Optimal control of interface problems with hp-finite elements

D. Wachsmuth, * J.-E. Wurst *

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Abstract

We investigate the optimal control of elliptic PDEs with jumping coefficients. As discretization we use interface concentrated finite elements on subdomains with smooth data. In order to apply convergence results, we prove higher regularity of the optimal solution using the concept of quasi-monotone coefficients and a domain that is injective modulo polynomials of degree 1 at each vertex. Numerical results are presented for a semi-linear control problem with a non-local radiation operator, which models the production process of silicon carbide single crystals.

Keywords. Optimal control, transmission problems, elliptic regularity, higher-order finite elements

MSC classification. 49M05, 65N30, 35J25

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1 Introduction

Let us introduce the class of optimal control problems that we will investigate. We consider the minimization of the objective functional

$$J(y,u) := \frac{1}{2}\| y - y_d \|^2_{L^2(\Omega)} + \frac{\nu}{2}\| u \|^2_{L^2(U)}$$

subject to box constraints on the control u and an elliptic partial differential equation (PDE) on a polygonal domain $\Omega \subset \mathbb{R}^2$ which consists of pairwise disjoint subsets Ω_i (also polygonal)

$$-\nabla(\kappa_i \nabla y_i) = f_i \quad \text{in } \Omega_i$$

where $\kappa_i > 0$. The control u acts on interfaces between subdomains. This setting is used to model physical applications with different materials, where on subdomain i the material i is used.
Due to the discontinuity of the coefficient κ across subdomain boundaries, we speak of transmission or interface problems. Their main characteristics are the transmission conditions

$$\begin{aligned} y_i - y_j &= g_{i,j}, \\ \kappa_i \partial_{n_i} y_i + \kappa_j \partial_{n_j} y_j &= h_{i,j} \quad \text{on } \partial\Omega_i \cap \partial\Omega_j \text{ with } i \neq j. \end{aligned}$$

*Institut für Mathematik, Universität Würzburg, 97074 Würzburg, Germany
D. Wachsmuth: daniel.wachsmuth@mathematik.uni-wuerzburg.de
J.-E. Wurst: jan-eric.wurst@mathematik.uni-wuerzburg.de

Existence and regularity of solutions have been thoroughly studied in literature. The homogeneous case is treated in [6, 28, 30] while inhomogeneous data is discussed for general elliptic operators in [26, 27]. The control will act on the interfaces through the condition $\kappa_i \partial_{n_i} y_i + \kappa_j \partial_{n_j} y_j = u$.
The application we have in mind is a semi-linear optimal control problem that models the production process of silicon carbide (SiC) single crystals. These crystals are often used in electronic applications because of their properties as semiconductor materials. SiC crystals are produced with the physical vapor transport method. Under high temperatures (2000-3000 K) and low pressure, polycrystalline powder at the bottom of a cavity inside a graphite crucible is caused to sublimate (see e.g. [16, 17, 18]).
On the interface between the solid and gas phases the radiation of heat is modeled as a source term in the transmission boundary condition. In order to optimize the production process, the gradient of the temperature is to be controlled. We formulate an optimal control problem with Neumann control at the outer boundary of the domain and report about numerical experiments in section 5.2. The case of distributed controls is treated in more detail with state or control constraints in [7, 22, 23, 24].
The aim of this paper is to apply a suitable discretization method to solve an optimal control problem subject to the elliptic problem described above. We will focus on the interface concentrated finite element method. This version of *hp*-FEM uses a priori information for mesh refinement, i.e. the regularity of the data and the domain itself. In order to be able to apply error estimates for the boundary concentrated finite element method (*bc*-FEM) of [15], we derive local and global regularity of solutions to the interface problem.
As the elliptic problem is posed on polygonal domains, singularities may appear at vertices that generally only allow for $H^{1+\delta}$-regular solutions with $\delta \in (0, 1]$. The expansion of solutions into a regular part and singular contributions located at the vertices of the domain is related to the seminal results of [20]. The monographs [5, 10, 11, 21] are classic in this field. In addition, the transmission conditions restrict the global regularity, which cannot exceed $H^{3/2}(\Omega)$ due to the jump in the normal derivative (even if $g_{i,j} = 0$). However, the solution to the state equation may display smoother behavior when it is restricted to a subdomain Ω_i.
Moreover, the presence of control constraints makes the application of higher order discretization techniques difficult, because the arising first order necessary conditions are non-smooth, which restrict the global regularity of the control to at most $C^{0,1}$. The resulting projection formula is challenging to implement for higher order trial functions.

The outline of this paper is as follows. After briefly introducing necessary functions spaces and notation, we exemplarily show in section 3 how the smoothness of a solution is related to an abstract eigenvalue problem. After rigorously defining the transmission problem we collect some results of the corresponding eigenvalue theory. The main point of this section is the formulation of an asymptotic expansion of the solution in the homogeneous case (Theorem 3.9).
Section 4 establishes a lower bound on the distribution of eigenvalues by means of a quasi-monotone distribution of the coefficients κ_i. The extension of the regularity result for inhomogeneous problems is obtained by the aid of the concept of injectivity modulo polynomials for PDEs posed on polygonal domains. Under the assumption that the interface control is from the space $H^{1/2}$ we can formulate an expansion result for the general case, which allows to deduce higher global and local regularity (Theorem 4.10, Corollary 4.11, 4.12).
In section 5 we present two optimal control problems, among them the semi-linear optimal control problem with non-local radiation operator, as mentioned before. We discuss $H^{1+\delta}$-regularity of the state y and adjoint q, which determines the convergence rates of the boundary concentrated finite element method (see [2, 3, 15]).

2 Preliminaries

The domain Ω is defined as an open, bounded subset of $\mathbb{R}^2$ whose boundary $\partial\Omega =: \Gamma$ is a polygon. This means that

$$\partial\Omega = \cup_{e=1}^{E} \bar{\gamma}_e, \quad E \in \mathbb{N},$$

for pairwise disjoint boundary parts γ_e. Each γ_e is a straight line segment, which is open with respect to the relative topology in $\mathbb{R}^2$. If the intersection $\bar{\gamma}_e \cap \bar{\gamma}_{e'}$ is nonempty, we refer to this point as a vertex. The set of all vertices is called $\mathcal{V}$.

We denote the space of p-times integrable functions by $L^p(\Omega)$. The functions whose weak derivatives of order k also lie in $L^p(\Omega)$ are collected in the Sobolev space $W^{k,p}(\Omega)$, where we write $H^k(\Omega)$ for $p = 2$. We also allow fractional exponents s. In this case a functions v lies in $H^s(\Omega)$ with

$$s > 0, \quad s = \lfloor s \rfloor + \sigma$$

if it has finite norm

$$\|v\|_{H^s(\Omega)} := \left(\int_\Omega \sum_{|\alpha| \leq \lfloor s \rfloor} |D^\alpha v|^2 \, \mathrm{d}x + \int_\Omega \int_\Omega \sum_{|\alpha| = \lfloor s \rfloor} \frac{|D^\alpha v(x) - D^\alpha v(y)|^2}{|x - y|^{2+2\sigma}} \, \mathrm{d}x \, \mathrm{d}y \right)^{1/2}. \tag{2.1}$$

It is well known that there is a bounded trace operator

$$T : H^s(\Omega) \to H^{s-1/2}(\Gamma_\mathcal{D}), \quad v \mapsto v|_{\Gamma_\mathcal{D}}$$

if $s - 1/2 > 0$ is not integer and $\Gamma_\mathcal{D} \subseteq \partial\Omega$, see [1, 11].

In order to incorporate homogeneous Dirichlet boundary conditions, we define

$$H^1_{\Gamma_\mathcal{D}}(\Omega) := \{v \in H^1(\Omega) \mid T(v) = 0\}.$$

In the sequel, we will need weighted Sobolev spaces with powers of the weight function

$$r(x) := \prod_{X \in \mathcal{V}} \min\{1, \mathrm{dist}(x, X)\}, \quad x \in \bar{\Omega}.$$

Define

$$C^\infty_\mathcal{V}(\bar{\Omega}) := \{v \in C^\infty(\bar{\Omega}) \mid \mathrm{supp}(v) \cap \mathcal{V} = \emptyset\}$$

and $V^{k,p}_\beta(\Omega)$ as the closure of $C^\infty_\mathcal{V}(\Omega)$ under the norm

$$\| v \|_{k,p,\beta} := \sum_{|\alpha| \leq k} \| r^{\beta + |\alpha| - k} D^\alpha v \|_{L^p(\Omega)}.$$

3 Expansion of solutions of the transmission problem

In order to investigate the global regularity of solutions to transmission problems, we built on the expansions of solutions into a regular part and singular parts corresponding to irregular functions at the vertices of Ω. As the procedure is complicated and tedious, we only sketch the basic ideas for a simpler case mainly following the exposition in [21].

3.1 Poisson's equation

We look for weak solutions to the Dirichlet problem

$$-\Delta y = f \quad \text{in } \Omega, \quad y = 0 \quad \text{on } \Gamma. \tag{3.1}$$

It is well known, that the Laplacian Δ in Cartesian coordinates transforms to

$$\frac{1}{r}\partial_r\left(r\partial_r\right) + \frac{1}{r^2}\partial_\theta^2 \tag{3.2}$$

in polar coordinates with $(x_1, x_2) = (r\cos\theta, r\sin\theta)$ and $r \geq 0,\ \theta \in [0, 2\pi)$. Analogous formulas are available for the n-dimensional case which allows for treating higher dimensional problems.
If we formally set $r\partial_r =: \lambda$, Poisson's equation becomes

$$(\lambda^2 + \partial_\theta^2)y = r^2 f.$$

Neglecting boundary and interface conditions, this equation is uniquely solvable if and only if

$$\lambda^2 v + \partial_\theta^2 v = 0 \tag{3.3}$$

has only trivial solutions $v \equiv 0$. This illustrates the important role of the non-linear eigenvalue problem (3.3).
Let us give a short but more rigorous outline of the derivation of the (Sturm-Liouville-)eigenvalue problem and the resulting expansion of the solution to (3.1). As regularity is a local concept, we only need to worry about the smoothness of y at the vertices of Ω. For interior balls

$$B_d(x_0) \quad \text{with} \quad x_0 \in \Omega, \quad d < \operatorname{dist}(x_0, \Gamma)$$

we know that $y \in H^2(B_d(x_0))$. The same is true for smooth parts of the boundary, which can be locally flattened and become half balls $B^+(x_0) := \{x \in \mathbb{R}^2 \mid x_2 = 0\}$. After the change of coordinates $y \in H^2(B_d^+(x_0))$ for d small enough and $x_0 \in \Gamma, x_0 \notin \mathcal{V}$.
For treating the irregularities in a vertex $X \in \mathcal{V}$ of the domain, we localize the problem using a smooth cut-off function $\eta_X = \eta_X(\| x - X \|_2) \in C^\infty(\mathbb{R}^2)$. We stipulate $0 \leq \eta \leq 1$ such that $\eta_X \equiv 1$ for all x near X and η_X decreases rapidly to 0 so that all other vertices are not 'visible'. Locally, a solution of (3.1) satisfies

$$-\Delta(\eta_X y) = g := -(\Delta\eta_X)y + \eta_X f + 2\nabla\eta_X \cdot \nabla y \tag{3.4}$$

where we can change the coordinates such that the domain becomes a cone with opening angle $\omega_X \in (0, 2\pi)$

$$C_X := \{(r, \theta) \in \mathbb{R}^2 \mid r \in \mathbb{R}^+, \theta \in (0, \omega_X)\}.$$

Applying this change to the differential operator yields the equivalent problem for the new variable $y := \eta_X y$ (we dispense with writing y_X everywhere)

$$\begin{aligned} -\left(\partial_r^2 y + \frac{1}{r}\partial_r y + \frac{1}{r^2}\partial_\theta^2 y\right) &= g \quad \text{in } \ C_X, \\ y(r, 0) = y(r, \omega_X) &= 0. \end{aligned} \tag{3.5}$$

The operation which manages to send $r\partial_r$ to $\lambda \in \mathbb{C}$ is the Mellin-transform. It reads for fixed $\theta \in (0, \omega_X)$

$$M[y(., \theta)](\lambda) = \frac{1}{\sqrt{2\pi}} \int_0^\infty r^{-\lambda-1} y(r, \theta)\mathrm{d}r =: Y(\lambda, \theta).$$

It is closely connected to the Fourier-Transform $\mathcal{F}[y(.,\theta)](z \in \mathbb{C})$ by Euler's change of variables, which substitutes $r =: e^\tau,\ \tau \in (-\infty, \infty)$. If we suppress the dependence on θ, which is assumed to be arbitrary but fixed in $[0, 2\pi)$, the use of the definitions of both transforms yields the relation

$$M[y](\lambda) = F[y](z), \quad z = -i\lambda.$$

Several known properties from the Fourier-Transform, therefore, carry over to the Mellin-Transform. We only state a few important ones (see [21]).

Theorem 3.1. *Let $\Re$ and $\Im$ denote the real and imaginary part of a complex number. For $\lambda \in \mathbb{C}$ and $h := -\Re(\lambda)$ fixed, the Mellin-Transform M*

- *is an isomorphism*

$$M : \left\{ f \mid \int_0^\infty |f(r)|^2 r^{2h-1}\ dx < \infty \right\} \to L^2(-h + i\mathbb{R}).$$

- *possesses an inverse mapping M_h^{-1} given by*

$$M_h^{-1}[U](r) := \frac{1}{i\sqrt{2\pi}} \int_{-h-i\infty}^{-h+i\infty} r^\lambda U(\lambda)\ d\lambda.$$

- *satisfies*

$$M[(r\partial_r)^k y](\lambda) = \lambda^k M[y](\lambda), \quad k \in \mathbb{N}.$$

We can apply M to (3.5) and solve the simpler problem for $Y(\lambda, \theta)$

$$\begin{aligned} \lambda^2 Y + \partial_\theta^2 Y &= M[-r^2 g], \quad \text{in } (0, \omega_X), \\ Y(\lambda, 0) = Y(\lambda, \omega_X) &= 0. \end{aligned} \tag{3.6}$$

In order to solve (3.6) with the help of Theorem 3.1, the integrability of $-r^2 g$ as defined in (3.5) has to be investigated. As the cut-off function η_X is smooth and $y \in H^1(\Omega)$, the behavior of f near the vertex X is crucial.

Let $f \in V_\beta^{0,2}(\Omega)$ with $\beta \geq 0$ and set $\Re(\lambda) = 1 - \beta = -h$, then

$$\infty > \int_{C_X} r^{2\beta} g(x)^2\ \mathrm{d}x = \int_0^{\omega_X} \int_0^\infty r^{2\beta} g(r,\theta)^2 r\ \mathrm{d}r\ \mathrm{d}\theta = \int_0^{\omega_X} \int_0^\infty r^{2h-1} |r^2 g(r,\theta)|^2\ \mathrm{d}r\ \mathrm{d}\theta. \tag{3.7}$$

This proves that the Mellin-Transform of $-r^2 g$ exists for $\Re(\lambda) \leq 1$. The case $\Re(\lambda) = 1$ corresponds to $f \in L^2(\Omega)$.

The inverse mapping of the Mellin-Transform works on lines parallel to the imaginary axis. We find a solution y of (3.4) if we apply the inverse mapping of Theorem 3.1 to solutions Y of (3.6) on a line $\{\Re(\lambda) = -h\}$ where

$$\begin{aligned} \lambda^2 V + \partial_\theta^2 V &= 0, \\ V(\lambda, 0) = V(\lambda, \omega_X) &= 0. \end{aligned} \tag{3.8}$$

has only trivial solutions (implying that Y is unique). The behavior of the resulting function for $r \to \infty$ hereby depends on the value of $\Re(\lambda) = 1 - \beta = -h$ which was chosen for the inverse transform. We have the following regularity ([20, 21])

$$M_h^{-1}[Y(\lambda)] \in V_\beta^{2,2}(C_X). \tag{3.9}$$

An expansion of the solution to Poisson's equation is obtained as follows. The solutions of (3.8) are given by

$$V = C\sin(\lambda\theta) + D\cos(\lambda\theta), \quad C, D \in \mathbb{C}.$$

The constants need to be adjusted to fit the boundary conditions, which implies that only the case $\lambda_k = k\pi/\omega$ allows non-trivial solutions for $k \in \mathbb{Z}\setminus\{0\}$, i.e. $V_k = \sin(\frac{k\pi}{\omega_X}\theta)$. Obviously, the eigenvalues are real and distributed symmetrically around zero.

For $\omega_X > \pi$ the lines $\{\Re(\lambda) = 1\}$ and $\{\Re(\lambda) = 0\}$ are free of eigenvalues. Due to [20], the original problem (3.5) has a solution in $V_1^{2,2}(\Omega)$ which corresponds to the inverse Mellin-Transform with $\Re(\lambda) = h = 0$ because of (3.9). Consequently, we need to evaluate

$$\frac{1}{i\sqrt{2\pi}} \int_{1-i\infty}^{1+i\infty} Y(\lambda,\theta) r^\lambda \, \mathrm{d}\lambda.$$

This is done with the help of the residue theorem and the box domain Q depicted in Figure 1.

$$\sqrt{2\pi} \lim_{L\to\infty} \int_Q Y r^\lambda \, \mathrm{d}\lambda = \frac{1}{i\sqrt{2\pi}} \int_{-i\infty}^{+i\infty} Y(\lambda,\theta) r^\lambda \, \mathrm{d}\lambda - \frac{1}{i\sqrt{2\pi}} \int_{1-i\infty}^{1+i\infty} Y(\lambda,\theta) r^\lambda \, \mathrm{d}\lambda$$
$$= \sqrt{2\pi} \sum_{\lambda\in Q} \mathrm{Res}(Y(\lambda,\theta) r^\lambda)$$

because the integrals for the horizontal parts of Q vanish in the limit ([21]). The only pole in the domain of integration is located at $\lambda_1 = \pi/\omega_X$ where the residue reads

$$c_X r^{\pi/\omega_X} \sin(\theta\pi/\omega_X), \quad c_X \in \mathbb{R}. \tag{3.10}$$

On account of the regularity property (3.9) we obtain the expansion

$$y(r,\theta) = w_X(r,\theta) + c_X r^{\pi/\omega_X} \sin(\theta\pi/\omega_X), \tag{3.11}$$

with $w_X \in H^2(C_X)$.
This procedure can be done for all $X \in \mathcal{V}$. Remember that we implicitly agreed on $y := \eta_X y$ before, so for the true solution y of (3.1) it follows that

$$y = \sum_{X\in\mathcal{V}} \eta_X^2 y + \left(1 - \sum_{X\in\mathcal{V}} \eta_X^2\right) y$$

where $\eta_X y$ has the form (3.11). Thus,

$$y = \sum_{X\in\mathcal{V}} \eta_X c_X \; r^{\pi/\omega_X} \sin\left(\theta\pi/\omega_X\right) + y_0 \tag{3.12}$$

with the regular part

$$y_0 = \sum_{X\in\mathcal{V}} \eta_X w_X + (1 - \sum_{X\in\mathcal{V}} \eta_X^2) y$$

being clearly in $H^2(\Omega)$.

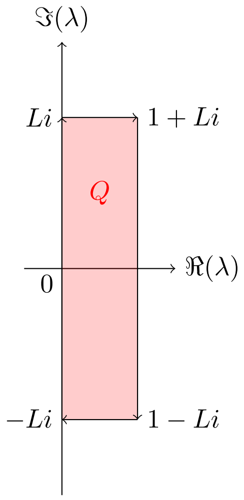

Figure 1: Domain of integration for evaluating inverse Mellin-Transforms.

Remark 3.2. *From the expansion* (3.12), *we see that the regularity of a solution* y *to* (3.1) *is limited to* $H^{1+\delta}(\Omega)$ *where*

$$\delta = \min_{X\in\mathcal{V}}\{\pi/\omega_X\} - \varepsilon, \quad \varepsilon > 0$$

on domains with re-entrant corners. On convex domains, there is no pole in Q *yielding a smooth solution* $y \in H^2(\Omega)$.

3.2 Transmission problems

In the following we generalize the setting of Poisson's equation to cover jumping coefficients in the elliptic operator. We then state the eigenvalue problem and provide solutions for several cases. Finally, we provide a regularity result in form of an asymptotic expansion of the solution. The following presentation is inspired by [26, 27].

Definition 3.3. *We speak of Ω as a $2d$-**network** if it consists of N pairwise disjoint domains Ω_i such that $\bar{\Omega} = \cup_{i=1}^{N} \bar{\Omega}_i$. The following notation is used*

$$\partial\Omega_i = \bigcup_{e=1}^{E_i} \bar{\gamma}_{i,e} \quad \textit{where} \quad \gamma_{i,e} \cap \gamma_{i,e'} = \emptyset \quad \textit{for } e \neq e'.$$

We further stipulate a compatibility condition among the subsets, i.e. exactly one of the following holds for $i, j \in \{1, \dots, N\}$ and $i \neq j$:

- $\bar{\Omega}_i \cap \bar{\Omega}_j = \emptyset$.
- $\bar{\Omega}_i \cap \bar{\Omega}_j$ *is a common vertex.*
- $\bar{\Omega}_i \cap \bar{\Omega}_j$ *is a common side, denoted by $\gamma_{i,j}$.*

*The boundary parts $\gamma_{i,j}$ are collected in $\mathcal{I}$ forming the **interface** $\Gamma_i = \cup_{\gamma_{i,j} \in \mathcal{I}} \gamma_{i,j}$.*
The set of all vertices is again called $\mathcal{V}$ which now comprises interior vertices as well.

In the context of elliptic PDE we are faced with boundary conditions and (in the case of transmission problems) interface conditions. Curves that lie on $\partial\Omega$ are collected in

$$\mathcal{E} := \mathcal{E}_{\mathcal{N}} \cup \mathcal{E}_{\mathcal{D}}$$

and divided into disjoint sets of Neumann and Dirichlet edges. The corresponding parts of the boundary are addressed by $\Gamma_{\mathcal{D}}, \Gamma_{\mathcal{N}}$. Restricting a function $y : \Omega \to \bar{\mathbb{R}}$ to one subdomain Ω_i is denoted by $y_i : \Omega_i \to \bar{\mathbb{R}}$. For a compact notation of the regularity of boundary functions on $\mathcal{E}, \mathcal{E}_{\mathcal{D}}, \mathcal{E}_{\mathcal{N}}$ or interface functions on $\mathcal{I}$ we define

$$u \in H^s(\mathcal{I}) \quad \Leftrightarrow \quad u|_{\gamma_{i,j}} \in H^s(\gamma_{i,j}) \quad \forall \gamma_{i,j} \in \mathcal{I}.$$

Assumption 3.4. *Assume that $\Gamma_{\mathcal{D}} \neq \emptyset$, $f_i \in L^2(\Omega_i)$, $h \in H^{1/2}(\Gamma_{\mathcal{N}})$ and $u \in H^{1/2}(\mathcal{I})$.*

The transmission problem (T) on a $2d$-network reads

$$\begin{aligned}
-\kappa_i \Delta y_i &= f_i && \text{in } \Omega_i, && (3.13a)\\
y_i - y_j &= 0 && \text{on } \gamma_{i,j} \in \mathcal{I}, && (3.13b)\\
\kappa_i \partial_{n_i} y_i + \kappa_j \partial_{n_j} y_j &= u && \text{on } \gamma_{i,j} \in \mathcal{I}, && (3.13c)\\
y_i &= 0 && \text{on } \gamma_i \in \mathcal{E}_{\mathcal{D}}, && (3.13d)\\
\kappa_i \partial_{n_i} y_i &= h_i && \text{on } \gamma_i \in \mathcal{E}_{\mathcal{N}} && (3.13e)
\end{aligned}$$

The function u will serve as a control variable in section 5. Note that in literature (3.13c) is often written in terms of the normal jump, i.e.

$$[\kappa \partial_n y(x)] := \lim_{\varepsilon \searrow 0} (\nabla y(x + \varepsilon n) - \nabla y(x - \varepsilon n)) \cdot n$$

which is independent of the sign of the normal vector n. With the different values of κ_i and the characteristic function χ for sets, we set

$$\kappa(x) = \sum_{i=1}^{N} \chi_{\Omega_i} \kappa_i$$

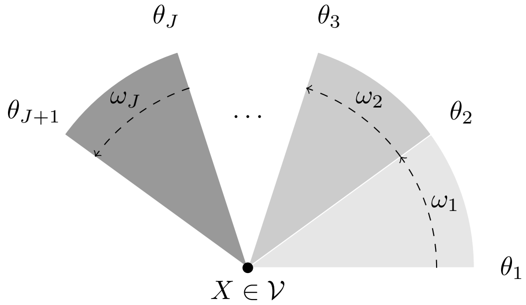

Figure 2: A vertex X in the domain Ω (after a change of variables) where J different materials meet.

and write down the weak formulation of the problem.

$$\int_\Omega \kappa \nabla y \cdot \nabla v \, \mathrm{d}x = \int_\Omega f v \, \mathrm{d}x + \sum_{\gamma_{i,j} \in \mathcal{I}} (u, v)_{L^2(\gamma_{i,j})} + \sum_{\gamma_i \in \mathcal{E}_\mathcal{N}} (h_i, v)_{L^2(\gamma_{i,j})}$$

for all $v \in H^1_{\Gamma_\mathcal{D}}(\Omega)$. The arising bi-linear form is bounded and coercive and the application of the Lemma of Lax-Milgram yields a unique solution (due to Assumption 3.4).
Proceeding as in Section 3.1, we obtain the following non-linear eigenvalue problem for $2d$-networks. Suppose J subdomains Ω_j meet at a vertex $X \in \mathcal{V}$, see Figure 2 for the notations. Then the non-linear eigenvalue problem is given by

$$\begin{aligned} \lambda^2 V + \partial_\theta^2 V &= 0 && \text{in } (\theta_j, \theta_{j+1}),\ j = 1, \ldots, J, && (3.14a) \\ V(\lambda, \theta_j + 0) &= V(\lambda, \theta_j - 0) && j = 2, \ldots, J, && (3.14b) \\ \kappa_i \partial_\theta V(\lambda, \theta_j + 0) &= \kappa_{j-1} \partial_\theta V(\lambda, \theta_j - 0) && j = 2, \ldots, J, && (3.14c) \end{aligned}$$

compare also (3.6). If no exterior boundary is involved, i.e. $X \cap \partial\Omega = \emptyset$, we set $\theta_{J+1} = \theta_1$ and let both sums in (3.14b),(3.14c) run from $1, \ldots, J$ with the convention $\kappa_0 = \kappa_J$. Otherwise, we additionally have boundary conditions

$$\begin{aligned} V(\lambda, \theta_1 = 0) &= 0 \quad \text{if } \partial\Omega_1 \cap \Gamma_\mathcal{D} \neq \emptyset && \vee && \partial_\theta V(\lambda, \theta_1 = 0) = 0 \quad \text{if } \partial\Omega_1 \cap \Gamma_\mathcal{N} \neq \emptyset && (3.14d) \\ V(\lambda, \theta_{J+1}) &= 0 \quad \text{if } \partial\Omega_J \cap \Gamma_\mathcal{D} \neq \emptyset && \vee && \partial_\theta V(\lambda, \theta_{J+1}) = 0 \quad \text{if } \partial\Omega_J \cap \Gamma_\mathcal{N} \neq \emptyset && (3.14e) \end{aligned}$$

A candidate for an eigensolution is (as for the Laplacian) the function

$$V_j = C_j \sin(\lambda(\theta - \theta_j)) + D_j \cos(\lambda(\theta - \theta_j)), \quad \theta \in (\theta_j, \theta_{j+1}). \tag{3.15}$$

The boundary and transmission conditions at the interface give rise to a system of equations for the unknowns C_j, D_j.

It is proved by induction ([26, Example 2.29]) that the Dirichlet-Dirichlet problem (3.14) with $V(\lambda, 0) = 0$ in (3.14d) is solved by

$$C_{j+1} = \frac{D_1}{\Pi_{\nu=2}^i \kappa_\nu} d_j^\mathcal{D}(\lambda), \quad D_{j+1} = \frac{D_1}{\Pi_{\nu=2}^{j+1} \kappa_\nu} d_j^\mathcal{M}(\lambda),$$

with the recursion formula

$$\begin{aligned} d_1^\mathcal{D}(\lambda) &= \sin(\lambda\omega_1), && (3.16a) \\ d_1^\mathcal{M}(\lambda) &= \kappa_1 \cos(\lambda\omega_1), && (3.16b) \\ d_j^\mathcal{D}(\lambda) &= \kappa_j \cos(\lambda\omega_j) d_{j-1}^\mathcal{D}(\lambda) + \sin(\lambda\omega_j) d_{j-1}^\mathcal{M}(\lambda), && (3.16c) \\ d_j^\mathcal{M}(\lambda) &= -\kappa_j^2 \sin(\lambda\omega_j) d_{j-1}^\mathcal{D}(\lambda) + \kappa_j \cos(\lambda\omega_j) d_{j-1}^\mathcal{M}(\lambda). && (3.16d) \end{aligned}$$

The Dirichlet condition $V(\lambda, \theta_{J+1}) = 0$ in (3.14e) is equivalent to $D_{J+1} = 0$. Hence, there are non-trivial solutions if and only if $d_J^{\mathcal{D}}(\lambda)$ is zero. Let us note that the condition $d_J^{\mathcal{M}}(\lambda) = 0$ determines the eigenvalues for the transmission problem with mixed boundary conditions, i.e. $V(\lambda, 0) = 0$ in (3.14d) and $\partial_\theta V(\lambda, \theta_{J+1}) = 0$ in (3.14e).

In an analogous way, the discriminant $d_J^{\mathcal{N}}(\lambda)$ for the Neumann-Neumann problem with $\partial_\theta V(\lambda, 0) = 0$ in (3.14d) and $\partial_\theta V(\lambda, \theta_{J+1}) = 0$ in (3.14e) can be derived. It involves the discriminant $d_J^{\mathcal{M}'}(\lambda)$ for the mixed transmission problem with $\partial_\theta V(\lambda, 0) = 0$ in (3.14d) and $V(\lambda, \theta_{J+1}) = 0$ in (3.14e). We find

$$C_{j+1} = \frac{C_1}{\Pi_{\nu=2}^{j}\kappa_\nu} d_j^{\mathcal{M}'}(\lambda), \quad D_{j+1} = -\frac{C_1}{\Pi_{\nu=2}^{j+1}\kappa_\nu} d_j^{\mathcal{N}}(\lambda),$$

with the recursion formula

$$d_1^{\mathcal{N}}(\lambda) = \kappa_1 \sin(\lambda\omega_1), \tag{3.16e}$$

$$d_1^{\mathcal{M}'}(\lambda) = \cos(\lambda\omega_1), \tag{3.16f}$$

$$d_j^{\mathcal{N}}(\lambda) = \kappa_j^2 \sin(\lambda\omega_j) d_{j-1}^{\mathcal{M}'}(\lambda) + \kappa_j \cos(\lambda\omega_j) d_{j-1}^{\mathcal{N}}(\lambda), \tag{3.16g}$$

$$d_j^{\mathcal{M}'}(\lambda) = \kappa_j \cos(\lambda\omega_j) d_{j-1}^{\mathcal{M}'}(\lambda) - \sin(\lambda\omega_j) d_{j-1}^{\mathcal{N}}(\lambda). \tag{3.16h}$$

Remark 3.5. *The eigenvalues of the transmission problem are real numbers because the problem can be written as a self-adjoint operator (see [25, Theorem 2.2]). Additionally, the set of eigenvalues is countable without a cluster point (see [9] with the result of [27, Theorem 3.4]). Furthermore, the roots of* $d_J^{\mathcal{D}}(\lambda), d_J^{\mathcal{N}}(\lambda), d_J^{\mathcal{M}}(\lambda), d_J^{\mathcal{M}'}(\lambda)$ *are symmetric around* 0.

Note that at interior vertices, the function $V \equiv$ const solves the eigenvalue problem for $\lambda = 0$ because there are no boundary conditions present.
Let us introduce some new notation and definitions that allow us to rigorously formulate the main result of this section, which is an asymptotic expansion for the homogeneous transmission problem. The concepts will also be used in section 4.

Definition 3.6. *Let* $X \in \mathcal{V}$ *and* $L_X(\lambda)$ *denote the differential operator corresponding to* (3.14a) *and* $B_X(\lambda)$ *denote the operator collecting* (3.14b)-(3.14e) *depending on the problem posed at vertex* X. *The eigenvalue problem is abbreviated by*

$$\mathcal{A}_X(\lambda) := (L_X(\lambda), B_X(\lambda)).$$

As the eigenvalue problem for $\mathcal{A}(\lambda)$ of Definition 3.6 is non-linear, we provide a generalized Definition of eigenvalues, eigensolutions and generalized Jordan chains. The following definitions are made under the assumption of one arbitrary, but fixed vertex $X \in \mathcal{V}$, which is why the dependency on X is suppressed.

Definition 3.7. *Let* $C^{\cap s} := C \cap \{r = 1\}$ *be the intersection of the cone at vertex* X *with the one-dimensional sphere. A number* $\lambda_0 \in \mathbb{C}$ *is an* ***eigenvalue*** *of the operator* $\mathcal{A}_X(\lambda)$ *if there is a non-trivial function* $s_{\lambda_0,0} \in H^2(C^{\cap s})$ *(called* ***eigensolution****) with*

$$\mathcal{A}_X(\lambda_0)s_{\lambda_0,0} = 0.$$

If λ_0 is an eigenvalue of $\mathcal{A}(\lambda)$, there are $\dim \mathrm{Ker}(\mathcal{A}_X(\lambda)) =: I_{\lambda_0}$ linearly independent eigensolutions $s_{\lambda_0,i,0}$ with $i = 1, \ldots, I_{\lambda_0}$. Besides them, there may exist $N_{\lambda_0,i}$ associated eigenfunctions $s_{\lambda_0,i,j}$.

Definition 3.8. *The system* $\{s_{\lambda_0,i,j}\}$ *with* $i = 1, \ldots I_{\lambda_0},\ j = 0, \ldots, N_{\lambda_0,i}$ *consists of eigensolutions and* ***associated eigensolutions*** *(called a system of Jordan chains) if*

$$\sum_{\nu=0}^{k} \frac{1}{\nu!} \partial_\lambda^\nu \mathcal{A}_X(\lambda_0) s_{\lambda_0,i,k-\nu} = 0$$

for $k = 0, \dots, N_{\lambda_0,i}$ *where* $N_{\lambda_0,i}$ *(decreasing with respect to* i*) denotes the* ***size of the Jordan chain****. An eigenvalue* λ_0 *is called* ***simple*** *if no associated eigensolutions exist, i.e.* $N_{\lambda_0} = 0$*.*

Theorem 3.9. *Let* $\lambda_{X,j},\ j = 1, \dots, N_X$ *denote all eigenvalues of* $\mathcal{A}_X(\lambda)$ *in* $(0,1]$ *and assume that* $\lambda_{X,j} \neq 1$*. Then the solution to* (T) *with* $u = 0$ *on a 2d-network* Ω *admits the expansion*

$$y = y_0 + \sum_{X \in \mathcal{V}} \sum_{j=1}^{N_X} c_{X,j}\ \eta_X\ r^{\lambda_{X,j}}\ s_{X,j}(\theta)$$

where $u_{0,i} \in H^2(\Omega_i),\ c_{X,j} \in \mathbb{R},\ s_{X,j} \in H^1(]0, \theta_{J(X)}[)$ *and* η_X *is a smooth cut-off function.*

This result comprises Remark 3.2 and is rigorously proved in [26, Theorem 2.27]. The eigenvalues of (3.14) are simple, which is why a similar result holds in weighted Sobolev spaces (see [26, Theorem 3.6]). An expansion of the solution y into a regular part y_0 and singular contributions can be derived for more general $2m$-coercive problems ($m \geq 1$) and transmission problems. The proofs are more involved and use (semi-)Fredholm properties of the general operators. At the core, however, a non-linear eigenvalue problem similar to (3.8) and its solvability is discussed on the infinite cone (see [26, 27] and references therein).

4 Higher regularity of solutions of the transmission problem

An expansion like the one provided in Theorem 3.9 allows to establish higher regularity (locally and globally) by bounding the eigenvalues from below. Since

$$r^\lambda s \in H^{1+\lambda-\varepsilon}(\Omega) \quad \text{but} \quad r^\lambda s \notin H^{1+\lambda}(\Omega)$$

(see [10, Thm. 1.2.18]), the lowest exponent in the singular functions decides on the regularity.

Corollary 4.1. *Assume there is a* $\delta \in (0,1]$ *such that* $\lambda_{X,j} > \delta$ *for all* $X \in \mathcal{V}$*. Then the solution* y *of* (T) *with* $u = 0$ *satisfies for all* $\varepsilon > 0$

$$y_i \in H^{1+\delta}(\Omega_i), \quad y \in H^{1+\min\{1/2-\varepsilon, \delta\}}(\Omega).$$

Proof. The first regularity result of the corollary follows from Theorem 3.9 in the case of $\lambda_{X,i} \neq 1$. Otherwise, we can rely on Sobolev embeddings and sharper results in L^p-spaces (see [28, Corollary 2.1] and references therein). $\square$

In this section we show that the homogeneous transmission problem is $H^{5/4}$-regular under the general assumption of a quasi-monotone distribution in the diffusion coefficients κ_i. After that, we establish higher regularity for the inhomogeneous case, where the control $u \neq 0$. This requires the introduction of the concept of injectivity modulo polynomials.

4.1 Quasi-monotone distributions

Under general assumptions it is impossible to find a lower bound for the eigenvalue distribution of $\mathcal{A}_X(\lambda)$, which the following example shows. For a mixed boundary value problem with $\omega_1 = \omega_2 = \pi/2$, it holds

$$d_2^{\mathcal{M}}(\lambda) = -\kappa_2^2 \sin^2(\lambda\pi/2) + \kappa_1\kappa_2 \cos^2(\lambda\pi/2).$$

A vanishing discriminant $d_2^{\mathcal{M}}(\lambda) = 0$ leads to

$$\tan(\lambda\pi/2) = \pm\sqrt{\frac{\kappa_1}{\kappa_2}}.$$

Letting $\kappa_2 \to \infty$ sends $\lambda \to 0$.
In order to avoid such phenomena, [28] used the concept of quasi-monotone diffusion coefficients, first introduced in [8].

Definition 4.2. *Let $\kappa_i > 0$ with $i = 1, \ldots, N$ be the distribution of diffusion coefficients for a 2d-network. Assume that*

$$i \neq j, \ \mathrm{meas}_1(\Omega_i \cap \Omega_j) > 0 \quad \Rightarrow \quad \kappa_i \neq \kappa_j.$$

*Let at $X \in \mathcal{V}$ meet J different domains with κ_j, $j = 1, \ldots, J$. We denote by $\kappa_{a_j}, \kappa_{b_j}$ the material constants of the domains which abut on material j with positive one dimensional measure (one of them being zero if there is only one neighbor). The distribution of κ_i is called **quasi-monotone** if the following assumptions hold for all $X \in \mathcal{V}$.*

- *If X lies in $\bar{\Omega} \setminus \Gamma_{\mathcal{D}}$, then*

$$\exists! \ j \in \{1, \ldots, J\} : \quad \kappa_j > max(\kappa_{a_j}, \kappa_{b_j}).$$

- *If X lies on $\Gamma_{\mathcal{D}}$, then $\kappa_j = max(\kappa_{a_j}, \kappa_{b_j})$ implies that* $\mathrm{meas}_1(\bar{\Omega}_j \cap \Gamma_{\mathcal{D}}) > 0$.

Remark 4.3. *Three materials meeting at an interior point are automatically distributed in a quasi-monotone way, i.e. the first condition only poses restrictions for $k \geq 4$. The second condition states that, locally, the domain with maximal material constant has to touch the Dirichlet boundary.*

Using this definition, [28] proved

Theorem 4.4. *If the coefficients κ_i are quasi-monotone, then we have*

$$\lambda_{X,i} > \frac{1}{4}.$$

This result answers the question on regularity for the homogeneous transmission problem. Global regularity of $H^{5/4}(\Omega)$ is achieved by requiring quasi-monotone coefficients κ_i.
If we restrict ourselves to only two materials the bound can be improved to achieve optimal global regularity.

Proposition 4.5. *Let Ω consist only of two subdomains Ω_1, Ω_2. For each $X \in \mathcal{V}$ and opening angle $\omega_X \in (0, 2\pi]$, we have in the case of $\mathcal{E}_{\mathcal{N}} = \emptyset$*

$$\lambda_{X,i} \geq \frac{1}{2}.$$

Proof. The result for $X \in \Gamma$ can be found in [4, Theorem 8.1]. For interior vertices, we refer to [19, section 2.2]. □

Two numerical examples for the eigenvalue distribution are shown in figure 3: there the dependence of eigenvalues of $\mathcal{A}_X(\lambda)$ on ω_1 is depicted for the two-material case, where two materials meet with angle ω_1 at a boundary and an interior vertex, respectively.

4.2 Injectivity modulo polynomials

Allowing non-homogeneous jumps in the normal derivative, i.e. $u \neq 0$ in (3.13c), seriously complicates the analysis. In order to formulate an existence result for the inhomogeneous problem, it is necessary to introduce the concept of injectivity modulo polynomials, which is described e.g. in [27].
For a cone C_X we define the restriction $C_{X,i}$ to be the part of C_X on which $\kappa = \kappa(\theta) = \kappa_i$. Furthermore, $y_i := y|_{C_{X,i}}$ for functions y defined on C_X.

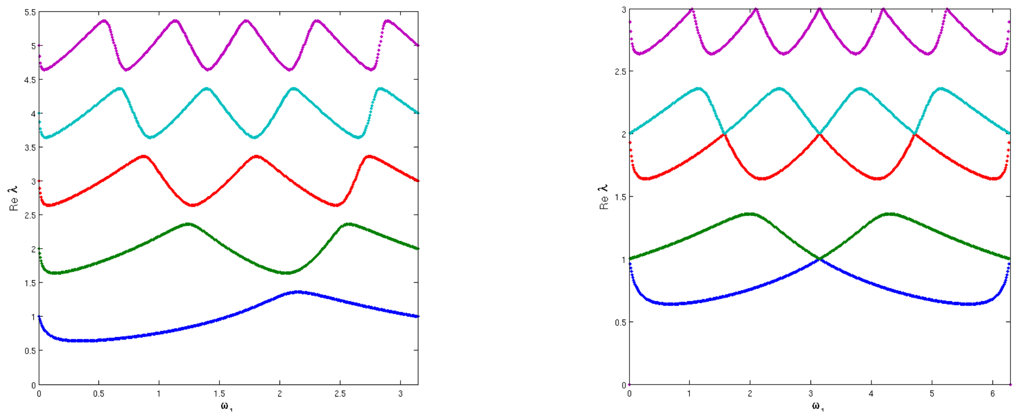

Figure 3: Eigenvalue distribution for a boundary (left) and interior (right) vertex with $\kappa_1 = 0.25, \kappa_2 = 5$.

Definition 4.6. *Let D be an open subset of $\mathbb{R}^n$ and let $l \in \mathbb{Z}$ and $X \in \mathcal{V}$. We define the* ***homogeneous polynomial spaces of degree*** *l as*

$$\begin{aligned} P_l^H(D) &:= \{q \mid q \text{ is a homogeneous polynomial of degree } l \text{ defined on } D\} \quad l \geq 0, \\ P_l^H(D) &:= \{0\} \quad l < 0, \\ P_l^H(C_X) &:= \{q : C_X \to \mathbb{R} \mid q_i \in P_l^H(C_{X,i})\}. \end{aligned}$$

For the data of our problem (P) we define the polynomial space

$$\Upsilon_l^H(C_X) := P_{l-2}^H(C_X) \times \prod_{\gamma_{ii'} \in \mathcal{E}_\mathcal{D}} P_l^H(\gamma_{i,i'}) \times \prod_{\gamma_{ii'} \in \mathcal{E}_\mathcal{N}} P_{l-1}^H(\gamma_{i,i'}) \times \prod_{\gamma_{i,i'} \in \mathcal{I}} P_l^H(\gamma_{i,i'}) \times \prod_{\gamma_{ii'} \in \mathcal{I}} P_{l-1}^H(\gamma_{i,i'}).$$

Definition 4.7. *We say $\mathcal{A}_X(\lambda)$ is* ***injective modulo polynomials of order*** *l (short i.m.p) for $l \in \mathbb{N}$ on C_X if and only if any solution w_X that solves problem (T) on the domain C_X with a right hand side in $\Upsilon_l^H(C_X)$ belongs to the space $P_l^H(C_X)$.*

Remark 4.8. *If the operator is injective modulo polynomials then every solution of the transmission problem (T) with polynomial data is itself polynomial.*

In order to answer the question on injectivity modulo polynomials in practice, a characterization of w_X is necessary.

Proposition 4.9. *Let w_X be a solution of the transmission problem (T) with polynomial data from $\Upsilon_l^H(C_X)$ with $l > 0$. Then the restriction to one subdomain Ω_i looks like (we suppress the index i for better readability)*

$$w_{X,l}(r, \theta) = P_{X,l}(r, \theta) + \sum_{\lambda_{X,j} = l} c_{X,j}\ r^l (\ln(r) s_{X,j}(\theta) + \theta \partial_\theta s_{X,j}(\theta)) \tag{4.1}$$

where $P_{X,l}$ is a polynomial of degree l.

For the proof, we refer the reader to [26, Theorem 3.10] where the result extends to $l \geq 0$. Note that general elliptic equations lead to higher powers of $\ln(r)$ due to the presence of more associated eigenfunctions (see [27, Lemma 7.1]).

A discussion of injectivity modulo polynomials for *elliptic boundary value problems* can be found in [5]. Under the assumption of injective modulo polynomials we have

Theorem 4.10. *Assume that $\mathcal{A}_X(\lambda)$ is i.m.p. of order 1 for all $X \in \mathcal{V}$ and the line $\{\Re(\lambda) = 1\}$ contains no eigenvalue of $\mathcal{A}(\lambda)$ except possibly at $\lambda = 1$. Then under Assumption 3.4, there exists a solution y to (T) that satisfies the expansion*

$$y = y_0 + \sum_{X \in \mathcal{V}} \sum_j c_{X,j}\ \eta_X\ r^{\lambda_{X,j}}\ s_{X,j}(\theta)$$

where $y_0 \in L^2(\Omega)$ and $y_{0,i} \in H^2(\Omega_i)$, $c_{X,j} \in \mathbb{R}$, $s_{X,j} \in H^2(]0, \sum_i \omega_{X,i}[)$ and η_X is a smooth cut-off function.

Proof. The proof is the same as [27, Theorem. 7.4] where we set $k = 0$, $m = 1$, $p = 2$ to cover the situation considered here. We only point out some important steps. The fact $u \in H^{1/2}(\Gamma_i)$ allows to construct a lift function $v \in V_0^{2,2}(\Omega)$ that exactly fulfills the transmission conditions [27, Lemma 4.3]. A unique solution and its expansion with a regular part in the weighted Sobolev space $V_0^{0,p}(\Omega)$ follows from [27, Corollary 4.4]. The result for $p = 2$ is then obtained by an interpolation argument which exploits the property of injectivity modulo polynomials of order 1. $\square$

Corollary 4.11. *Suppose that the coefficients κ_i are distributed in a quasi-monotone way and that the domain is i.m.p of order 1. Under Assumption 3.4, the solution of (T) lies in $H^{5/4}(\Omega)$.*

Proof. Applying Theorem 4.10 gives us an expansion of the solution where the eigenvalues are bound from below by 1/4 (Theorem 4.4). Just as in the proof of Corollary 4.1, we argue that $y \in H^{1+1/4}(\Omega)$. $\square$

Corollary 4.12. *Suppose that there is a $\delta \in (0, 1]$ such that for each $X \in \mathcal{V}$ the eigenvalues of $\mathcal{A}_X(\lambda)$ satisfy $\lambda_{X,i} > \delta$. Under Assumption 3.4, the solution y to the transmission problem satisfies*

$$y \in H^{1+\delta}(\Omega_i), \quad y \in H^{\min\{1/2-\varepsilon,\delta\}}(\Omega)$$

for arbitrary $\varepsilon > 0$ and $i = 1, \dots, N$.

Proof. The result immediately follows from the expansion in Theorem 4.10 combined with the results and argumentation of Corollary 4.1. $\square$

Let us discuss the concept of injectivity modulo polynomials of order 1 for the transmission problem (T) with $\mathcal{E}_\mathcal{N} = \emptyset$ and some showcase vertices $X \in \mathcal{V}$.
Let C_X be the cone at an exterior vertex $X \in \mathcal{V}$ with Dirichlet-Dirichlet boundary conditions where two materials meet (see Figure 4).

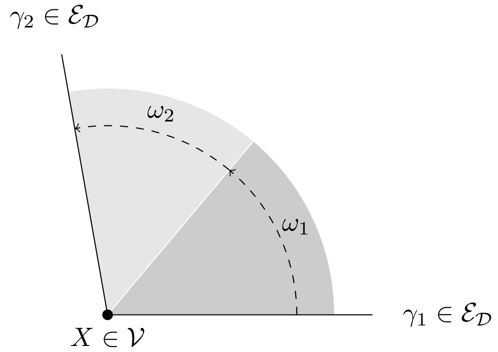

Figure 4: Dirichlet-Dirichlet problem at a conical point with two materials.

From (3.16c) we get

$$d_2^{\mathcal{D}}(\lambda) = \kappa_2 \cos(\lambda\omega_2)\sin(\lambda\omega_1) + \kappa_1 \sin(\lambda\omega_2)\cos(\lambda\omega_1).$$

For $\omega_1 = \omega_2$ it is obvious that $\lambda = 1$ is an eigenvalue if $\sin(\omega_1) = 0$, i.e. $\omega_1 = \pi/2$. We find with (3.15) that

$$s_{X,1} = \sin(\theta), \quad s_{X,2} = \cos(\theta - \pi/2) = \sin(\theta)$$

in (4.1).
Observing that

$$P_X = \begin{cases} \frac{1}{\kappa_1} r\cos(\theta) & \theta \in (0, \pi/2) \\ -\frac{1}{\kappa_2} r\cos(\theta) & \theta \in (\pi/2, \pi) \end{cases}$$

is a polynomial that solves (3.14a)-(3.14e) with polynomial data from $\Upsilon_1^H(C_X)$, we set

$$w_{X,i} = P_{X,i} + \frac{r}{\kappa_i}(\ln(r)\sin(\theta) + \theta\cos(\theta)).$$

A simple calculation shows that $\Delta w_X = 0$. Continuity of w_X at $\theta = \pi/2$ is also fulfilled as well as the jump in the normal derivative

$$\kappa_1 \partial_\theta w_{X,1} = -r - \pi/2 = -(r + \pi/2) = -\kappa_2 \partial_\theta w_{X,2}.$$

So w_X solves a problem with polynomial data, but is itself non-polynomial. Consequently, the operator $A(\lambda)$ is not i.m.p. of order 1 at such a vertex $X \in \mathcal{V}$.

The situation is different if 1 is no eigenvalue of $\mathcal{A}_X(\lambda)$. Then the sum in (4.1) is empty and Proposition 4.9 yields a unique (polynomial) solution which in turn guarantees i.m.p. of order 1.
This can be also seen in the left diagram of figure 3. There, eigenvalues λ were computed for

$$\kappa_1 = 0.25, \quad \kappa_2 = 5,$$
$$0 < \omega_1 < \pi, \quad \omega_1 + \omega_2 = \pi.$$

According to figure 3, $\lambda = 1$ is only an eigenvalue if $\omega_1 = \pi/2$.
As vertices with only one material do not pose a problem due to [5, section 4], the operator $\mathcal{A}(\lambda)$ is i.m.p. on S^1 for the domain shown in figure 5.

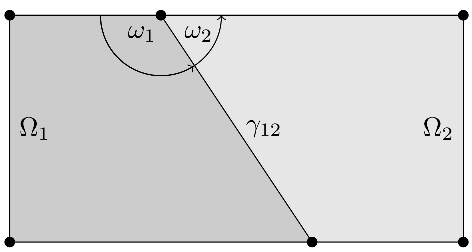

Figure 5: A suitably shaped domain to apply Theorem 4.10.

For two materials and an interior vertex, $\lambda = 1$ is never an eigenvalue. This can be seen as follows. Setting $J = 2$ in (3.14) and inserting the solution candidate from (3.15) yields a system of equation with the determinant (see also [26, Example 2.30])

$$d(\lambda) = (\kappa_1 - \kappa_2)^2 \sin^2(\lambda(\pi - \omega_1)) + (\kappa_1 + \kappa_2)^2 \sin^2(\lambda\pi).$$

Assume $d(1) = 0$, then it follows

$$\omega_1 = 0 \quad \vee \quad \omega_1 = \pi,$$

which can also be observed in the right diagram of figure 3. However, these two cases do not allow for an interior vertex with two materials. Hence, the operator $\mathcal{A}(\lambda)$ is i.m.p on the model domain of Figure 6.

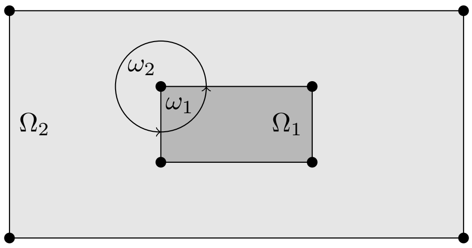

Figure 6: A suitably shaped domain to apply Theorem 4.10.

5 Optimal control problems

We study a linear quadratic optimal control problems with interface control and underlying box constraints. The state equation is the transmission problem of (T) of chapter 3.

The full optimization problem (P) reads

$$(P) \quad \begin{cases} \text{minimize} & J(y,u) := \frac{1}{2}\| y - y_d \|^2_{L^2(\Omega)} + \frac{\nu}{2}\| u \|^2_{L^2(\mathcal{I})} \\ \text{subject to } (T) & \\ & \begin{aligned} -\nabla(\kappa_i \nabla y) &= f_i && \text{in } \Omega_i, \\ y_i &= y_j && \text{on } \gamma_{i,j} \in \mathcal{I}, \\ \kappa\partial_{n_i} y_i + \kappa_j \partial_{n_j} y_j &= u && \text{on } \gamma_{i,j} \in \mathcal{I}, \\ y_i &= 0 && \text{on } \gamma_i \in \mathcal{E}_{\mathcal{D}}, \\ \kappa_i \partial_{n_i} y_i &= h && \text{on } \gamma_i \in \mathcal{E}_{\mathcal{N}}. \end{aligned} \\ \text{and} & \\ & u_a \le u \le u_b \quad \text{a.e. on } \mathcal{I}. \end{cases}$$

Existence of a solution and first-order necessary conditions can be derived in a standard way [29]. **Let $(y^*, u^*) \in H^1_{\Gamma_{\mathcal{D}}}(\Omega) \times L^2(\mathcal{I})$ denote a solution. Then, there exists $q^* \in H^1_{\Gamma_{\mathcal{D}}}(\Omega)$ satisfying**

$$\begin{aligned} -\nabla(\kappa_i \nabla q^*) &= y^* - y_d && \textbf{in } \Omega_i, \\ q_i^* &= q_j^* && \textbf{on } \gamma_{i,j} \in \mathcal{I}, \\ \kappa\partial_{n_i} q_i^* + \kappa_j \partial_{n_j} q_j^* &= 0 && \textbf{on } \gamma_{i,j} \in \mathcal{I}, \\ q_i^* &= 0 && \textbf{on } \gamma_i \in \mathcal{E}_{\mathcal{D}}, \\ \kappa_i \partial_{n_i} q_i^* &= 0 && \textbf{on } \gamma_i \in \mathcal{E}_{\mathcal{N}} \end{aligned} \tag{5.1}$$

such that

$$u^* = P_{U_{ad}}\left(-\frac{1}{\nu} q^*\right) \in H^{1/2}(\mathcal{I}) \tag{5.2}$$

holds. We solve the problem numerically with the boundary concentrated finite element method for piecewise analytic data ([2, section 3.5]). Moreover, we use the variational discretization concept of [12] combined with a semi-smooth Newton method (see also [3, 14, 29]). The latter method solves the

optimality system consisting of the state equation of (P), adjoint equation (5.1), and the projection equation (5.2).
In order to to prove a priori error estimates, piecewise analytic data is stipulated for the state equation and adjoint equation.

Assumption 5.1. *Assume that there exists a constant $\delta \in (0,1]$ such that $f_i, y_{d,i}$ are analytic on Ω_i for $i = 1, \ldots, N$ and satisfy*

$$\| r^{p+1-\delta} \nabla^p y_d \|_{L^2(\Omega)} + \| r^{p+1-\delta} \nabla^p f \|_{L^2(\Omega)} \leq C_f \gamma_f p! \quad \forall p \in \mathbb{N}_0.$$

Together with the results of section 4 we can derive an a priori error bound for the discrete solution of (P).

Theorem 5.2. *Let Ω be a 2d-network with N materials and denote by (y_h^*, u_h^*) the discrete approximation of the solution (y^*, u^*) of (P). Assume that $\mathcal{A}_X(\lambda)$ is i.m.p. of order 1 and satisfies $\lambda_{X,j} > \delta$ for all vertices $X \in \mathcal{V}$ with δ from Assumption 5.1. Then, the following error bound holds on a geometric mesh with sufficiently large polynomial slope (see [2])*

$$\| y^* - y_h^* \|_{L^2(\Omega)} + \sqrt{\nu} \| u^* - u_h^* \|_{L^2(\mathcal{I})} \leq C h^{\delta}. \tag{5.3}$$

Proof. Let q^* be the adjoint variable to (y^*, u^*) and q_h^* its approximation corresponding to (y_h^*, u_h^*). The error between the numerical result (y_h^*, u_h^*) and the optimal solution pair (y^*, u^*) can be bounded by the approximation error of the discretization technique (see [13, Theorem 3.1]).

$$\| y^* - y_h^* \|^2_{L^2(\Omega)} + \nu \| u^* - u_h^* \|^2_{L^2(\mathcal{I})} \leq \| y^h - y^* \|^2_{L^2(\Omega)} + \frac{1}{\nu} \| q^h - q^* \|^2_{L^2(\mathcal{I})} \tag{5.4}$$

where y^h (respectively q^h) denotes the *bc*-FEM solution the the state (respectively adjoint) equation with data $u^*, (y^*)$.

The optimality system (5.2) yields $u^* \in H^{1/2}(\mathcal{I})$ because the bounds u_a, u_b are from $H^{1/2}(\mathcal{I})$ as well. The same holds true for u_h^* since it is variationally discretized and *bc*-FEM gives rise to conform approximation space (a subspace of $H^1_{\Gamma_{\mathcal{D}}}(\Omega)$). Moreover, $f_i \in B^2_{1-\delta}(\Omega)$ (Assumption 5.1) implies $f \in L^2(\Omega_i)$ which verifies Assumption 3.4.
Therefore, we can apply Corollary 4.12 and find

$$y_i^* \in H^{1+\delta}(\Omega_i).$$

Assumption 5.1 provides additional regularity for the solution to the state equation (see [15, Theorem 1.4])

$$y_i^* \in H^{1+\delta}(\Omega_i) \cap B^2_{1-\delta}(\Omega_i).$$

The *bc*-FEM approximation error (see [15, Theorem 2.13] and also [2, section 3.5]) reads

$$\| y^h - y^* \|_{H^1(\Omega_i)} \leq C h^{\delta}. \tag{5.5}$$

An analogous line of reasoning applies to the adjoint variable $q^* \in H^{1+\delta}(\Omega_i) \cap B^2_{1-\delta}(\Omega_i)$. The refined approximation result [2, Theorem 3.7]) yields the approximation error

$$\| q^* - q^h \|_{L^2(\mathcal{I})} \leq C h^{\delta + 1/2}. \tag{5.6}$$

Plugging the estimates (5.5),(5.6) in (5.4) and adapting the constant C leads to

$$\| y^* - y_h^* \|^2_{L^2(\Omega)} + \nu \| u^* - u_h^* \|^2_{L^2(\mathcal{I})} \leq C(h^{2\delta} + h^{2\delta+1}). \tag{5.7}$$

Taking the square root concludes the proof. □

In the following we apply *bc*-FEM to two optimal control problems. For the visualization of results, we used a software library developed at the TU Chemnitz. [1]

[1] http://www-user.tu-chemnitz.de/~pester/graf2d/

5.1 Linear-quadratic problem

We investigate the theoretical findings for a simple example of problem (P):

$$\text{minimize } J(y,u) := \frac{1}{2}\| y - y_d \|^2_{L^2(\Omega)} + \frac{\nu}{2}\| u \|^2_{L^2(\partial\Omega_1)} \tag{5.8a}$$

subject to the transmission problem (T)

$$-\kappa_i \Delta y_i = f_i \qquad \text{in } \Omega_i, \tag{5.8b}$$
$$y_i = y_j \qquad \text{on } \partial\Omega_1 \tag{5.8c}$$
$$\kappa_1 \partial_{n_1} y_1 + \kappa_2 \partial_{n_2} y_2 = u \qquad \text{on } \partial\Omega_1, \tag{5.8d}$$
$$y = 0 \qquad \text{on } \partial\Omega_2, \tag{5.8e}$$

where $i = 1,2$ and the domain $\bar{\Omega} = \bar{\Omega}_1 \cup \bar{\Omega}_2 = [0,2]^2$ looks as follows.

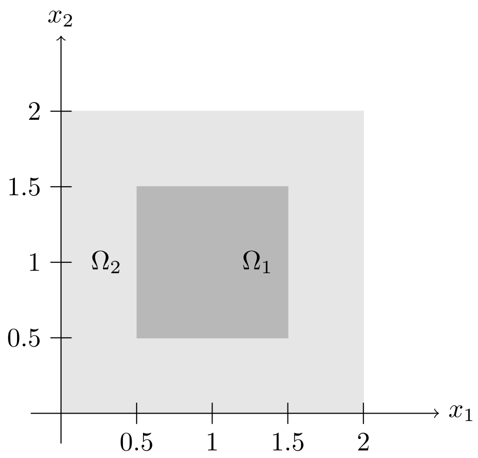

Figure 7: The domain Ω for problem (5.7).

The data is chosen as

$$\kappa_1 = 5, \qquad f_1 = 10,$$
$$\kappa_2 = 0.25, \qquad f_2 = 10,$$

with $\nu = 0.01$ and the desired state

$$y_d|_{\Omega_1} = 16, \quad y_d|_{\Omega_2} = 10.$$

Box constraints are omitted.

A general lower bound δ for the eigenvalues of $\mathcal{A}_X(\lambda)$ is obtained by applying Corollary 4.11 ($\delta = 1/4$) or the refined estimate in Proposition 4.5 ($\lambda_{X,j} \geq 1/2$). By numerically evaluating the eigenvalues at the interior vertices of Ω, we find

$$\lambda_1 = 0.70114949, \quad \lambda_2 = 1.2988505, \quad \lambda_3 = 2.7011495, \quad \dots$$

which indicates that, locally, $y_i^* \in H^{1+\lambda_1-\varepsilon}(\Omega_i)$ (Corollary 4.12). Obviously, the same holds true for the adjoint variable q^*.

Because of Theorem 5.2 we expect the following error decay

$$\| y^* - y_h^* \|_{L^2(\Omega)} + \sqrt{\nu} \| u^* - u_h^* \|_{L^2(\partial\Omega_1)} \lesssim Ch^{0.7}.$$

We show the errors and convergence rate for the state (respectively adjoint) variable in Table 1 (respectively 2). The experimental order of convergence (EOC) with respect to a given norm is computed by taking the solution on the finest discretization as reference (see Figure 8,9).
The EOC for the state y in the $H^1(\Omega)$-norm is in very good compliance with the theoretical results and the estimate of $\delta = \lambda_1 \approx 0.7$. It is still open to prove that the $L^2(\Omega)$-error decays like $\mathcal{O}(h^{2\delta})$ for *bc*-FEM, because the Aubin-Nitsche trick cannot be applied directly.

h	$\|y_h^* - y^*\|_{L^2(\Omega)}$	$\mathrm{EOC}(y, L^2(\Omega))$	$\|y_h^* - y^*\|_{H^1(\Omega)}$	$\mathrm{EOC}(y, H^1(\Omega))$
0.25	$3.04 \cdot 10^{-1}$	-	5.7	-
0.125	$1.04 \cdot 10^{-1}$	1.55	3.52	$6.94 \cdot 10^{-1}$
0.0625	$3.85 \cdot 10^{-2}$	1.44	2.14	$7.19 \cdot 10^{-1}$
0.0312	$1.41 \cdot 10^{-2}$	1.45	1.28	$7.44 \cdot 10^{-1}$
0.0156	$5.14 \cdot 10^{-3}$	1.45	$7.76 \cdot 10^{-1}$	$7.2 \cdot 10^{-1}$
0.00781	$1.87 \cdot 10^{-3}$	1.46	$4.72 \cdot 10^{-1}$	$7.16 \cdot 10^{-1}$
0.00391	$6.73 \cdot 10^{-4}$	1.48	$2.85 \cdot 10^{-1}$	$7.3 \cdot 10^{-1}$
0.00195	$2.28 \cdot 10^{-4}$	1.56	$1.66 \cdot 10^{-1}$	$7.76 \cdot 10^{-1}$
0.000488	-	-	-	-

Table 1: Numerical results for the state variable y and problem (5.7).

h	$\|q_h^* - q^*\|_{L^2(\partial\Omega_1)}$	$\mathrm{EOC}(q, L^2(\partial\Omega_1))$	$\|q_h^* - q^*\|_{H^1(\Omega)}$	$\mathrm{EOC}(q, H^1(\Omega))$
0.25	$3.01 \cdot 10^{-3}$	-	2.45	-
0.125	$1.13 \cdot 10^{-3}$	1.42	1.29	$9.18 \cdot 10^{-1}$
0.0625	$4.62 \cdot 10^{-4}$	1.29	$5.99 \cdot 10^{-1}$	1.11
0.0312	$2.1 \cdot 10^{-4}$	1.14	$2.42 \cdot 10^{-1}$	1.31
0.0156	$9.77 \cdot 10^{-5}$	1.1	$9.29 \cdot 10^{-2}$	1.38
0.00781	$4.47 \cdot 10^{-5}$	1.13	$3.59 \cdot 10^{-2}$	1.37
0.00391	$1.98 \cdot 10^{-5}$	1.18	$1.48 \cdot 10^{-2}$	1.28
0.00195	$8.14 \cdot 10^{-6}$	1.28	$6.7 \cdot 10^{-3}$	1.14
0.000488	-	-	-	-

Table 2: Numerical results for the state variable q and problem (5.7).

The convergence for the adjoint variable q and the $H^1(\Omega)$ norm is significantly faster, which could be explained by the fact that the optimal adjoint is close to zero in Ω_1 (see Figure 8). The singularities at the interior vertices, therefore, do not have much impact on the approximation quality. It is proved in [2, Theorem 3.7] that the error $\| q^* - q_h^* \|_{L^2(\partial\Omega_1)}$ decays at best like $\mathcal{O}(h^{\delta+1/2})$. This rate can be observed in Table 2.
Since no control constraints are present, it holds $u^* = -\frac{1}{\nu} q^*$ and $u_h^* = -\frac{1}{\nu} q_h^*$. Consequently, the observed rate of convergence of $\| u^* - u_h^* \|_{L^2(\partial\Omega_1)}$ coincides with that of $\| q^* - q_h^* \|_{L^2(\partial\Omega_1)}$.

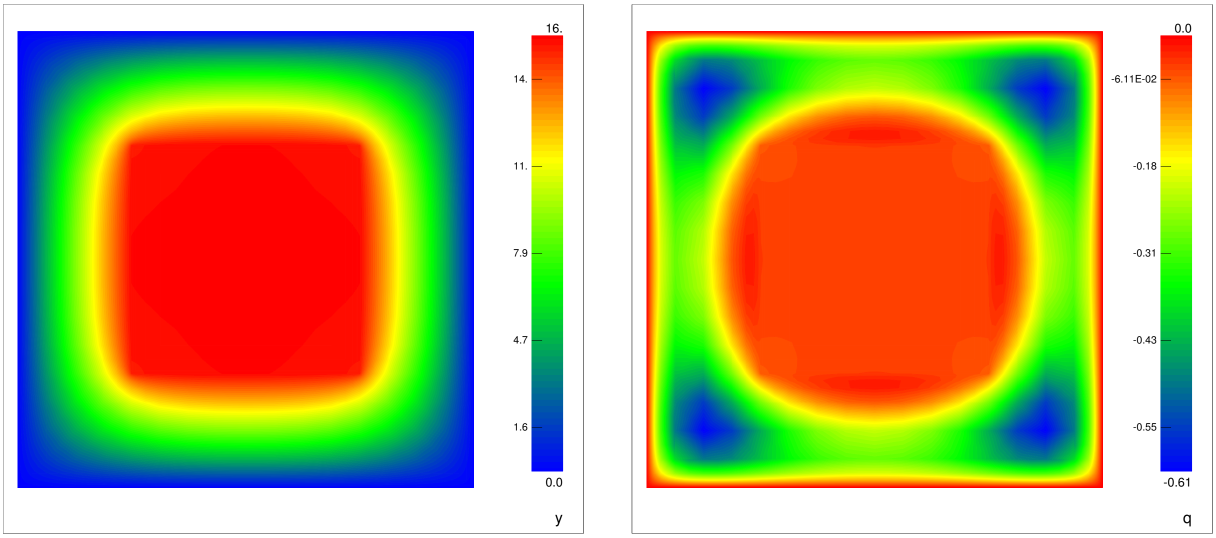

Figure 8: Optimal state (left) and adjoint (right) for problem (5.7).

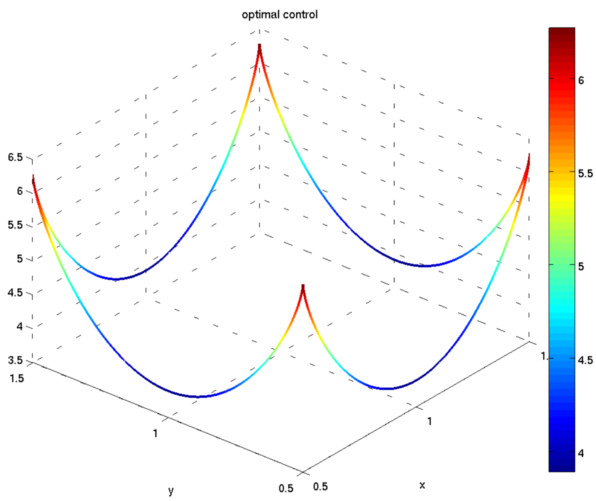

Figure 9: The optimal control for problem (5.7).

5.2 Semi-linear control problem with non-local radiation

We will now report about the results when applying the interface concentrated finite element method to the optimal control of the crystal growth problem. The model domain is shaped like in the previous example (see Figure 6). In order to comply with the notation of [22], we set $\Omega_g := \Omega_1$ with Γ_r being the interface $\partial\Omega_1$ where the radiation takes place. The boundary $\Gamma_0 := \partial\Omega$ is used for the Neumann control. Let ∂_n be the unit normal vector of Γ_r that points into the interior of Ω_g and ∂_{n_0} the standard outward unit normal of Γ_0.

Let us briefly describe the modeling of the radiation problem. The non-local radiation operator G is defined by

$$G\sigma|y|^3 y = (I - K)(I - (1-\varepsilon)K)^{-1}\varepsilon\sigma|y|^3 y$$

where the two dimensional integral operator K is given by

$$(Kv)(x) = \int_{\Gamma_r} \Xi(x,z) \frac{[n(z)\cdot(x-z)][n(x)\cdot(z-x)]}{2|z-x|^3} v(z)\ \mathrm{d}s_z$$

with the visibility factor

$$\Xi(x,z) := \begin{cases} 0 & \text{if } \overline{xz} \cap \Omega_s \neq \emptyset \\ 1 & \text{if } \overline{xz} \cap \Omega_s = \emptyset \end{cases}$$

The radiation problem (R) reads

$$(R) \qquad \begin{cases} \text{minimize} & J(y,u) := \frac{1}{2}\int_{\Omega_g} |\nabla y - z|^2\ \mathrm{d}x + \frac{\nu}{2}\int_{\Gamma_0} u^2\ \mathrm{d}s \\ \text{subject to} & \\ & \begin{aligned} -\nabla(\kappa_s \nabla y) &= f_s && \text{in } \Omega_s, \\ -\nabla(\kappa_g \nabla y) &= f_g && \text{in } \Omega_g, \\ \kappa_g \partial_n y_g - \kappa_s \partial_n y_s &= G\sigma|y|^3 y && \text{on } \Gamma_r, \\ \kappa_s \partial_{n_0} y + \varepsilon\sigma|y|^3 y &= \varepsilon\sigma y_0^4 + u && \text{on } \Gamma_0, \end{aligned} \\ \text{and} & \\ & u_a \leq u \leq u_b \text{ a.e. on } \Gamma_0. \end{cases}$$

The emissivity constant of the materials is denoted by ε and σ signifies the Stefan-Boltzmann constant. The Tychonov regularization parameter ν is positive, as well as the two coefficients κ_g, κ_s.
More details on the physics behind the model problem and derivation of the state equation can be found in [16, 17, 18, 22, 23, 24].
In order to apply the existence results of [22] we require

Assumption 5.3. *Let $f \in L^2(\Omega_s), z \in L^2(\Omega_g)^2$. The bounds $u_a \leq u_b$ are assumed to be in $L^4(\Gamma_0)$ and the external temperature $y_0 \in L^{16}(\Gamma_0)$. Finally, $\sigma\varepsilon y_0^4 + u \geq \xi > 0$ a.e. on Γ_0.*

The last assumption is no restriction since the term represents a temperature, which is naturally greater than zero. It is required for proving a maximum principle allowing existence results for the linearized state equations.

Theorem 5.4. *[22, Theorem 3.7] Under Assumption 5.3, the state equation of (R) possesses a unique solution $y \in H^1(\Omega) \cap L^4(\Gamma_r \cup \Gamma_0)$ which satisfies*

$$\| y \|_{L^\infty(\Omega)} + \| y \|_{L^\infty(\Gamma_r \cup \Gamma_0)} \leq C(1 + \| f \|_{L^2(\Omega)} + \| y_0 \|^4_{L^{16}(\Gamma_0)} + \| u \|_{L^4(\Gamma_0)}).$$

The optimal control problem (R) admits a solution which can be characterized by first order necessary conditions. Introducing an adjoint variable q which solves a linearized version of the state equation, the optimality conditions take the familiar form $u^* = P_{U_{ad}}(-q^*/\nu)$. This can be proved by adapting the results of [22, chapter 3.3].
We solved the problem numerically with

$$\begin{aligned} \kappa_g &= 0.08, & f_g &= 0, \\ \kappa_s &= 24, & f_s &= 125000, \\ u_a &= 241, & u_b &= 20000. \end{aligned}$$

The desired gradient is set to $z = (0, -10)$ and the regularization parameter reads $\nu = 5 \cdot 10^{-8}$. The emissivity is chosen as $\varepsilon = 0.8$ with the Stefan-Boltzmann constant $\sigma = 5.6696 \cdot 10^{-8}$.

A numerical evaluation of the eigenvalues of $\mathcal{A}_X(\lambda)$ gives

$$\lambda_1 = 0.66910618, \quad \lambda_2 = 1.3308938, \quad \lambda_3 = 2.6691062.$$

It is known that the radiation operator G is a bounded linear mapping from $L^p(\Gamma_r) \to L^p(\Gamma_r)$ for $1 \leq p \leq \infty$ ([22, Lemma 3.1]). However, it is open whether G retains higher regularity and maps into $H^{1/2}(\Gamma_r)$. In the positive case we can apply Corollary 4.12 and achieve higher local regularity $y \in H^{1+\lambda_1-\varepsilon}(\Omega_i)$.
This motivates the discretization with boundary concentrated finite elements. As the problem requires a fine discretization to get reasonable results, we dispense with showing experimental convergence rates on a set of nested discretizations. Let us emphasize that the benefit of using *bc*-FEM is the good approximation quality with respect to the number of unknowns (see [15]).
Problem (R) is solved with an SQP method where the quadratic subproblems are dealt with by a primal dual active set strategy. In order to globalize the algorithm, we use a projected gradient method with Armijo linesearch. For a detailed description regarding the discretization of the non-local radiation operator, the SQP method and the arising linearized state equations, together with their optimality systems, see [22].
We used the direct sparse LU-solver UMFPACK for the arising system of equations because the regularization parameter ν is chosen very small which leads to ill-conditioned matrices and slow convergence rates in iterative solvers.

The geometric mesh shown in Figure 11 was additionally h-refined at the four vertices of Γ_r to get a better resolution of the adjoint variable, which displays peaks (see Figure 10). This behavior was already noticed by [22] where the area around the vertices were strongly refined as well.

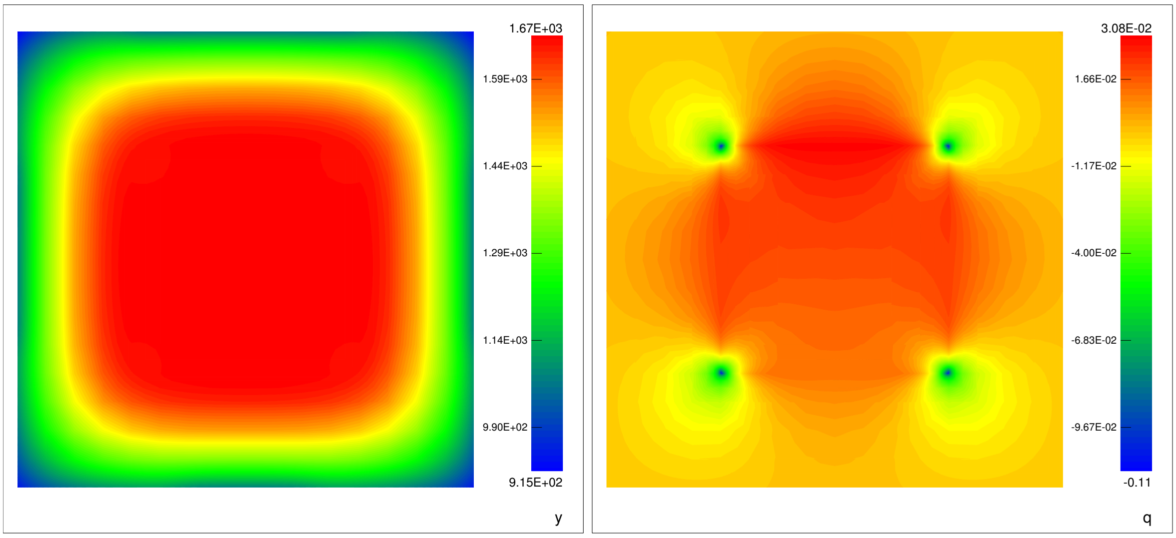

Figure 10: Optimal state (left) and adjoint (right) of the radiation problem (R).

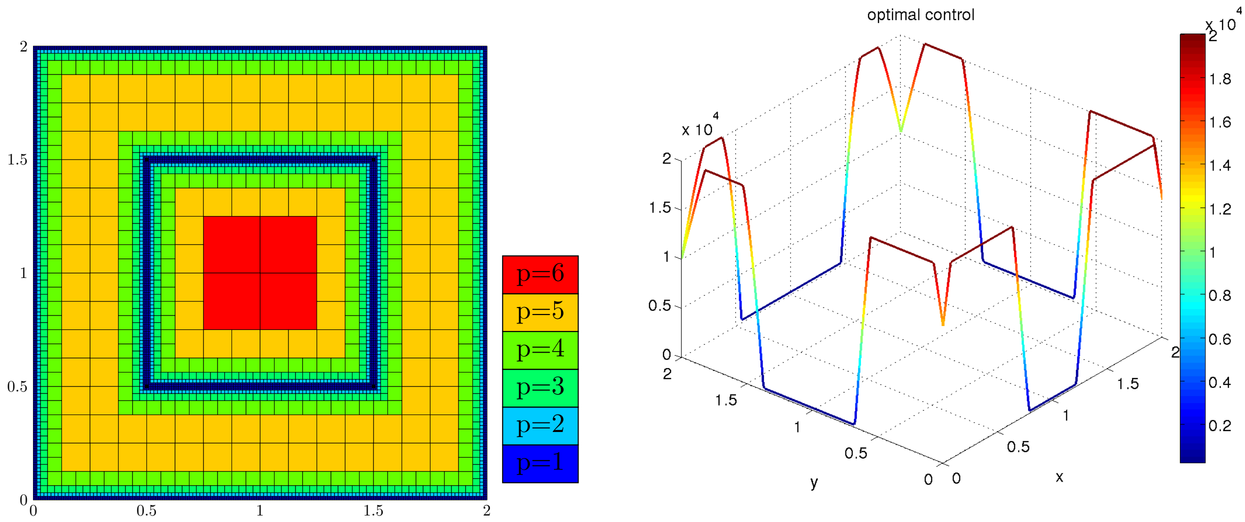

Figure 11: The geometric mesh (left) used for computing the optimal control (right) of the radiation problem (R).

6 Final remarks

We applied the *bc*-FEM method to different optimal control problems. In order to incorporate bounds on the control, we restricted ourselves to interface or boundary controls. Global and local $H^{1+\delta}$-regularity was discussed for elliptic equations by means of solutions expansions. The numerical results are consistent with the theory.

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