Chapter 1

Introduction

We are concerned with elliptic problems in a domain Ω in $R^d,\ d = 2, 3$ which can be written in the strong form as

$$\nabla \cdot (k(x)\nabla u(x)) = f(x) \in L^2(\Omega) \quad \forall x \in \Omega \ ,$$

where the diffusion coefficient k is bounded by

$$\delta \le k(x) \le \delta^{-1} \quad \forall x \in \Omega$$

for some $\delta > 0$. Such problems arise from diffusive processes as for instance the heat transfer in a workpiece or the transport of groundwater in a saturated aquifer and will be called *interface problems* for the Laplacian. If the workpiece consists of different materials or if the aquifer consists of different types of soil, the diffusion coefficient will depend on the material. We will make the assumption that the *diffusion coefficient* k is piecewise constant on Lipschitz subdomains $\Omega_i \subset \Omega$.
This work is divided into three parts concerning

- analytical results about regularity of the solution u
- a-posteriori error estimators for the numerical approximation with Finite Elements
- numerical experiments.

In the first part (chapter 2) we investigate the piecewise H^s-regularity, $1 < s \le 2$, of the solution u of an interface problem with homogeneous boundary conditions of Dirichlet- and Neumann-type. Due to discontinuities of k and boundary conditions the solution u will not have the optimal piecewise regularity $H^2(\Omega_i)$ implied by the load function $f \in L^2(\Omega)$. Regularity is important from the analytical point of view, but it is also a valuable information in numerical analysis or mechanics. We want to mention its application in the approximation theory of Finite Elements or convergence theory for Multigrid Methods.
Known regularity results, which hold independently of the shape of the subdomains, restrict the partition of Ω into subdomains Ω_i to the case that the maximum number of subdomains which meet in a point is 2 for points on the boundary and 3 for interior

points. In our regularity results there are *no restrictions* on the maximum number of subdomains which share a point.
In the following we assume that the space dimension is $d = 2$. Vertices of the *interface* $\Gamma = Cl(\bigcup \partial\Omega_i / \partial\Omega)$ will be called *singular points*. In Figure 1.1 a) we depict a domain consisting of two subdomains. A singular point is denoted by x.
The most important analytical tool used in chapter 2 is a decomposition theorem [33], stating that the regularity of the solution u is perturbed by *singular functions* ψ_x that are part of the solution u. The singular function ψ_x is defined in a neighbourhood U of the singular point x and has piecewise regularity $\psi_x \notin H^{1+\lambda_x}(U \cap \Omega_i)$ and $\psi_x \in H^{1+s}(U \cap \Omega_i)$ for certain $\lambda_x \in (0, 1]$ and any $s < \lambda_x$. The smallest positive value λ_x for given x is called singular exponent. Thus, regularity of u is determined by the regularity of the singular functions that means by the smallest of the singular exponents λ_x of all singular points.

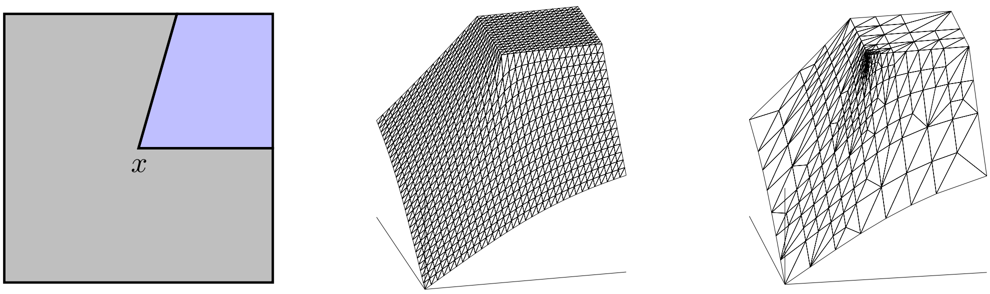

Figure 1.1: a) two subdomains b) the singular function c) the approximation of the singular function on an a-posteriori adapted grid

The dependence of the smallest positive singular exponent λ_x for a given singular point x on the diffusion coefficient and the subdomains is complicated and λ_x may take every value from $(0, 1)$ as can be shown using a special singular function defined in [34].
In order to obtain the regularity results, we use the fact that the singular exponents λ_x are related to the real, positive eigenvalues λ_x^2 of a *Sturm-Liouville eigenvalue problem*. In contrast to approaches of [34] [61] [36], we do not try to evaluate the eigenvalues, which are given by a system of transcendent equations, directly, but instead investigate the structure of the according eigenfunctions.
To show regularity we use a criterion on the diffusion coefficient that was originally used for Finite Element applications, *the quasi-monotonicity condition* [24]. We prove the quasi-monotonicity condition to be *necessary and sufficient* for piecewise regularity

$$u \in H^{1+1/4}(\Omega_i) \ , \ \ i = 1, .., n$$

independent of δ. In several special situations we are able to show better regularity results. As it turns out, all regularity results, known to the author, are covered by our approach and the quasi-monotonicity condition is a useful tool for analyzing regularity. Roughly speaking, the function k is quasi-monotone, if its trace on a sphere around each singular point has only one local maximum. If a singular point belongs to the boundary, there is a different condition.

In the general case, when no conditions on the structure of the diffusion coefficient are imposed, u has piecewise regularity $H^{1+s}(\Omega_i)$ for any positive s which is smaller than $\lambda := \min_x(\lambda_x)$ where x runs over all singular points x. But it is known that $\lambda > 0$ can be arbitrary small if $\delta \to 0$. To our knowledge until now no bound of λ from below in terms of the diffusion coefficient k has been known. We show in section 2.6.2 for the general case, where no special conditions on k and on the subdomains Ω_i are imposed, the inequality $1/(2\pi)\ \delta < \lambda$ which implies piecewise regularity

$$u \in H^{1+\delta/(2\pi)}(\Omega_i) \ \ , \ \ i = 1, .., n \quad .$$

Moreover, we can show slightly improved lower bounds which we show to be sharp using a special singular function ψ_2. In other words, we prove that the singular function ψ_2 has the lowest regularity, among all singular functions, with no restrictions on the number and interior angles of the subdomains and with the only restriction $\delta \leq k \leq \delta^{-1}$. Similar results hold for singular points on the boundary.
We address shortly vertex- and edge-singularities occuring in three space dimensions (section 2.7). As edge singularities are closely related to singularities in 2D one can use the results already derived.
The second part of this thesis (chapter 3) is devoted to the approximation of interface problems with *Finite Elements*. The non-optimal regularity usually causes large approximation errors. There are several approaches which improve the convergence. One could *a-priori* locally refine the mesh around a singularity [47] [32] [5] or add special functions to the Galerkin space [56] [20]. In all of these approaches one needs some data depending on the singularities in order to get the best performance. Except for some special cases, these data are not known explicitly. A further drawback of methods that rely on a-priori refining the grid, is, that one does not know how much to refine around particular singular points, since different singular functions have a different impact on the solution; the impact may even vanish.
To reduce the approximation error, we propose adaptive mesh refinement on the basis of *a-posteriori error estimators*. The calculation of the a-posteriori error estimators goes without the knowledge of parameters depending on the singularities and uses only available data. Additionally the error estimators allow for a control of the approximation error in the numerical simulation which is important for technical applications. Grid refinement is organized in such a way that simplices with large local a-posteriori error estimators are subsequently refined. See Figure 1.1 c), where an adapted grid is shown. It can be seen that refinement of the grid occurs around the singular point.
For the derivation of the error estimators we exploit the interpolation properties of Finite Elements in some norms depending on the diffusion k (section 3.5). Here it is crucial that the factor δ does not enter into the approximation inequalities. It is known that this is not possible for arbitrary data k [62], and we note that this it true only for the class of quasi-monotone diffusion coefficients. Within the class of quasi-monotone diffusion coefficients we can derive a-posteriori error bounds (section 3.6) where δ does not enter into the error bounds. We address a-posteriori error estimators which are based on local problems and propose a new estimator (section 3.6.3). In section 3.8 we extend the a-posteriori error estimators for problems with an additional mass term and Cauchy boundary conditions.

Our results are similar to the very recent paper [11]. There an equivalent a-posteriori error estimator was independently derived for a class of diffusion coefficients that is smaller than the class of quasi-monotone diffusion coefficients (see remarks 3.3, 3.4). For recent independent results for the case of essentially two subdomains see [21]. Deriving the a-posteriori error estimators we use the framework developed in [57].
In the third part of the this work we test the error estimators using various singular functions in numerical experiments (chapter 4). The results obtained for a 2D model problem with regularity $H^{1+3/4}$ confirmed robustness of the error estimates and led to a reduction of the error which is *optimal with respect to the number of nodes*.
We pay special attention to the performance of the error estimators, when in a different model problem the quasi-monotonicity condition is violated and the regularity deteriorates (section 4.5). The preasymptotic efficiency index seems to be dependent on the problem. The reason for this behaviour is the strong singularity together with an underestimated local efficiency index at the singularity.
It is interesting to note that the asymptotic efficiency index reaches for all of the model problems under consideration *the same value* independent of the regularity.
Calculations done with “real life” problems, coming from groundwater flow simulation, show that the error estimators are robust and lead to an optimal error reduction rate (section 4.6).
Numerical experiments for 3D problems show an optimal error reduction rate and a moderately constant efficiency index (section 4.7).