma)} = \sup_{0 \neq v \in H^{-s}(\Gamma)} \frac{|u(v)|}{\|v\|_{H^{-s}(\Gamma)}} .$$

Additionally, we need some spaces which are only defined on a part of the boundary. Let $\Gamma_0$ be an open part of the sufficiently smooth boundary $\Gamma$. For $s \geq 0$, we set the Sobolev space

$$H^s(\Gamma_0) = \left\{ u = \widetilde{u}|_{\Gamma_0} : \widetilde{u} \in H^s(\Gamma) \right\}$$

with the norm

$$\|u\|_{H^s(\Gamma_0)} = \inf_{\widetilde{u} \in H^s(\Gamma) : \widetilde{u}|_{\Gamma_0} = u} \|\widetilde{u}\|_{H^s(\Gamma)} .$$

Furthermore, let

$$\widetilde{H}^s(\Gamma_0) = \left\{ u = \widetilde{u}|_{\Gamma_0} : \widetilde{u} \in H^s(\Gamma), \ \operatorname{supp} \widetilde{u} \subset \Gamma_0 \right\} ,$$

and for $s < 0$, we set $H^s(\Gamma_0)$ as the dual space of $\widetilde{H}^s(\Gamma_0)$. Finally, we define a Sobolev space over the boundary with piecewise regularity. Therefore, let

$$\Gamma = \bigcup_{i=1}^{p} \overline{\Gamma}_i , \qquad \Gamma_i \cap \Gamma_j = \varnothing \quad \text{for } i \neq j ,$$

and define

$$H^s_{\mathrm{pw}}(\Gamma) = \left\{ u \in H^{\min\{\frac{d-1}{2}, s\}}(\Gamma) : u|_{\Gamma_i} \in H^s(\Gamma_i),\ i = 1, \dots, p \right\} .$$

This space is equipped with the norm

$$\|u\|_{H^s_{\mathrm{pw}}(\Gamma)} = \left( \sum_{i=1}^{p} \|u|_{\Gamma_i}\|^2_{H^s(\Gamma_i)} \right)^{1/2} .$$

#### 1.3.1.3 Properties of Sobolev Spaces

To state some properties of Sobolev spaces, we have to guarantee certain regularities of the domain $\Omega$ and its boundary $\Gamma$. Therefore, we take from [87] the following definition.

**Definition 1.1** Let $\Omega$ be an open subset of $\mathbb{R}^d$. We say that its boundary $\Gamma$ is continuous (respectively Lipschitz, continuously differentiable, of class $C^{k,1}$, $k$ times differentiable) if for every $\mathbf{x} \in \Gamma$ there exists a neighbourhood $U$ of $\mathbf{x}$ in $\mathbb{R}^d$ and new orthogonal coordinates $\{\xi_1, \dots, \xi_d\}$ such that

1. $U$ is an hypercube in the new coordinates:

$$U = \{(\xi_1, \dots, \xi_d) : -c_i < \xi_i < c_i,\ i = 1, \dots, d\} ,$$

2. there exists a continuous (respectively Lipschitz, continuous differentiable, of class $C^{k,1}$, $k$ times continuously differentiable) function $f$, defined in

$$U' = \{(\xi_1, \dots, \xi_{d-1}) : -c_i < \xi_i < c_i,\ i = 1, \dots, d-1\} ,$$

and such that

$$|f(\xi')| \le c_d/2 \quad \text{for every } \xi' = (\xi_1, \dots, \xi_{d-1}) \in U' ,$$
$$\Omega \cap U = \{\xi = (\xi', \xi_d) \in U : \xi_d < f(\xi')\} ,$$
$$\Gamma \cap U = \{\xi = (\xi', \xi_d) \in U : \xi_d = f(\xi')\} .$$

If $\Omega$ has a Lipschitz boundary, we call $\Omega$ a Lipschitz domain. From now on, we restrict ourselves to bounded domains $\Omega$. So, the boundary $\Gamma$ is compact, and thus there is a finite cover of $\Gamma$, which can be used to construct a parametrisation as given in (1.2). We state the famous Sobolev embedding theorem, see, e.g., [1, 49].

**Theorem 1.2 (Sobolev Embedding)** *Let $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$ be a bounded domain with Lipschitz boundary and let $2k > d$ with $k \in \mathbb{N}$. For $u \in H^k(\Omega)$, it is*

*$u \in C^0(\overline{\Omega})$ and there exists a constant $C_S > 0$ such that*

$$\|u\|_{C^0(\overline{\Omega})} \le C_S \|u\|_{H^k(\Omega)} \quad \text{for } u \in H^k(\Omega) \; .$$

*Remark 1.3* In [49], it is shown that for convex domains $\Omega$ with diameter smaller or equal to one, the constant in Theorem 1.2 has the form

$$C_S = c\,|\Omega|^{-1/2}$$

with a constant $c > 0$ which only depends on $d$ and $k$.

Next, we give some results for traces of functions in Sobolev spaces. For sufficiently smooth functions $u$ over $\overline{\Omega}$, we set the trace operator $\gamma_0$ as restriction of $u$ to the boundary $\Gamma$, i.e.

$$\gamma_0 u = u\big|_\Gamma \; .$$

This operator has continuous extensions such that the following theorems taken from [61] and [128] are valid.

**Theorem 1.4** *If the bounded subset $\Omega$ of $\mathbb{R}^d$ has a boundary $\Gamma$ of class $C^{k-1,1}$ and if $1/2 < s \le k$, then*

$$\gamma_0 : H^s(\Omega) \to H^{s-1/2}(\Gamma)$$

*is a bounded linear operator, i.e.*

$$\|\gamma_0 u\|_{H^{s-1/2}(\Gamma)} \le c_T \; \|u\|_{H^s(\Omega)} \quad \text{for } u \in H^s(\Omega) \; .$$

*This operator has a continuous right inverse*

$$\mathfrak{E} : H^{s-1/2}(\Gamma) \to H^s(\Omega)$$

*with $\gamma_0 \mathfrak{E} v = v$ for all $v \in H^{s-1/2}(\Gamma)$ and*

$$\|\mathfrak{E} v\|_{H^s(\Omega)} \le c_{IT} \; \|v\|_{H^{s-1/2}(\Gamma)} \quad \text{for } v \in H^{s-1}(\Gamma) \; .$$

**Theorem 1.5** *If $\Omega \subset \mathbb{R}^d$ is a bounded domain with Lipschitz boundary $\Gamma$, then the trace operator $\gamma_0$ is bounded for $\frac{1}{2} < s < \frac{3}{2}$.*

### *1.3.2 Galerkin Formulations*

At several places in this book, we are concerned with operator equations and in particularly with weak formulations of differential equations. These are treated by means of Galerkin formulations in the continuous as well as in the discretized versions. We also call these formulations variational problems. In the following, we give a summary on this topic.

Let $V$ be a Hilbert space with inner product $(\cdot,\cdot)_V$ and corresponding induced norm $\|\cdot\|_V = \sqrt{(\cdot,\cdot)_V}$. The abstract setting of a Galerkin formulation is

$$\text{Find } u \in V: \quad a(u,v) = \ell(v) \quad \forall v \in V\ , \tag{1.3}$$

where $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ denotes a bilinear and $\ell(\cdot) : V \to \mathbb{R}$ a linear form. The bilinear form is said to be continuous or bounded on $V$ if there exists a constant $c_1 > 0$ such that

$$|a(u,v)| \le c_1 \|u\|_V \|v\|_V \quad \text{for } u, v \in V\ .$$

Furthermore, $a(\cdot,\cdot)$ is called $V$-elliptic if there is another constant $c_2 > 0$ such that

$$a(v,v) \ge c_2 \|v\|_V^2 \quad \text{for } v \in V\ .$$

Analogously, $\ell(\cdot)$ is said to be continuous if

$$|\ell(v)| \le c_\ell \|v\|_V \quad \text{for } v \in V\ ,$$

for a constant $c_\ell > 0$. Hence, a continuous linear form is a bounded functional on $V$ and therefore, it belongs to the dual space of $V$.

**Theorem 1.6 (Lax–Milgram Lemma)** *Let $V$ be a Hilbert space, $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ be a continuous $V$-elliptic bilinear form, and let $\ell : V \to \mathbb{R}$ be a continuous linear form. The abstract variational problem* (1.3) *has one and only one solution.*

In the proof of the Lax–Milgram Lemma, the Riesz representation theorem is utilized, see, e.g., [58] or the original work [121].

**Theorem 1.7 (Riesz Representation Theorem)** *Let $V'$ be the dual space of $V$ equipped with the norm*

$$\|\ell\|_{V'} = \sup_{0 \ne v \in V} \frac{|\ell(v)|}{\|v\|_V}\ .$$

*For each $\ell \in V'$, there exists a unique $u \in V$ such that*

$$(u,v)_V = \ell(v) \quad \textit{for } v \in V$$

*and*

$$\|u\|_V = \|\ell\|_{V'}\ .$$

In the numerics, it is not possible to work with the space $V$ directly. Therefore, a finite dimensional subspace $V_h$ of $V$ is introduced and the discrete Galerkin formulation

$$\text{Find } u_h \in V_h : \quad a(u_h, v_h) = \ell(v_h) \quad \forall v_h \in V_h \tag{1.4}$$

is considered. Since $V_h \subset V$, the method is said to be conforming. Due to the finite dimension of $V_h$, we can introduce a basis $\Psi$ with $V_h = \operatorname{span} \Psi$ and $\dim V_h = n$ for some $n \in \mathbb{N}$. Next, we express $u_h$ as linear combination of basis functions

$$u_h = \sum_{\psi \in \Psi} u_\psi \psi \ ,$$

and we have to test (1.4) only with $v_h = \varphi$ for all $\varphi \in \Psi$. Consequently, we end up with a system of linear equations to compute the unknown coefficients $u_\psi$ of $u_h$. More precisely, let $\underline{u}_h$ be the vector with components $u_\psi$, i.e. $\underline{u}_h = \big(u_\psi\big)_{\psi \in \Psi}$. We obtain

$$A\underline{u}_h = b \tag{1.5}$$

with

$$A = \big(a(\psi, \varphi)\big)_{\varphi,\psi \in \Psi} \in \mathbb{R}^{n \times n} \quad \text{and} \quad b = \big(\ell(\varphi)\big)_{\varphi \in \Psi} \in \mathbb{R}^n \ .$$

The system matrix $A$ is positive definite because of the $V$-ellipticity of the bilinear form $a(\cdot,\cdot)$. Therefore, the $n \times n$ system of linear equations admits a unique solution. If the system (1.5) of linear equations is small, we use an efficient direct solver of LAPACK [6]. In case of large systems, however, iterative solvers are preferable. For symmetric matrices we apply the conjugate gradient method (CG) [90] and for non-symmetric matrices we utilize GMRES [150].

Nevertheless, the question remains how the Galerkin formulations (1.3) and (1.4) are related to each other. Céa's Lemma gives the answer. The discrete Galerkin formulation (1.4) yields the quasi-best approximation of the solution of (1.3).

**Lemma 1.8 (Céa's Lemma)** *Let $V$ be a Hilbert space and $V_h \subset V$ a finite dimensional subspace of $V$, let $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ be a continuous $V$-elliptic bilinear form, and let $\ell : V \to \mathbb{R}$ be a continuous linear form. Furthermore, let $u \in V$ be the solution of* (1.3) *and $u_h \in V_h$ be the solution of* (1.4)*. The abstract error estimate*

$$\|u - u_h\|_V \le \frac{c_1}{c_2} \min_{v_h \in V_h} \|u - v_h\|_V \tag{1.6}$$

*holds.*

Consequently, we can estimate the error of the Galerkin approximation by studying interpolation properties of the finite dimensional subspace. More precisely, we can estimate the minimum on the right hand side of (1.6) by inserting an interpolation of $u$ in the space $V_h$. Thus, we have to introduce interpolation operators and to prove interpolation error estimates. This yields error estimates for the Galerkin approximation of the form

$$\|u - u_h\| \le c\, \mathfrak{h}^s\, |||u|||$$

with certain norms $\|\cdot\|$ and $|||\cdot|||$, where $s \in \mathbb{R}$ and $\mathfrak{h}$ corresponds either to the characteristic mesh size $h$, defined later, or to the number of degrees of freedom (DoF) in the system of linear Eq. (1.5). We say in this case that the error in the norm $\|\cdot\|$ converges with order $s$ with respect to $\mathfrak{h}$. In our computational tests, we verify the theoretical orders of convergence. Therefore, let $V_h$ and $V_{h_*}$ be two approximation spaces with corresponding $\mathfrak{h}$ and $\mathfrak{h}_*$. We compute the numerical order of convergence (noc) as

$$\frac{\log(\|u - u_h\|) - \log(\|u - u_{h_*}\|)}{\log(\mathfrak{h}) - \log(\mathfrak{h}_*)}\,, \tag{1.7}$$

which is an approximation on $s$ in the error model

$$\|u - u_h\| \approx c\, \mathfrak{h}^s\, |||u|||\,.$$

An important analytical tool in order to prove interpolation error estimates is the Bramble–Hilbert Lemma, see [58] and below. Beside of this, we extensively apply the triangle and reverse triangle inequality,

$$\|x + y\| \le \|x\| + \|y\| \qquad \text{and} \qquad |\,\|x\| - \|y\|\,| \le \|x + y\|\,,$$

for all kinds of norms, as well as the Cauchy–Schwarz inequality

$$|(x, y)| \le \|x\|\|y\|\,,$$

where the norm $\|\cdot\|$ is induced by the inner product $(\cdot,\cdot)$, i.e. $\|\cdot\| = \sqrt{(\cdot,\cdot)}$. Here, $x$ and $y$ might refer to vectors, functions or vector valued functions depending on the context of the inequality.

**Theorem 1.9 (Bramble–Hilbert Lemma)** *Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain. For some integer $k \ge 0$, let $\mathbf{f}$ be a continuous linear form on the space $H^{k+1}(\Omega)$ with the property that*

$$\mathbf{f}(p) = 0 \quad \forall p \in \mathscr{P}^k(\Omega)\,.$$

*There exists a constant $C(\Omega)$ such that*

$$|\mathbf{f}(v)| \le C(\Omega)\, \|\mathbf{f}\|_*\, |v|_{H^{k+1}(\Omega)}\,,$$

*where $\|\cdot\|_*$ is the norm in the dual space of $H^{k+1}(\Omega)$.*