Functional Optimization- and Integro-Partial Differential Equations-Based Mathematical Modeling and Numerical Simulation

Applications to Heat Transfer, Crack Propagation, and Shape Design

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Preface

This thesis consists of the following nine selected refereed articles [1, 2, 3, 4, 5, 6, 7, 8, 9], previously published in the period 2005–2012, preceded by an Introduction.

The following list provides the bibliographic information for the mentioned papers in the order they are included in the thesis. The actual papers can be found after the sections containing the Introduction and further relevant references.

Except [6, 7], all included articles constitute collaborations. I have contributed original numerical code for the included papers [1, 2, 4, 5, 7, 9]. In particular, I have been the initial principal developer of the numerical simulation software *WIAS-HiTNIHS* (cf. Sec. 1.1.5 of Introduction). In my judgment, all coauthors have contributed about equal shares to the joint papers [1, 2, 3, 4, 8]. My main contribution to [9] is [9, Sec. 3].

Bibliography of Included Papers

[1] C. Meyer and P. Philip. *Optimizing the temperature profile during sublimation growth of SiC single crystals: Control of heating power, frequency, and coil position.* Crystal Growth & Design **5** (2005), 1145–1156.

[2] J. Geiser, O. Klein, and P. Philip. *Influence of anisotropic thermal conductivity in the apparatus insulation for sublimation growth of SiC: Numerical investigation of heat transfer.* Crystal Growth & Design **6** (2006), 2021–2028.

[3] C. Meyer, P. Philip, and F. Tröltzsch. *Optimal Control of a Semilinear PDE with Nonlocal Radiation Interface Conditions.* SIAM J. Control Optim. **45** (2006), 699–721.

[4] J. Geiser, O. Klein, and P. Philip. *A finite volume scheme designed for anisotropic heat transfer in general polyhedral domains.* Advances in Mathematical Sciences and Applications (AMSA) **18** (2008), 43–67.

[5] O. Klein, Ch. Lechner, P.-É. Druet, P. Philip, J. Sprekels, Ch. Frank-Rotsch, F.-M. Kiessling, W. Miller, U. Rehse, and P. Rudolph. *Numerical simulations of the influence of a traveling magnetic field, generated by an internal heater-magnet module, on liquid encapsulated Czochralski crystal growth.* Magnetohydrodynamics **45** (2009), 257–267, Special Issue: Selected papers of the International Scientific Colloquium Modelling for Electromagnetic Processing, Hannover, Germany, October 27-29, 2008.

[6] P. Philip. *A Quasistatic Crack Propagation Model Allowing for Cohesive Forces and Crack Reversibility.* Interaction and Multiscale Mechanics: an International Journal (IMMIJ) **2** (2009), 31–44.

[7] P. Philip. *Analysis, Optimal Control, and Simulation of Conductive-Radiative Heat Transfer.* Mathematics and its Applications / Annals of AOSR **2** (2010), 171–204.

[8] P.-É. Druet and P. Philip. *Noncompactness of integral operators modeling diffuse-gray radiation in polyhedral and transient settings.* Integral Equations and Operator Theory (IEOT) **69** (2011), 101–111.

[9] P. Philip and D. Tiba. *Shape Optimization via Control of a Shape Function on a Fixed Domain: Theory and Numerical Results*, pp. 285–299 in *Numerical Methods for Differential Equations, Optimization, and Technological Problems: Celebration proceedings dedicated to Prof. Pekka Neittaanmaki's 60th birthday.* Springer, 2012, in press.

Contents

1 Introduction

1.1 Conductive-Radiative Heat Transfer

1.1.1 Model Equations

Except for [6, 9], the included papers are all in some way related to the topic of mathematical modeling of conductive-radiative heat transfer, with special focus on numerical simulation and control. The need for modeling, simulation, and control of conductive-radiative heat transfer arises from industrial applications such as single crystal growth from vapor or melt (see references in the included papers, in particular in [1, 5, 7]).

Transient conductive heat transfer is modeled by

$$\frac{\partial \varepsilon(x,\theta)}{\partial t} - \operatorname{div}\big(\kappa(x,\theta)\,\nabla\,\theta\big) = f(t,x) \quad \text{in }]0,T[\times\Omega, \tag{1}$$

where $T > 0$ represents the final time, $\theta(x,t)$ represents absolute temperature depending on the space variable x and the time variable t, $\varepsilon > 0$ represents internal energy, $\kappa > 0$ represents thermal conductivity, and f models heat sources or sinks. The stationary variant of (1), where the term $\frac{\partial \varepsilon(x,\theta)}{\partial t}$ is missing and θ, f do not depend on t, namely

$$-\operatorname{div}\big(\kappa(x,\theta)\,\nabla\,\theta\big) = f(x) \quad \text{in } \Omega, \tag{2}$$

is also of interest and is considered as well. The space domain $\Omega \subseteq \mathbb{R}^3$ is assumed to consist of two parts $\Omega_{\rm s}$ and $\Omega_{\rm g}$, where $\Omega_{\rm s}$ represents an opaque solid and $\Omega_{\rm g}$ represents a transparent gas:

$$\overline{\Omega} = \overline{\Omega}_{\rm s} \cup \overline{\Omega}_{\rm g}, \quad \Omega_{\rm s} \cap \Omega_{\rm g} = \emptyset, \quad \Sigma := \overline{\Omega}_{\rm s} \cap \overline{\Omega}_{\rm g}. \tag{3}$$

This decomposition of Ω is to facilitate the modeling of radiative heat transfer, where nonlocal radiative heat transport is considered between points on the surface Σ of $\Omega_{\rm g}$. The open sets Ω, $\Omega_{\rm s}$, $\Omega_{\rm g}$ need to satisfy a number of geometrical regularity assumptions, see, e.g., [7, Sec. 2.1], which also has illustrating figures.

Continuity of the normal component of the heat flux on the interface Σ between solid and gas, where one needs to account for radiosity R and for irradiation J, yields the following interface condition for (2) (the same works for (1) after replacing the space domains by the corresponding time-space cylinders):

$$\big(\kappa(x,\theta)\,\nabla\,\theta\big)\restriction_{\overline{\Omega}_{\rm g}} \cdot \mathbf{n}_{\rm g} + R(\theta) - J(\theta) = \big(\kappa(x,\theta)\,\nabla\,\theta\big)\restriction_{\overline{\Omega}_{\rm s}} \cdot \mathbf{n}_{\rm g} \quad \text{on } \Sigma. \tag{4}$$

Here, $\mathbf{n}_{\rm g}$ denotes the unit normal vector pointing from gas to solid and $\restriction$ denotes restriction (or trace). Thus, effectively, (2) consists of two equations, one on $\Omega_{\rm s}$ and one on $\Omega_{\rm g}$, coupled via (4) (and analogously for (1)).

In the context of diffuse-gray radiation, where reflection and emittance are taken to be independent of the angle of incidence and independent of the wavelength, R is modeled via the well-known radiosity equation

$$\big(\operatorname{Id} - (1-\epsilon)K\big)(R) = \epsilon\sigma|\theta|^3\theta, \tag{5}$$

where Id denotes the identity operator, $\sigma \in \mathbb{R}^+$ represents the Boltzmann radiation constant, $\epsilon = \epsilon(x,\theta) \in [0,1]$ represents the emissivity of the solid surface, and K denotes the nonlocal integral radiation operator defined by

$$K(\rho)(x) := \int_\Sigma V(x,y)\,\omega(x,y)\,\rho(y)\,\mathrm{d}y \quad \text{for a.e. } x \in \Sigma, \tag{6}$$

$$\omega(x,y) := \frac{\big(\mathbf{n}_{\rm s}(y)\cdot(x-y)\big)\,\big(\mathbf{n}_{\rm s}(x)\cdot(y-x)\big)}{\pi\big((y-x)\cdot(y-x)\big)^2} \quad \text{for a.e. } (x,y) \in \Sigma\times\Sigma, \tag{7}$$

$$V(x,y) := \begin{cases} 0 & \text{if } \Sigma \cap]x,y[\neq \emptyset, \\ 1 & \text{if } \Sigma \cap]x,y[= \emptyset \end{cases} \quad \text{for each } (x,y) \in \Sigma\times\Sigma, \tag{8}$$

where ω is called view factor, V is called visibility factor (being 1 if, and only if, x and y are mutually visible), and $\mathbf{n}_{\mathrm{s}}$ denotes the outer unit normal to the solid domain Ω_{s}, existing almost everywhere if the interface Σ is Lipschitz.

If θ is to represent absolute temperature, then it must be always positive. However, it is also mathematically interesting to study equations (1), (2), and (5) in situations, where the solution θ can be negative. For that reason, it is often desirable to keep the problem formulation sufficiently flexible, such that it makes sense even if $\theta \geq 0$ can not be guaranteed. In particular, functions depending on θ should be (extended to be) defined also for $\theta < 0$, and, due to its monotonicity properties, using $|\theta|^3\theta$ in (5) instead of θ^4 is more suitable for the mathematical theory in situations, where θ can become negative.

It is well-known that, for each $1 \leq p \leq \infty$, the operator $K : L^p(\Sigma) \longrightarrow L^p(\Sigma)$ given by (6) is well-defined, linear, bounded, and positive with $\|K\| = 1$ (see [Tii97a, Lem. 1], [Tii97b, Lem. 2]). If the geometry of the domains is such that Σ is at least $C^{1,\alpha}$, $\alpha > 0$, then K is also known to be compact on $L^p(\Sigma)$ (see [Tii97b, Dru08]). However, compactness of K fails in many relevant cases:

Theorem 1. *For Σ being polyhedral, K is noncompact on $L^p(\Sigma)$ for each $p \in [1, \infty]$. Moreover, for $p < \infty$, K can never be compact when reinterpreted as a linear bounded operator $K : L^p(0, T, L^p(\Sigma)) \longrightarrow L^p(0, T, L^p(\Sigma))$ in a transient setting (regardless of the regularity of Σ).*

Proof. See [8, Ths. 2.1, 3.1, 3.2]. ■

The following Th. 2 allows to solve the radiosity equation (5) for R.

Theorem 2. *Let $p \in [1, \infty]$, assume* [7, (A-1)–(A-3)] *regarding Ω, Ω_{s}, Ω_{g}, and ϵ; and assume* [7, (A-4)] *regarding K (where K compact or Σ polyhedral is sufficient for* [7, (A-4)] *to hold). Then the operator $\mathrm{Id} - (1 - \epsilon)K$ has an inverse in the Banach space $\mathcal{L}(L^p(\Sigma), L^p(\Sigma))$ of bounded linear operators, and the operator*

$$G := (\mathrm{Id} - K)\big(\mathrm{Id} - (1 - \epsilon)K\big)^{-1}\epsilon \tag{9}$$

is an element of $\mathcal{L}(L^p(\Sigma), L^p(\Sigma))$.

Proof. For compact K, see [LT01, Lem. 2]; for noncompact K, see [8, Th. 2.4]. ■

Corollary 3. *Under the hypotheses of Th. 2, given $\theta \in L^4(\Sigma)$, the radiosity equation (5) has the unique solution $R(\theta) = \big(\mathrm{Id} - (1 - \epsilon)K\big)^{-1}(\epsilon\sigma|\theta|^3\theta) \in L^1(\Sigma)$ (recall $\sigma > 0$ and $\epsilon \in L^\infty(\Sigma)$).* ■

Using (9) together with the Stefan-Boltzmann law and Kirchhoff's law, one easily obtains (cf. [7, (15)])

$$R(\theta) - J(\theta) = G(\sigma|\theta|^3\theta) \quad \text{on } \Sigma, \tag{10}$$

such that (4) becomes

$$\big(\kappa(x,\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_\mathrm{g}} \cdot \mathbf{n}_\mathrm{g} + G(\sigma|\theta|^3\theta) = \big(\kappa(x,\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_\mathrm{s}} \cdot \mathbf{n}_\mathrm{g} \quad \text{on } \Sigma. \tag{11}$$

Assuming the domain Ω to be exposed to a black body environment (e.g. a large isothermal room) radiating at θ_ext (given absolute temperature), the Stefan-Boltzmann law provides the outer boundary condition

$$\kappa(x,\theta)\,\nabla\theta \cdot \mathbf{n}_\mathrm{s} - \sigma\,\epsilon\,(\theta_\mathrm{ext}^4 - |\theta|^3\theta) = 0 \quad \text{on } \partial\Omega. \tag{12}$$

1.1.2 Optimal Control of Heat Sources

When modeling heat transfer for industrial applications such as crystal growth, one is usually not merely interested in determining the temperature distribution θ, but one aims at optimizing θ according to a suitable objective functional. For example, during sublimation growth of silicon carbide, small horizontal temperature gradients in the gas domain Ω_g are desirable to avoid defects of the growing crystal, while sufficiently large vertical temperature gradients are required to guarantee a material transport from the silicon source to the seed crystal [SKM+00, MZPD02]. This background led to the optimal control problem considered in [3]:

$$\text{minimize} \quad J(\theta,u) := \frac{1}{2}\int_{\Omega_\mathrm{g}} \|\,\nabla\theta - z\|_2^2 + \frac{\nu}{2}\int_{\Omega_\mathrm{s}} u^2 \tag{13a}$$

$$\text{subject to} \quad \text{system (14) with } f = \begin{cases} u & \text{on } \Omega_\mathrm{s}, \\ 0 & \text{on } \Omega_\mathrm{g}, \end{cases} \tag{13b}$$

$$\text{and} \quad 0 < u_a \le u \le u_b \quad \text{in } \Omega_\mathrm{s}, \tag{13c}$$

where $z : \Omega_\mathrm{g} \longrightarrow \mathbb{R}^3$ is a given desired distribution for the temperature gradient, $\nu > 0$ is a regularization parameter, and system (14) is the summarized stationary model of Sec. 1.1.1, namely

$$-\operatorname{div}\big(\kappa(x,\theta)\,\nabla\theta\big) = f(x) \qquad \text{in } \Omega, \tag{14a}$$

$$\big(\kappa(x,\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_\mathrm{g}} \cdot \mathbf{n}_\mathrm{g} + G(\sigma|\theta|^3\theta) = \big(\kappa(x,\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_\mathrm{s}} \cdot \mathbf{n}_\mathrm{g} \qquad \text{on } \Sigma, \tag{14b}$$

$$\kappa(x,\theta)\,\nabla\theta \cdot \mathbf{n}_\mathrm{s} - \sigma\,\epsilon\,(\theta_\mathrm{ext}^4 - |\theta|^3\theta) = 0 \qquad \text{on } \partial\Omega, \tag{14c}$$

an integro-differential boundary value problem for the unknown $\theta : \overline{\Omega} \longrightarrow \mathbb{R}$. In particular, (13b) imposes the condition of no heat sources in the gas region Ω_g, motivated

by the application of induction heating. The control constraints (13c) reflect the fact that only heating (and no cooling) is considered, and they take into account that, due to technical limitations, an actual heating device can not produce heat sources of arbitrarily large values.

Actually, from the point of view of the application, a control problem like (13), where the heat sources f are controlled directly, is only the first step. In practice, the heat sources are generated by a heating mechanism such as induction heating, i.e. f itself is again the solution to some equation. A coupled system, where f is obtained as a solution to Maxwell's equations describing induction heating has been solved numerically in the context of industrial applications in [2, 5], which will be elaborated upon in Sections 1.1.3, 1.1.4, and 1.1.5 below. Moreover, a control problem for such a coupled system has been solved numerically in [1], cf. Sec. 1.1.3 below.

The mathematical theory of (13) obviously requires a theory for the existence, uniqueness, and regularity of solutions to (14). Results regarding the existence, uniqueness, and regularity of solutions to (14) and also of solutions to the transient variant of (14) are surveyed in [7]. The essence of these results is the existence and uniqueness of weak solutions to (14) and its transient counterpart under suitable hypotheses, where stronger hypotheses can guarantee, in particular, the continuity of the weak solution, see [7, Ths. 9,12] for details. Here, only [7, Ths. 9] is reproduced as Th. 6 below, as it is technically easier to state and relevant to the stationary control problem (13). Still, we need some preparations:

Notation 4. For $p, q \in [1, \infty]$, let

$$V^{p,q}(\Omega) := \big\{ u \in W^{1,p}(\Omega) : u \in L^q(\Sigma \cup \partial\Omega) \big\}, \tag{15}$$

simply writing u instead of $\mathrm{tr}(u)$ when considering u on $\Sigma \cup \partial\Omega$, suppressing the trace operator tr.

Definition 5. Define $\theta \in V^{s,4}(\Omega)$ for some $s \in [1, \infty]$ to be a *weak solution* to (14) if, and only if,

$$\int_\Omega \kappa(\cdot, \theta)\, \nabla\, \theta \cdot \nabla\, \psi + \int_{\partial\Omega} \sigma\epsilon|\theta|^3\theta\psi + \int_\Sigma G(\sigma|\theta|^3\theta)\psi = \int_\Omega f\psi + \int_{\partial\Omega} \sigma\epsilon\theta_{\mathrm{ext}}^4\psi \tag{16}$$

for each $\psi \in V^{s',\infty}(\Omega)$, where $s' \in [1, \infty]$ is the conjugate exponent to s, i.e. $\frac{1}{s} + \frac{1}{s'} = 1$.

Theorem 6. *Assume* [7, (A-1)–(A-4), (A-6)–(A-11)].

(a) *If $f \in L^p(\Omega)$, where $p > \frac{9}{7}$ or just $p > 1$ under the additional assumption that Σ is $C^{1,\alpha}$, $\alpha > 0$, then (14) has a weak solution θ. If $f \geq 0$, then $\theta \geq \operatorname{ess\,inf} \theta_{\mathrm{ext}}$. Moreover, regarding the regularity of θ, if $p \geq \frac{3}{2}$ and $\theta_{\mathrm{ext}} \in L^8(\partial\Omega)$, then $|\theta|^r \in$*

$W^{1,2}(\Omega)$ *for each* $r \in [1,\infty[$. *If* $p \in]\frac{9}{7},\frac{3}{2}[$ *and* $\theta_{\text{ext}} \in L^{8p/(3-p)}(\partial\Omega)$, *then* $\theta \in V^{2,2p/(3-2p)}(\Omega)$ *with* $2p/(3-2p) > 6$. *If* Σ *is* $C^{1,\alpha}$, $\alpha > 0$, $p \in [\frac{6}{5},\frac{9}{7}]$ *and* $\theta_{\text{ext}} \in L^{8p/(3-p)}(\partial\Omega)$, *then* $\theta \in V^{2,(9-5p)/(3-2p)}(\Omega)$ *with* $5 \le (9-5p)/(3-2p) \le 6$. *If* Σ *is* $C^{1,\alpha}$, $\alpha > 0$, $p \in]1,\frac{6}{5}[$ *and* $\theta_{\text{ext}} \in L^{8p/(3-p)}(\partial\Omega)$, *then* $\theta \in V^{3p/(3-p),(9-5p)/(3-2p)}(\Omega)$ *with* $\frac{3}{2} < 3p/(3-p) < 2$.

(b) *If* $f \in L^1(\Omega)$, Σ *is* $C^{1,\alpha}$, $\alpha > 0$, *and* $\epsilon < 1$, *then* (14) *has a weak solution* $\theta \in \bigcap_{s\in[1,\frac{3}{2}[} V^{s,4}(\Omega)$.

(c) *If* $\theta_{\text{ext}} \in L^\infty(\partial\Omega)$, $f \in L^p(\Omega)$ *with* $p > \frac{3}{2}$, *and all* $\partial\Omega_i$ *are* C^1, *then* (14) *has a weak solution* $\theta \in W^{1,q}$ *with* $q := 2p > 3$ *(in particular, the solution is Hölder continuous,* $\theta \in C^\gamma(\overline{\Omega})$, $\gamma > 0$*). This solution is unique provided* κ *is piecewise Lipschitz continuous (cf.* [7, (A-6), Th. 9(c)]*).*

Proof. For (a) see [Dru09, Th. 5.1], for (b) see [Dru09, Th. 6.1], and for (c) see [DKS$^+$11, Lem. 3.6] and its proof. ■

Definition 7. Under the assumptions of Th. 6(c), define the *control-to-state operator* $S : L^2(\Omega_{\text{s}}) \longrightarrow W^{1,q}(\Omega) \subseteq C^\gamma(\overline{\Omega}) \subseteq L^\infty(\Omega)$ ($q > 3$ as in Th. 6(c), $\gamma > 0$), $u \mapsto \theta$, assigning to $u \in L^2(\Omega_{\text{s}})$ the unique weak solution θ of (14) with $f := \begin{cases} u & \text{on } \Omega_{\text{s}}, \\ 0 & \text{on } \Omega_{\text{g}}, \end{cases}$ provided by Th. 6(c).

Definition 8. Employing the control-to-state operator of Def. 7, and letting

$$U_{\text{ad}} := \big\{u \in L^\infty(\Omega_{\text{s}}) : \, u_a \le u \le u_b\big\}, \tag{17}$$

$(\bar\theta,\bar u) \in W^{1,q}(\Omega) \times U_{\text{ad}}$ ($q > 3$ as in Th. 6(c)) is called an *optimal control* for (13) if, and only if, $\bar\theta = S(\bar u)$, and $\bar u$ minimizes the reduced objective functional

$$j : L^2(\Omega_{\text{s}}) \longrightarrow \mathbb{R}_0^+, \quad j(u) := J\big(S(u),u\big) \tag{18}$$

on U_{ad}.

—

The following theorem provides the existence of an optimal control for (13) under the simplifying assumption of θ-independent κ:

Theorem 9. *Under the assumptions of Th.* 6(c) *plus* $z \in L^2(\Omega_{\text{g}},\mathbb{R}^3)$, $u_a, u_b \in L^\infty(\Omega_{\text{s}})$, $0 < u_a \le u_b$, κ *θ-independent, and* $\operatorname{ess\,inf} \theta_{\text{ext}} > 0$, *there exists an optimal control* $(\bar\theta,\bar u)$ *for* (13).

Proof. See [3, Th. 5.2]. ■

Next, the differentiability of the control-to-state operator is considered as well as first-order necessary optimality conditions for (13), which are related to weak solutions to the linearized form of (14):

Definition 10. Under the assumptions of Th. 6(c) plus $\operatorname{ess\,inf}\theta_{\text{ext}} > 0$, let $\bar{u} \in L^2(\Omega_{\text{s}})$, $\bar{u} \geq 0$, $\bar{\theta} := S(\bar{u}) \in W^{1,q}(\Omega)$ with $q > 3$ as in Th. 6(c). Given $\mathcal{F}$ in the dual of $W^{1,q'}(\Omega)$ (q' the conjugate exponent to q), a function $\theta \in W^{1,q}(\Omega)$ is called a *weak solution* to the *linearized form* of (14) (or (16)) with right-hand side $\mathcal{F}$ if, and only if,

$$\begin{aligned}&\int_\Omega \kappa(\cdot,\bar{\theta})\,\nabla\theta\cdot\nabla\psi + \int_\Omega \frac{\partial\kappa}{\partial\theta}(\cdot,\bar{\theta})\theta\,\nabla\bar{\theta}\cdot\nabla\psi\\ &+4\int_{\partial\Omega}\sigma\epsilon|\bar{\theta}|^3\theta\psi + 4\int_\Sigma G(\sigma|\bar{\theta}|^3\theta)\psi = \mathcal{F}(\psi)\end{aligned}\tag{19}$$

for each $\psi \in W^{1,q'}(\Omega)$ (recall $G:\ L^\infty(\Sigma) \longrightarrow L^\infty(\Sigma)$ according to Th. 2).

Theorem 11. *Under the assumptions of Th.* 6(c) *plus* $\operatorname{ess\,inf}\theta_{\text{ext}} > 0$, *and* κ *being piecewise* C^1 *with bounded derivative in the sense of* [7, (A-6), (A-15)] *(*θ*-independence is* not *needed here), the control-to-state operator of Def.* 7 *is Fréchet differentiable on* $L^2_+(\Omega_{\text{s}}) := \{\bar{u} \in L^2(\Omega_{\text{s}}) :\ \bar{u} > 0\}$. *Moreover, for* $\bar{u} \in L^2_+(\Omega_{\text{s}})$, $\bar{\theta} = S(\bar{u})$, *and* $u \in L^2(\Omega_{\text{s}})$, *one has* $\theta := S'(\bar{u})(u)$ *given by the weak solution to the linearized form of* (14) *(i.e. of* (19)*) with right-hand side* $\mathcal{F}(\psi) := \mathcal{F}_u(\psi) := \int_{\Omega_{\text{s}}} u\psi$.

If $z \in L^2(\Omega_{\text{g}},\mathbb{R}^3)$, $u_a, u_b \in L^\infty(\Omega_{\text{s}})$, $0 < u_a \leq u_b$, *then* $(\bar{\theta},\bar{u}) \in W^{1,q}(\Omega)\times U_{\text{ad}}$ *(*$q > 3$ *as in Th.* 6(c)*) being an optimal control for* (13) *implies the necessary condition*

$$j'(\bar{u})(u-\bar{u}) = \langle\nabla\bar{\theta} - z, \nabla\theta\rangle_{L^2(\Omega_{\text{g}})} + \nu\langle\bar{u},(u-\bar{u})\rangle_{L^2(\Omega_{\text{s}})} \geq 0 \quad \textit{for each } u \in U_{\text{ad}},\tag{20}$$

with j *as in* (18), $\bar{\theta} = S(\bar{u})$, *and* $\theta = S'(\bar{u})(u-\bar{u})$.

Proof. See [3, Th. 7.1] and [7, Th. 18]. The proof is based on the implicit function theorem and makes use of [DKS$^+$11, Th. 4.4] which, under the above hypotheses, provides a unique weak solution $\theta \in W^{1,q}(\Omega)$ to (19), where this solution also satisfies $\|\theta\|_{W^{1,q}(\Omega)} \leq c\,\|\mathcal{F}\|$ for some $c > 0$. ■

1.1.3 Induction Heating: Model and Control

As stated before, from the point of view of industrial applications such as crystal growth, a control problem like (13), where the heat sources f are controlled directly, is only the first step. In practice, the heat sources are generated by a heating mechanism such as induction heating, i.e. f itself is again the solution to some equation. A control problem, where f is obtained as a solution to Maxwell's equations describing induction

heating, has been treated numerically in [1] for axisymmetric geometries. In [1], the heat sources f are obtained due to induction heating, generated by finitely many coil rings located outside the domain Ω. The heat sources are numerically computed according to the following model, where all materials in Ω_{s} are considered as potential conductors, whereas Ω_{g} is treated as a perfect insulator (see [KPS04, Sec. 2.6] for details; due to the axisymmetry, cylindrical coordinates (r, z) are used):

$$f(r,z) = \frac{|j(r,z)|^2}{2\,\sigma_{\mathrm{c}}(r,z)}, \tag{21}$$

$$j = \begin{cases} -i\omega\,\sigma_{\mathrm{c}}\,\phi \;+\; \frac{\sigma_{\mathrm{c}}\,v_k}{2\pi r} & \text{in the } k\text{-th coil ring,} \\ -i\omega\,\sigma_{\mathrm{c}}\,\phi & \text{in } \Omega_{\mathrm{s}}, \end{cases} \tag{22}$$

where σ_{c} denotes the electrical conductivity, v_k is the voltage imposed in the kth coil ring, ω is the common angular frequency of the imposed voltages, and i is the imaginary unit. The potential ϕ is determined from the following system of elliptic partial differential equations:

$$-\nu\,\mathrm{div}\,\frac{\nabla(r\phi)}{r^2} \qquad\qquad\qquad\qquad = 0 \quad \text{in } \Omega_{\mathrm{g}}, \tag{23a}$$

$$-\nu\,\mathrm{div}\,\frac{\nabla(r\phi)}{r^2} \qquad + \frac{i\,\omega\sigma_{\mathrm{c}}\phi}{r} \qquad = \frac{\sigma_{\mathrm{c}}\,v_k}{2\pi r^2} \quad \text{in the } k\text{-th coil ring,} \tag{23b}$$

$$-\nu\,\mathrm{div}\,\frac{\nabla(r\phi)}{r^2} \qquad + \frac{i\,\omega\sigma_{\mathrm{c}}\phi}{r} \qquad = 0 \quad \text{in } \Omega_{\mathrm{s}}, \tag{23c}$$

where ν denotes the magnetic reluctivity. The system (23) is completed by the interface conditions

$$\left(\frac{\nu\restriction_{\overline{\Omega}_i}}{r^2}\,\nabla(r\phi)\restriction_{\overline{\Omega}_i}\right) \bullet \mathbf{n}_{\Omega_i} = \left(\frac{\nu\restriction_{\overline{\Omega}_j}}{r^2}\,\nabla(r\phi)\restriction_{\overline{\Omega}_j}\right) \bullet \mathbf{n}_{\Omega_i}, \tag{24}$$

and the assumption that $\phi = 0$ both on the symmetry axis $r = 0$ and sufficiently far from the growth apparatus (imposed as Dirichlet boundary condition).

The domain used for the numerical computations of [1] represents an apparatus for silicon carbide single crystal growth via sublimation by physical vapor transport. The precise domain and its dimensions are provided in [1, Figs. 1,3]. During sublimation growth of silicon carbide, small horizontal temperature gradients in the gas domain Ω_{g} (more precisely in the part of Ω_{g} close to the surface of the growing crystal) are desirable to avoid defects of the growing crystal, while sufficiently large vertical temperature gradients are required to guarantee a material transport from the silicon source to the seed crystal [SKM$^+$00, MZPD02].

The control problem solved numerically in [1] is similar to (13). However, for the optimization of the temperature field θ in [1], the heat sources were not controlled directly

as in (13), but they were computed according to (21) – (24), whereas the quantities heating power P, vertical upper rim z_{rim} of the induction coil (cf. [1, Fig. 1]), and the frequency $f = \omega/(2\pi)$ of the heating voltage were used as control parameters, which is more realistic from the point of view of the considered crystal growth application. The control parameters, thus, result in a temperature distribution $\theta(P, z_{\mathrm{rim}}, f)$ via (21) – (24) and (14) (see [1] for details; one should not get confused by the fact that $f = \omega/(2\pi)$ denotes the frequency in [1] and not, as in (21) and previous equations above, the heat sources occurring on the right-hand side of the heat equation).

While [1, Fig. 7(a)] depicts the numerically computed temperature field for a generic, unoptimized situation as a reference, the objective functional minimized in [1, Fig. 7(b)] is

$$\mathcal{F}_r(\theta) := \left(\int_\Gamma 2\pi\, r\, \partial_r \theta(r,z)^2 \,\mathrm{d}r \right)^{1/2}, \tag{25}$$

aiming at minimizing the radial temperature gradient on the lower surface Γ of the growing SiC crystal. The objective functional minimized in [1, Fig. 7(c)] is

$$\frac{1}{2}\mathcal{F}_r(\theta) - \frac{1}{2}\mathcal{F}_z(\theta), \quad \mathcal{F}_z(\theta) := \left(\int_A 2\pi\, r\, \partial_z \theta(r,z)^2 \,\mathrm{d}(r,z) \right)^{1/2}, \tag{26}$$

aiming at minimizing the radial temperature gradient on Γ, while simultaneously maximizing the vertical temperature gradient inside the region A between the SiC crystal and the SiC powder, to guarantee material transport from the powder to the crystal (cf. [1, Fig. 2]).

The optimization is subject to a number of state constraints on θ, motivated by the crystal growth application: (a) The maximal temperature in the apparatus must not surpass a prescribed bound $\theta_{\max}$; (b) the temperature at the crystal surface Γ needs to stay within a prescribed range $[\theta_{\min,\Gamma}, \theta_{\max,\Gamma}]$; (c) the temperature gradient between source and seed must be negative, and must not surpass a prescribed value $\Delta_{\max} < 0$:

$$\max_\Omega(\theta) \le \theta_{\max}, \tag{27a}$$

$$\theta_{\min,\Gamma} \le \min_\Gamma(\theta) \le \max_\Gamma(\theta) \le \theta_{\max,\Gamma}, \tag{27b}$$

$$\max_A (\partial_z \theta) \le \Delta_{\max} < 0. \tag{27c}$$

A Nelder-Mead method was used for the numerical optimization as described in [1, Sec. 3]. The simulation software *WIAS-HiTNIHS* (cf. Sec. 1.1.5 below) was used for the required repeated numerical solution of the coupled state system (14), (21) – (24).

The main difference between the generic solution of [1, Fig. 7(a)] and the optimized solutions shown in [1, Figs. 7(b),(c)] is the gained homogeneity of the temperature inside

the SiC crystal in the optimized solutions (favorable with respect to low thermal stress and few crystal defects) as well as the isotherms below the crystal's surface becoming more parallel to that surface (as intended by the minimization of $\mathcal{F}_r(\theta)$). As expected, in [1, Fig. 7(c)], the maximization of $\mathcal{F}_z(\theta)$ leads to an increased number of isotherms between the crystal and the source powder. Summarizing the results, the radial and the vertical gradient can be effectively tuned simultaneously.

In [1, Figs. 4–6], the paper [1] also provides contour plots of the values of the objective functionals depending on the control parameters $\theta(P, z_{\mathrm{rim}}, f)$, illustrating the effect of the state constraints as well as the location of the numerically determined optimal controls.

1.1.4 Anisotropic Thermal Conductivity

The included articles [2, 4] deal with the numerical simulation of conductive-radiative heat transfer in the presence of anisotropic thermal conductivity. This is relevant to crystal growth applications since it is not unusual for the thermal insulation of growth apparatus to possess an anisotropic thermal conductivity (e.g. in the case of graphite felt, where the fibers are aligned in one particular direction). In generalization of (2), stationary heat conduction in anisotropic materials is described by

$$-\operatorname{div}\big(K_m(\theta)\,\nabla\,\theta\big) = f_m \quad \text{in } \Omega_m \qquad (m \in M), \tag{28}$$

where the symmetric and positive definite matrix K_m represents the thermal conductivity tensor in material m, f_m represents heat sources in material m, Ω_m is the domain of material m, and M is a finite index set. The papers [2, 4] consider the case where the thermal conductivity tensor is a diagonal matrix with temperature-independent anisotropy, i.e.

$$K_m(\theta) = \big(\kappa^m_{i,j}(\theta)\big), \quad \text{where} \quad \kappa^m_{i,j}(\theta) = \begin{cases} \alpha^m_i\,\kappa^m_{\mathrm{iso}}(\theta) & \text{for } i = j, \\ 0 & \text{for } i \neq j, \end{cases} \tag{29}$$

$\kappa^m_{\mathrm{iso}}(\theta) > 0$ being the thermal conductivity of the isotropic case (allowed to depend on the temperature θ), and $\alpha^m_i > 0$ being anisotropy coefficients. The material domains Ω_m are supposed to satisfy the geometric assumptions [4, (A-1)], restated below:

Assumption 12. $\overline{\Omega} = \bigcup_{m\in M} \overline{\Omega}_m$, $\Omega_{m_1} \cap \Omega_{m_2} = \emptyset$ for each $(m_1, m_2) \in M^2$ such that $m_1 \neq m_2$, and each of the sets Ω, Ω_m, $m \in M$, is a nonvoid, connected, polyhedral, bounded, and open subset of $\mathbb{R}^2$ (even though (28) holds in three dimensions, in the axisymmetric context of [2, 4], it suffices to consider the two-dimensional case, cf. [4, Sec. 3.6]).

The modification of the interface condition (4) for interfaces between anisotropic materials m_1 and m_2, $m_1 \neq m_2$, reads

$$\big(K_{m_1}(\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_{m_1}} \bullet \mathbf{n}_{m_1} = \big(K_{m_2}(\theta)\,\nabla\theta\big)\restriction_{\overline{\Omega}_{m_2}} \bullet \mathbf{n}_{m_1} \quad \text{on } \overline{\Omega}_{m_1} \cap \overline{\Omega}_{m_2}, \tag{30}$$

where the anisotropic materials are taken as opaque, such that no radiative contributions R, J are present in (30). The unit normal vector $\mathbf{n}_{m_1}$ in (30) points from material m_1 to material m_2.

In [4], a finite-volume discretization suitable for the numerical solution of (29), (30) with suitable boundary conditions is developed. The presented scheme was implemented in the software *WIAS-HiTNIHS* and used to compute the numerical results in [2, 4]. An admissible discretization of material domain Ω_m, $m \in M$, consists of a finite family $\Sigma_m := (\sigma_{m,i})_{i\in I_m}$ of subsets of Ω_m satisfying the following Assumptions 13 and 15.

Assumption 13. For each $m \in M$, $\Sigma_m = (\sigma_{m,i})_{i\in I_m}$ forms a finite conforming triangulation of Ω_m. In particular, for each $i \in I_m$, $\sigma_{m,i}$ is an open triangle. Moreover, letting $I := \bigcup_{m\in M} I_m$, $\Sigma := (\sigma_i)_{i\in I}$ forms a conforming triangulation of Ω.

—

For each $\sigma_{m,i}$, let $V(\sigma_{m,i}) = \big\{v^m_{i,j} : j \in \{1,2,3\}\big\}$ denote the set of vertices of $\sigma_{m,i}$, and let $V := \bigcup_{m\in M,\, i\in I_m} V(\sigma_{m,i})$ be the set of all vertices in the triangulation. One can then define the control volumes as the Voronoï cells with respect to the vertices. Using $\|\cdot\|_2$ to denote Euclidean distance, define

$$\text{for all } v \in V: \qquad \omega_v := \big\{x \in \Omega : \|x - v\|_2 < \|x - z\|_2 \text{ for each } z \in V \setminus \{v\}\big\}, \tag{31a}$$

$$\text{for all } m \in M: \quad \omega_{m,v} := \omega_v \cap \Omega_m, \quad V_m := \{z \in V : \omega_{m,z} \neq \emptyset\}. \tag{31b}$$

Letting $\mathcal{T} := (\omega_v)_{v\in V}$, $\mathcal{T}_m := (\omega_{m,v})_{v\in V_m}$, $m \in M$, $\mathcal{T}$ forms a partition of Ω, and $\mathcal{T}_m$ forms a partition of Ω_m.

Remark 14. Since $\mathcal{T}$ is a Voronoï discretization, each intersection $\partial\omega_v \cap \partial\omega_z$, $(v,z) \in V^2$, $v \neq z$, is contained in the set $\{x \in \Omega : \|v - x\|_2 = \|z - x\|_2\}$. In particular, $\frac{z-v}{\|z-v\|_2} = \mathbf{n}_{\omega_v}\restriction_{\partial_{\mathrm{reg}}\omega_v \cap \partial_{\mathrm{reg}}\omega_z}$, where ∂_{reg} denotes the regular boundary of a polyhedral set, i.e. the points of the boundary, where a unique outer unit normal vector exists, $\partial_{\mathrm{reg}}\emptyset := \emptyset$; and $\mathbf{n}_{\omega_v}\restriction_{\partial_{\mathrm{reg}}\omega_v \cap \partial_{\mathrm{reg}}\omega_z}$ is the outer unit normal to ω_v restricted to the face $\partial_{\mathrm{reg}}\omega_v \cap \partial_{\mathrm{reg}}\omega_z$ (see [4, Fig. 2]).

Assumption 15. For each $m \in M$, the triangulation Σ_m has the constrained Delaunay property: If $\tilde{V}_m := \bigcup_{i\in I_m} V(\sigma_{m,i})$; then, for each $(v,z) \in \tilde{V}_m^2$ such that $v \neq z$, the following conditions (a) and (b) are satisfied:

(a) If the boundaries of the Voronoï cells corresponding to v and z have a one-dimensional intersection, then the line segment $[v,z]$ is an edge of at least one $\sigma \in \Sigma_m$.

(b) If $[v, z]$ is an edge of at least one $\sigma \in \Sigma_m$, then the boundaries of the corresponding Voronoï cells have a nonempty intersection.

Due to the two-dimensional setting, the constrained Delaunay property can be expressed equivalently in terms of the angles in the triangulation: For each $m \in M$, if γ is an interior edge of the triangulation Σ_m, and α and β are the angles opposite to γ, then $\alpha + \beta \leq \pi$. If $\gamma \subseteq \partial\Omega_m$ is a boundary edge of Σ_m, and α is the angle opposite γ, then $\alpha \leq \pi/2$. Also see [4, Fig. 2].

Remark 16. Using Rem. 14, it is not hard to show that Assumptions 13 and 15 imply the following assertions (a) and (b):

(a) For each $m \in M$, the set V_m defined in (31b) is identical to the set $\tilde{V}_m$ defined in Assumption 15.

(b) Let Γ be a one-dimensional material interface: $\Gamma = \partial\Omega_m \cap \partial\Omega_{\tilde{m}}$. For each $v \in V$, if some $\overline{\omega}_v$ has a one-dimensional intersection with the interface Γ, then it lies on both sides of the intersection; in other words, $\partial_{\mathrm{reg}}\omega_{m,v} \cap \Gamma = \partial_{\mathrm{reg}}\omega_{\tilde{m},v} \cap \Gamma$.

—

As usual, the finite volume scheme for (28), (30) is constructed by integrating (28) over $\omega_{m,v}$, applying the Gauss-Green integration theorem to obtain

$$-\int_{\partial\omega_{m,v}} (K_m(\theta)\,\nabla\theta) \bullet \mathbf{n}_{\omega_{m,v}} = \int_{\omega_{m,v}} f_m \tag{32}$$

(where $\mathbf{n}_{\omega_{m,v}}$ denotes the outer unit normal vector to $\omega_{m,v}$), and by using (30) followed by suitable approximations for the integrals. In the context of (14), the construction and further references can be found in [7, Sec. 4]. The novelty of [4] lies in the approximation of the heat flux integrals $\int_{\partial\omega_{m,v}\cap\Omega_m} (K_m(\theta)\,\nabla\theta) \bullet \mathbf{n}_{\omega_{m,v}}$ in the presence of anisotropic thermal conductivity, so only the main particularities of this approximation are briefly included below.

Notation 17. For each $m \in M$ and each $(v, w) \in M^2$, let $\gamma_{m,v,w} := \partial\omega_{m,v} \cap \partial\omega_{m,w}$ denote the interface of the two Voronoï cells inside the material domain Ω_m (of course, in general, $\gamma_{m,v,w}$ can be empty).

—

For the approximation of $\int_{\partial\omega_{m,v}\cap\Omega_m} (K_m(\theta)\,\nabla\theta) \bullet \mathbf{n}_{\omega_{m,v}}$, the set $\partial\omega_{m,v} \cap \Omega_m$ is partitioned further, namely into the interfaces with all neighboring Voronoï cells. Up to null sets with respect to one-dimensional Lebesgue measure λ_1

$$\partial\omega_{m,v} \cap \Omega_m = \bigcup_{w \in \mathrm{nb}_m(v)} \gamma_{m,v,w}, \tag{33}$$

where $\mathrm{nb}_m(v) := \{w \in V_m \setminus \{v\} : \lambda_1(\gamma_{m,v,w}) \neq 0\}$ is the set of m-neighbors of v (cf. [4, Fig. 3]).

Using (33), it remains to approximate $(K_m(\theta)\,\nabla\,\theta) \bullet \mathbf{n}_{\omega_{m,v}}$ on $\gamma_{m,v,w}$. According to the assumed form (29) of the $K_m(\theta)$, the approximation can be broken down into two parts: (a) Approximation of the temperature-dependent, isotropic part. (b) Approximation of the temperature-independent, anisotropic part.

Approximation of the temperature-dependent, isotropic part

The quantity $\kappa^m_{\mathrm{iso}}(\theta)$ on $\gamma_{m,v,w}$ is approximated by the mean

$$\kappa^m_{\mathrm{iso}}(\theta)\restriction_{\gamma_{m,v,w}} \approx \frac{1}{2}\left(\kappa^m_{\mathrm{iso}}(\theta_v) + \kappa^m_{\mathrm{iso}}(\theta_w)\right) \tag{34}$$

(cf. remark after [4, (14)]).

Approximation of the temperature-independent, anisotropic part

For the anisotropic part, it remains to approximate $(A_m\,\nabla\,\theta) \bullet \mathbf{n}_{\omega_{m,v}}$ on $\gamma_{m,v,w}$, where A_m is the constant diagonal matrix

$$A_m = (a^m_{i,j}), \qquad a^m_{i,j} := \begin{cases} \alpha^m_i & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases} \tag{35}$$

The approximation of [4] is devised such that it is exact provided θ is affine on each $\sigma \in \Sigma$ and provided Σ has the strong Delaunay property (all angles are less than or equal to $\pi/2$). If θ is affine on $\sigma \in \Sigma$, then

$$\nabla\,\theta\restriction_\sigma = \sum_{v \in V(\sigma)} \theta(v)\ \nabla\,\phi_{\sigma,v}, \tag{36}$$

where $\phi_{\sigma,v} : \sigma \longrightarrow [0,1]$, $v \in V(\sigma)$, are the affine coordinates on the triangle σ with respect to its 3 vertices.

Given $m \in M$, $(v,w) \in V_m^2$, $v \neq w$, such that $[v,w]$ is an edge of some $\sigma \in \Sigma_m$, let

$$\Sigma_{m,v,w} := \left\{\sigma \in \Sigma_m : \{v,w\} \subseteq V(\sigma)\right\} \tag{37}$$

be the set of triangles in Σ_m having $[v,w]$ as an edge. Since Σ_m is a conforming triangulation of Ω_m by Assumption 13, if $[v,w]$ is a boundary edge, then $\Sigma_{m,v,w}$ has precisely one element; otherwise, it has precisely two elements, lying on different sides of $[v,w]$. For each $\sigma \in \Sigma_{m,v,w}$, let $H_{v,w,\sigma}$ be the half-space that lies on the same side of

the line through $[v, w]$ as σ. Even though Assumption 15 guarantees $\lambda_1(\gamma_{m,v,w}) \neq 0$, [4, Fig. 3] shows that $\gamma_{m,v,w}$ can lie entirely on one side of $[v, w]$. However, letting

$$\Sigma_{\gamma_{m,v,w}} := \big\{\sigma \in \Sigma_{m,v,w} : \lambda_1(H_{v,w,\sigma} \cap \gamma_{m,v,w}) \neq 0\big\}, \tag{38}$$

one can decompose $\gamma_{m,v,w}$ according to (cf. [4, Fig. 3])

$$\gamma_{m,v,w} = \bigcup_{\sigma \in \Sigma_{\gamma_{m,v,w}}} \overline{\sigma} \cap \gamma_{m,v,w}. \tag{39}$$

Using (36) together with Rem. 14 yields, for each $\sigma \in \Sigma_{\gamma_{m,v,w}}$:

$$(A_m \nabla \theta)\restriction_\sigma \bullet \mathbf{n}_{\omega_v}\restriction_{\gamma_{m,v,w}} = \sum_{\tilde{v} \in V(\sigma)} \theta(\tilde{v}) \, (A_m \nabla \phi_{\sigma,\tilde{v}}) \bullet \frac{w - v}{\|w - v\|_2}. \tag{40}$$

Together with (34) and (39), (40) provides the approximation of the normal heat flux across $\gamma_{m,v,w}$ (cf. (41) below). Formula (40) constitutes the key difference to and improvement over previously published schemes (see Introduction and paragraphs following (20) in [4]).

Combining the temperature-dependent and temperature-independent parts

Combining the approximations of the temperature-dependent and the temperature-independent parts, i.e. combining (34), (39), and (40) yields

$$\begin{aligned} &\int_{\gamma_{m,v,w}} (K_m(\theta) \nabla \theta) \bullet \mathbf{n}_{\omega_{m,v}} \\ &\approx \sum_{\sigma \in \Sigma_{\gamma_{m,v,w}}} \frac{1}{2} \left(\kappa^m_{\mathrm{iso}}(\theta_v) + \kappa^m_{\mathrm{iso}}(\theta_w)\right) \\ &\qquad \sum_{\tilde{v} \in V(\sigma)} \theta_{\tilde{v}} \, (A_m \nabla \phi_{\sigma,\tilde{v}}) \bullet \frac{w - v}{\|w - v\|_2} \, \lambda_1(H_{v,w,\sigma} \cap \gamma_{m,v,w}). \end{aligned} \tag{41}$$

Numerical Results Using the New Scheme

Numerical results verifying the new scheme in comparison with exactly computable closed-form solutions can be found in [4, Sec. 4.2], showing second-order convergence in a single-material domain and first-order convergence in a multi-material domain with discontinuous thermal conductivity coefficients.

In [2], the new scheme is employed to compute temperature fields in realisticly modeled crystal growth apparatus with thermally anisotropic insulation material. The numerical

results in [2, Sections 4.2 and 5] show that, depending on the insulation's orientation, even a moderate anisotropy in the insulation can result in temperature variations of more than 100 K at the growing crystal's surface, which need to be taken into account for an accurate simulation as well as for the design of the growth apparatus.

1.1.5 Numerical Simulation Software WIAS-HiTNIHS[1]

Except [3, 6, 8], all included papers present numerical simulation results computed using the software *WIAS-HiTNIHS*. At WIAS Berlin, I was the head developer of *WIAS-HiTNIHS* in the period 1997 – 2006. Since I left WIAS Berlin, the role of head developer was taken over by Dr. Olaf Klein.

WIAS-HiTNIHS constitutes a tool for both stationary and transient simulations of heat transport in axisymmetric technical systems that are subject to heating by induction. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature, e.g. employing temperature-dependent laws of thermal and electrical conductivity. Using a band model, *WIAS-HiTNIHS* can treat materials as semi-transparent. Anisotropic thermal conductivity can be accounted for during the computations as in [2, 4]. It is also possible to use *WIAS-HiTNIHS* just to compute axisymmetric magnetic scalar potentials and the resulting heat sources. An optimization module allows the control of parameters such as heating power and coil position with the objective of minimizing functionals such as the max-norm of the radial temperature gradient in a neighborhood of the growing crystal's surface as in [1]. The simulator is designed to deal with complicated axisymmetric setups having a polygonal 2-dimensional projection.

From a more abstract perspective, *WIAS-HiTNIHS* is a solver for two-dimensional potentially nonlinear elliptic and parabolic PDE in both Cartesian and cylindrical coordinates. Multi-material, polyhedral domains are allowed, and all material functions can depend nonlinearly on the solution. Fourier law type interface conditions are implemented as well as nonlocal radiative interface conditions. Implemented outer boundary conditions include time- and space-dependent Dirichlet conditions, Neumann and Robin conditions, emission conditions, and nonlocal radiative conditions. A shape optimization module enables numerical PDE-driven shape optimization via optimal control of a shape function on a (larger) fixed domain as described in [9].

The PDE solver in *WIAS-HiTNIHS* employs a finite volume discretization [7, Sec. 4]. *WIAS-HiTNIHS* is based on the program package *pdelib* [FKL01], it employs the grid generator *Triangle* [She96, She02] to produce constrained Delaunay triangulations of the domains, and it uses the sparse matrix solver *PARDISO* [SG04, SGF00] to solve the linear system arising from the finite volume scheme.

[1] **Hi**gh **T**emperature **N**umerical **I**nduction **H**eating **S**imulator; pronunciation: ∼hit-nice.

In the included paper [5], *WIAS-HiTNIHS* is used to aide the industrial application of liquid encapsulated Czochralski crystal growth of GaAs under the influence of a traveling magnetic field. It is used to compute electromagnetic fields as well as temperature fields in realistic growth apparatus, assessing the influence of the Lorentz force on the melt, e.g. regarding the damping of the temperature oscillations below the crystal, desirable for high-quality growth.

1.2 Crack Propagation

The included paper [6] is aimed at improving the understanding of brittle fracture formation and propagation in materials. While the classical theory of Griffith [Gri21] constitutes the foundation of modern understanding of brittle fracture, it still has a number of significant shortcomings: Griffith theory does not predict crack initiation and path and it suffers from the presence of unphysical stress singularities. While the former problem is addressed, e.g., in [FM98, DFT05], and the latter problem is addressed, e.g., in [SMS05], [6] is directed at including the ideas of [SMS05] for the removal of stress singularities into the framework of [FM98, DFT05].

The approach of [FM98, DFT05] has the advantage that it does not need to prescribe the presence of a crack or its path a priori, but the potential crack as well as its path are part of the problem's solution. It is founded on the global minimization of energy functionals acting on spaces of functions of bounded variations, where the cracks are related to the discontinuity sets of such functions. The model of [6] formulates modified energy functionals that account for molecular interactions in the vicinity of crack tips and the cohesive forces in the spirit of [SMS05]. In contrast to [FM98, DFT05], the model also allows for crack reversibility and considers local minimizers of the energy functionals, employing different time scales. Solving the model for a simple one-dimensional example with a dead load, it is shown that the local energy minimization yields the physically expected result in a situation where the global minimization according to [FM98] fails.

The goal in [6] is to model a strained and cracked body quasistatically using a time- and space-dependent function u, representing the body's displacement field with respect to an uncracked *reference configuration* $\Omega \subseteq \mathbb{R}^N$, $N \in \{1, 2, 3\}$, assumed to be nonempty, bounded, open, connected, with Lipschitz boundary $\partial\Omega$. The considerations in [6] culminate in the formulation of two versions of a quasistatic evolution model, one based on global energy minimization in [6, Sec. 2.5.5] and one based on local energy minimization in [6, Sec. 2.5.6]. Both versions will be restated here, followed in each case by summaries of the involved concepts. Previously unexplained notation occurring in the following Def. 18 will also be made clear after the definition statement below.

Definition 18. Let $T > 0$. A *quasistatic evolution of globally minimizing energy configurations* (*QEGMEC*) is a function $u : [0, T] \longrightarrow SBV^\infty(\Omega, \mathbb{R}^N)$ satisfying the

following conditions:

(a) For each $t \in [0,T]$: $u(t) \in \mathrm{AD}(t)$.

(b) For each $t \in [0,T]$: $\mathcal{E}(t)(u_{u(t)}) \leq \mathcal{E}(t)(u_v)$ for every $v \in \mathrm{AD}(t)$.

(c) $W_{\mathrm{ext}}(t)(u) - W_{\mathrm{ext}}(s)(u) = \mathcal{E}(t)(u) - \mathcal{E}(s)(u)$ for each $(s,t) \in [0,T]^2$, $s < t$.

—

In Def. 18, the variables $s, t \in [0,T]$ represent time, $SBV^\infty(\Omega,\mathbb{R}^N) := SBV(\Omega,\mathbb{R}^N) \cap L^\infty(\Omega,\mathbb{R}^N)$, $SBV(\Omega,\mathbb{R}^N)$ denoting the space of *special functions of bounded variation*, and the set $\mathrm{AD}(t)$ in Def. 18(a),(b) is the set of *admissible displacement fields* satisfying a Dirichlet boundary condition on $\partial_{\mathrm{D}}\Omega \subseteq \partial\Omega$ (see [6, Sec. 2.5.1, Sec. 2.3]):

$$\mathrm{AD}(t) := \big\{ u \in SBV^\infty(\Omega,\mathbb{R}^N) : \operatorname{tr}_{\partial_{\mathrm{D}}\Omega} u = u_{\mathrm{D}}(t) \in L^\infty(\partial_{\mathrm{D}}\Omega,\mathbb{R}^N) \ \text{ given} \big\}. \tag{42}$$

The model requires $u(t) \in L^\infty(\Omega,\mathbb{R}^N)$, since unbounded displacements are not physically reasonable, and the requirement $u(t) \in SBV(\Omega,\mathbb{R}^N)$ is reasonable in the context of crack modeling as explained in [6, Sec. 2.1.2]. In particular, for a fixed time t, the set $\Gamma(u,r) \subseteq \Omega$ of present cracks can be defined by

$$\Gamma(u,r) := r^{-1}\{1\} \cup \big\{ x \in J_u : \big([u](x)\big) \bullet \mathbf{n}_{J_u}(x) > 0 \big\}, \tag{43}$$

where J_u is the so-called *jump set* of $u := u(t) \in SBV(\Omega,\mathbb{R}^N)$, $\mathbf{n}_{J_u}$ denotes the normal vector with respect to J_u,

$$[u] : J_u \longrightarrow \mathbb{R}^N, \quad [u](x) := u_+(x) - u_-(x), \tag{44}$$

u^+ and u^- being the one-sided limits of u with respect to J_u. Moreover, the *crack reversibility function* $r : \Omega \longrightarrow \{0,1\}$ occurring in (43) is an accounting tool that, for each $x \in \Omega$, records if there is an irreversible crack at x or not: $r(x) = 1$ if, and only if, there is an irreversible crack at x (thus, if $r(x) = 0$, then there is either no crack at x, or there is a reversible crack at x). According to the model of [6], irreversibility is triggered by a crack having opened more than a threshold value $a_{\mathrm{th}} > 0$. Thus, more precisely, r depends on time and space, $r : [0,T] \times \Omega \to \{0,1\}$, and, given u and a_{th},

$$r_u(t,x) = \begin{cases} 0 & \text{if } \big([u](t,x)\big) \bullet \mathbf{n}_{J_{u(t)}}(x) < a_{\mathrm{th}} \text{ for all } s \leq t, \\ 1 & \text{otherwise.} \end{cases} \tag{45}$$

In consequence, r_u can be seen as a *memory* function for u: The energy at time t does not only depend on $u(t)$, but also on $r_u(t)$, i.e. on the history of u. It is also noted that

the crack (43) is determined by u and r, i.e. it does not have to be specified separately as in Francfort-Marigo theory [FM98].

The functional $\mathcal{E}(t)$ in Def. 18(b),(c) represents the total energy at time t. As described in [6, Sec. 2.4.5], there are several contributions to the total energy, namely the energy of the crack, the bulk energy, the energy of the body forces, and the energy of the surface forces. Only the formula for determining the energy of the crack is new in [6, Sec. 2.4.1] and is summarized here (see [6, Sec. 2.4.2 – Sec. 2.4.4] for the remaining contributions): The energy $\mathcal{E}_{\mathrm{cr}}$ of the crack is defined by

$$\mathcal{E}_{\mathrm{cr}}(u,r) := \int_{\Gamma(u,r)} \kappa\big(x, \mathbf{n}_\Gamma(x), [u](x), r(x)\big)\, \mathrm{d}\mathcal{H}^{N-1}(x), \tag{46}$$

where $\mathcal{H}^{N-1}$ denotes the restriction of $(N-1)$-dimensional Hausdorff measure to $\Gamma(u,r)$, and

$$\kappa : \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \{0,1\} \longrightarrow \mathbb{R}_0^+ \cup \{\infty\} \tag{47}$$

is a function modeling the material's toughness, $\mathbb{S}^{N-1}$ denoting the $(N-1)$-dimensional unit sphere. The dependence of κ on x and $\mathbf{n}_\Gamma(x)$ describes the location- and direction-dependent toughness of the material. The dependence of κ on its third variable allows to account for Barenblatt-type energies corresponding to cohesive forces depending on the normal distance of the crack lips. Permitting κ to depend on the entire jump $[u](x)$ instead of just on the jump in the normal direction allows to include energy barriers for slip dislocations (jumps of u parallel to the crack). The dependence on $r(x)$ allows to account for crack reversibility: The idea is to use this as a switch for the dependence of κ on its third variable: As cohesive forces should play no role once the crack has become irreversible, κ should depend nontrivially on the third variable if, and only if, the fourth variable is 0. For an example of a toughness function κ based on a Lennard-Jones potential, see [6, (10),(11)] and [6, Fig. 2]. According to the reasoning in [6, Sec. 2.4.1], κ should, at least, have the following properties:

(a) $\kappa(x,\mathbf{n},z,r) < \infty$ for each $(x,\mathbf{n},z,r) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \{0,1\}$ such that $z \bullet \mathbf{n} \geq 0$.

(b) $\kappa(x,\mathbf{n},z_1,1) = \kappa(x,\mathbf{n},z_2,1)$ for each $(x,\mathbf{n},z_1,z_2) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N \times \mathbb{R}^N$ such that $z_1 \bullet \mathbf{n} \geq 0$ and $z_2 \bullet \mathbf{n} \geq 0$.

(c) For each $(x,\mathbf{n}) \in \Omega \times \mathbb{S}^{N-1}$, the function $z \mapsto \kappa(x,\mathbf{n},z,0)$ is continuous on the set $\{z \in \mathbb{R}^N : 0 \leq z \bullet \mathbf{n} \leq a_{\mathrm{th}}\}$.

(d) $\kappa(x,\mathbf{n},z,0) = \kappa(x,\mathbf{n},z,1)$ for each $(x,\mathbf{n},z) \in \Omega \times \mathbb{S}^{N-1} \times \mathbb{R}^N$ such that $z \bullet \mathbf{n} = a_{\mathrm{th}}$.

—

Condition Def. 18(b) is the condition of global energy minimization (cf. [6, Sec. 2.5.2]): For each $t \in [0,T]$, $u(t)$ needs to be a minimizer of the total energy $\mathcal{E}(t)$ among all

admissible $v \in \mathrm{AD}(t)$. Due to the presence of the reversibility function, to be able to formulate the condition at time t, one has to make use of the function u already defined for times smaller than t: Let $v \in \mathrm{AD}(t)$ be an admissible displacement field at time t, and let $u : [0,t[\longrightarrow SBV^\infty(\Omega,\mathbb{R}^N)$ be given. Then u can be extended to time t by v:

$$u_v : [0,t] \longrightarrow SBV^\infty(\Omega,\mathbb{R}^N), \quad u_v(s) := \begin{cases} u(s) & \text{for } s < t, \\ v & \text{for } s = t. \end{cases} \tag{48}$$

Finally, condition Def. 18(c) states the energy balance: For each time interval, the increment in stored energy plus the energy spent in crack increase (or recovered by crack closure) needs to equal the work W_{ext} of the external forces, where, in general, W_{ext} has the three contributions listed in [6, Sec. 2.5.4].

We now come to the model of [6, Sec. 2.5.6], which is based on *local* energy minimization. It is restated as Def. 19, followed by further explanations.

Definition 19. Let $T > 0$. A *quasistatic evolution of locally minimizing energy configurations* (*QELMEC*) is a function $u : [0,T] \longrightarrow SBV^\infty(\Omega,\mathbb{R}^N)$ satisfying the following conditions:

(a) For each $t \in [0,T]$: $u(t) \in \mathrm{AD}(t)$.

(b) For each $t \in [0,T]$, there is $\epsilon > 0$ such that $\mathcal{E}(t)(u_{u(t)}) \le \mathcal{E}(t)(u_v)$ for each $v \in \mathrm{AD}(t)$ satisfying $\|u(t) - v\|_{\infty,1} < \epsilon$.

(c) There exists a finite sequence of times $0 = t_0 < \cdots < t_n = T$ such that u is continuous with respect to the $\|\cdot\|_{\infty,1}$-norm on each interval $[t_{\nu-1}, t_\nu[$, $\nu \in \{1,\dots,n\}$, and, for each $\nu \in \{1,\dots,n\}$, there is $v_\nu \in \mathrm{AD}(t_\nu)$ such that the map

$$u_\nu : [t_{\nu-1}, t_\nu] \longrightarrow SBV^\infty(\Omega,\mathbb{R}^N), \quad u_\nu(t) := \begin{cases} u(t) & \text{for } t < t_\nu, \\ v_\nu & \text{for } t = t_\nu, \end{cases}$$

is continuous with respect to the $\|\cdot\|_{\infty,1}$-norm on the entire closed interval $[t_{\nu-1}, t_\nu]$, and such that there is an admissible path $p_\nu \in P_{t_\nu}\big(v_\nu, u(t_\nu)\big)$ connecting v_ν and $u(t_\nu)$.

(d) $W_{\mathrm{ext}}(t)(u) - W_{\mathrm{ext}}(s)(u) = \mathcal{E}(t)(u) - \mathcal{E}(s)(u)$ for each $(s,t) \in [0,T]^2$, $s < t$.

—

Conditions Def. 19(a),(d) were already present in Def. 18. Condition Def. 19(b) is the local analogue of the global minimization condition Def. 18(b): For each $t \in [0,T]$,

$u(t)$ now needs to be a local minimizer of the total energy $\mathcal{E}(t)$ among all admissible $v \in \mathrm{AD}(t)$, local with respect to the norm

$$\|u\|_{\infty,1} := \|u\|_\infty + \|\nabla u\|_1, \tag{49}$$

where ∇u denotes the absolutely continuous part of the distributional derivative of u with respect to Lebesgue measure (see [6, Sec. 2.5.3] regarding the choice or norm).

Condition Def. 19(c) states that the quasistatic evolution must be energetically admissible, where, for a fixed time $t \in [0,T]$, given $u : [0,t[\longrightarrow SBV^\infty(\Omega,\mathbb{R}^N)$, the set $P_t(v_1,v_2)$ of *admissible paths* between states v_1 and v_2, $(v_1,v_2) \in \mathrm{AD}(t) \times \mathrm{AD}(t)$, is defined as the set of maps $p : [0,1] \longrightarrow \mathrm{AD}(t)$ continuous with respect to $\|\cdot\|_{\infty,1}$ such that $p(0) = v_1$, $p(1) = v_2$, and such that the map $a \mapsto \mathcal{E}(t)\big(u_{p(a)}\big)$ is nonincreasing on $[0,1]$. According to [6, Sec. 2.5.3], condition Def. 19(c) arises from considering different scales for the time dependence: First, assume that the local minima in Def. 19(b) are strict. Then, the macro time scale is active as long as $u(t)$ "naturally" sits in a local minimum for the energy according to Def. 19(b). This is the case inside each interval $[t_{\nu-1}, t_\nu[$. The energy of $u(t)$ can actually increase with t, but, at each t, it is smaller than for any state in some $\|\cdot\|_{\infty,1}$-neighborhood of $u(t)$. Since $\mathcal{E}(t)$ changes with time, so does the energy landscape. At the times t_ν, $\nu \in \{1,\dots,n\}$, it has changed so much that what used to be a strict local minimum is no longer a strict local minimum, and there exists an admissible path in $\mathrm{AD}(t_\nu)$ to some state of lower energy. The assumption of quasistatic evolution means that the system follows such a path on the micro time scale, finding a new local energetic minimum. This happens instantaneously on the macro time scale, namely at time t_ν. The consideration of nonstrict, plateau-type local minima is somewhat more subtle and can be found in [6, Sec. 2.5.3].

In [6, Sec. 3], both the global and local version of the new model are solved for a concrete one-dimensional example. The example considers a dead load of the type [FM98, Sec. 5.2]. The issue discussed in [FM98, Sec. 5.2] is basically that the energy minimization yields an unphysical result, namely failure for an arbitrarily small nonzero load. This problem is due to the global energy minimization, and [6, Sec. 3.2] shows that introducing reversibility and cohesive forces does nothing to change the situation. However, the local version of the energy minimization considered in Sec. [6, Sec. 3.3] yields the physically expected result that failure occurs only once the load surpasses a critical value.

1.3 Shape Design

The included paper [9] formulates a fixed-domain method for the solution of shape design problems governed by elliptic PDE, including a numerical algorithm and corresponding numerical results.

Let $E \subseteq D \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, be some given bounded domains with Lipschitz boundary. Let $\Omega \subseteq D$ be some (unknown) set and $y \in H_0^1(\Omega)$ be the weak solution of the following PDE defined in Ω:

$$\underset{v \in H_0^1(\Omega)}{\forall} \quad \int_\Omega \left(\sum_{i,j=1}^{d} a_{ij} \frac{\partial y}{\partial x_i} \frac{\partial v}{\partial x_j} + a_0 y v \right) = \int_\Omega f v, \tag{50}$$

where a_{ij}, $a_0 \in L^\infty(D)$, $(a_{ij})_{i,j=1,d}$ elliptic and $f \in L^2(D)$.

A general shape optimization problem associated to (50) consists of the minimization of a cost functional of the form

$$F(y, \Omega) = \int_\Lambda j\big(x, y(x), \nabla y(x)\big)\, \mathrm{d}x\,, \tag{51}$$

where Λ may be E, Ω, or D and y is the solution of the corresponding state equation (50) (extended by 0 to the whole D for $\Lambda = D$). An important special case is the quadratic functional

$$J(\Omega) = \alpha \int_\Lambda |y - y_d|^2 \,\mathrm{d}x \, + \beta \int_\Lambda \|\nabla y - \nabla y_d\|_2^2, \tag{52}$$

where α, $\beta \in \mathbb{R}_0^+$, $\alpha + \beta > 0$, $y_d \in H^1(D)$ are given.

Various constraints may be imposed as well. For instance, if $\Lambda = E$, then impose

$$\Omega \supseteq E \tag{53}$$

for any admissible domain Ω, such that (51), (52) make sense.

The domains Ω are encoded using so-called shape functions g according to

$$\Omega = \Omega_g = \mathrm{int}\{x \in D : \, g(x) \geq 0\}. \tag{54}$$

Using g one can put further constraints on the set of admissible domains by imposing $g \in X(D)$, $X(D)$ being a subspace of piecewise continuous mappings defined in D. More precisely, the piecewise continuity means there exists $l \in \mathbb{N}$ and $\Omega_i \subseteq D$, $i \in \{1, \ldots, l\}$, open subsets such that $\Omega_i \bigcap \Omega_j = \varnothing$, $i \neq j$, $\overline{D} = \bigcup_{i=1}^{l} \overline{\Omega_i}$, and $g_i \in C(\overline{D})$ such that $g\restriction_{\Omega_i} = g_i\restriction_{\Omega_i}$ for each $i \in \{1, \ldots, l\}$.

If the constraint (53) is to be imposed as well, then one requires

$$g \geq 0 \quad \text{in} \quad E. \tag{55}$$

Even though the shape functions $g \in X(D)$ are also known as level functions, as explained in [9], the fixed domain approach used in [9] and summarized below is quite

different from the well-known methods of Sethian [Set96], Osher and Sethian [OS88]. An approximation property specific to PDE with Dirichlet boundary conditions is at the base of the method used in [9]. Denote by $H^\varepsilon : \mathbb{R} \longrightarrow \mathbb{R}$ the following differentiable regularization of the Yosida approximation of the maximal monotone extension in $\mathbb{R}\times\mathbb{R}$ of the Heaviside function H:

$$H^\varepsilon(r) := \begin{cases} 1 & \text{for } r \geq 0, \\ \dfrac{\varepsilon(r+\varepsilon)^2 - 2r(r+\varepsilon)^2}{\varepsilon^3} & \text{for } -\varepsilon < r < 0, \\ 0 & \text{for } r \leq -\varepsilon. \end{cases} \tag{56}$$

Then (50) is approximated by

$$\underset{v\in H_0^1(D)}{\forall} \quad \int_D \left(\sum_{i,j=1}^d a_{ij} \frac{\partial y_\varepsilon}{\partial x_i} \frac{\partial v}{\partial x_j} + a_0 y_\varepsilon v + \frac{1}{\varepsilon}\big(1 - H^\varepsilon(g)\big) y_\varepsilon v \right) = \int_D f v, \tag{57}$$

now always integrating over the larger fixed domain D, penalizing nonzero values of $y_\varepsilon \in H_0^1(D)$ in $D \setminus \Omega_g$ via the additional term on the left-hand side of (57).

Results regarding the convergence $y_\varepsilon|_{\Omega_g} \to y_g$ for $\varepsilon \to 0$ are surveyed in [9, Sec. 2] as well as results regarding the differentiability of the control-to-state mapping $g \mapsto y_\varepsilon = y_\varepsilon(g)$. Only [9, Th. 3(i)] is reproduced here as Th. 20, as it provides the basis for the adjoint equation and the descent directions used in the numerical algorithm.

Theorem 20. *The mapping $g \mapsto y_\varepsilon = y_\varepsilon(g)$ defined by (57) is Gâteaux differentiable between $X(D)$ and $H_0^1(D)$ and $z = \nabla y_\varepsilon(g)w \in H_0^1(D)$ satisfies the equation in variations:*

$$\underset{v\in H_0^1(D)}{\forall} \quad \int_D \left(\sum_{i,j=1}^d a_{ij} \frac{\partial z}{\partial x_i} \frac{\partial v}{\partial x_j} + a_0 z v + \frac{1}{\varepsilon}\big(1 - H^\varepsilon(g)\big) z v \right) = \frac{1}{\varepsilon} \int_D (H^\varepsilon)'(g) w y_\varepsilon v. \tag{58}$$

—

The variations occurring in the directional derivatives of the above control-to-state map are of the form $g + \lambda w$, $\lambda \in \mathbb{R}$; g, $w \in X(D)$. They allow for simultaneous changes of the boundary and of the topological characteristic of the searched domain.

All the numerical experiments of [9, Sec. 3] use the square fixed domain

$$D :=]-1, 1[\times]-1, 1[\subseteq \mathbb{R}^2 \tag{59a}$$

with fixed subdomain

$$E :=]-\tfrac{1}{2}, \tfrac{1}{2}[\times]-\tfrac{1}{2}, \tfrac{1}{2}[\subseteq D \tag{59b}$$

in case the shape function constraint (55), restated as

$$g \in U(D) := \{g \in X(D) : \, g \geq 0 \ \text{ on } \ E\}, \tag{60}$$

is used. In each experiment, the state equation for $y_\varepsilon \in H_0^1(D)$ is a special case of (57), having the form

$$\underset{v \in H_0^1(D)}{\forall} \quad \int_D \left(\frac{\partial y_\varepsilon}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial y_\varepsilon}{\partial x_2} \frac{\partial v}{\partial x_2} + \frac{1}{\varepsilon} \left(1 - H^\varepsilon(g)\right) y_\varepsilon \, v \right) = \int_D f v. \tag{61}$$

The cost functionals considered for the shape optimization have the general form

$$J : \, X(D) \longrightarrow \mathbb{R}, \quad g \mapsto J(g) = F(S(g), g), \tag{62}$$

where $F : \, H_0^1(D) \times X(D) \longrightarrow \mathbb{R}$ and $S : \, X(D) \longrightarrow H_0^1(D)$, $S(g) = y_\varepsilon(g)$, is the control-to-state operator corresponding to (61).

The shape optimization algorithm of [9, Sec. 3.1] is summarized as follows ($\varepsilon > 0$ is fixed throughout the algorithm):

Step 1 Set $n := 0$ and choose an admissible initial shape function $g_0 \in X(D)$.

Step 2 Compute the solution to the state equation $y_n = y_\varepsilon = S(g_n)$.

Step 3 Compute the solution to the corresponding adjoint equation $p_n = p_\varepsilon$.

Step 4 Compute a descent direction $w_{\mathrm{d},n} = w_{\mathrm{d},n}(y_n, p_n)$.

Step 5 Set $\tilde{g}_n := g_n + \lambda_n \, w_{\mathrm{d},n}$, where $\lambda_n \geq 0$ is determined via line search, i.e. as a solution to the minimization problem

$$\lambda \mapsto J(g_n + \lambda \, w_{\mathrm{d},n}) \to \min . \tag{63}$$

(numerically accomplished by a golden section search for results in [9, Sec. 3]).

Step 6 Set $g_{n+1} := \pi_{U(D)}(\tilde{g}_n)$, where $\pi_{U(D)}$ denotes the projection

$$\pi_{U(D)} : \, X(D) \longrightarrow U(D), \quad \pi_{U(D)}(g)(x) := \begin{cases} \max\{0, g(x)\} & \text{for } x \in E, \\ g(x) & \text{for } x \in D \setminus E \end{cases} \tag{64}$$

(and $U(D) = X(D)$, $\pi_{U(D)}(g) = g$ if no constraints are imposed).

Step 7 RETURN $g_{\mathrm{fin}} := g_{n+1}$ if the change of g and/or the change of $J(g)$ are below some prescribed tolerance parameter (see [9, Sec. 3.1] for details). Otherwise: Increment n, i.e. $n := n + 1$ and GO TO Step 2.

The state equations as well as the adjoint equations that need to be solved numerically during the above algorithm are linear elliptic PDE with homogeneous Dirichlet boundary conditions. For the numerical simulations in [9, Sec. 3], an augmented version of the software *WIAS-HiTNIHS* (cf. Sec. 1.1.5) has been employed to this end.

In Example 1 of [9, Sec. 3.2] the cost functional J is as in (62) with

$$F(y,g) := \frac{1}{2}\int_E (y-y_d)^2 \,\mathrm{d}x\,, \tag{65a}$$

$$y_d(x_1,x_2) := -\left(x_1-\frac{1}{2}\right)^2 - \left(x_2-\frac{1}{2}\right)^2 + \frac{1}{16}, \tag{65b}$$

$f \equiv 1$ is used on the right-hand side of the state equation, the descent direction used in Step 4 is $w_{\mathrm{d}}(y,p) = -\frac{1}{\varepsilon}yp$ (see [9, (20)] for the corresponding adjoint equation), and $g \geq 0$ on E is imposed.

The results depicted in [9, Figs. 1–3] show the convergence to the optimal shape $\Omega_{g_{\mathrm{fin}}} = E$ for three different initial shape functions g_0. For a fixed g_0, [9, Table 1], shows the convergence of the final value $J(g_{\mathrm{fin}})$ of the objective functional for $\varepsilon \to 0$.

In Example 2 of [9, Sec. 3.2], a different objective functional is used: As before, J has the form (62), but now with

$$F(y,g) := \int_D H^\varepsilon(g)(y-y_d) \,\mathrm{d}x\,, \tag{66a}$$

$$y_d(x_1,x_2) := -\left(x_1-\frac{1}{2}\right)^2 - \left(x_2-\frac{1}{2}\right)^2 + \frac{1}{8}. \tag{66b}$$

Note that (66a) is an approximation for $\int_\Omega (y-y_d)\,\mathrm{d}x$. In this example $\varepsilon = 10^{-5}$ is fixed as well as $f \equiv 1$, and, for the descent direction of Step 4,

$$w_{\mathrm{d}}(y,p) = -\left(H^\varepsilon(g)(y-y_d) + \frac{1}{\varepsilon}yp\right) \tag{67}$$

is used (see [9, (25)] for the corresponding adjoint equation).

The results in [9, Figs. 4–6] show a slight dependence of the final shape $\Omega_{g_{\mathrm{fin}}}$ on the initial shape function g_0, which is not unexpected due to the nonconvexity of the situation and since, in general, only local minima are found during the line searches of Step 5. It is also noted that (66) and (67) are symmetric with respect to exchanging x_1 and x_2, and this symmetry can be observed in the shapes in [9, Figs. 4,5], whereas the symmetry is slightly broken in [9, Figs. 6] due to the initial condition.

In Example 3 of [9, Sec. 3.2], a nonconstant right-hand side is used, namely

$$f:\ D \longrightarrow \mathbb{R}, \quad f(x_1,x_2) := -x_1^2\,x_2^2 + 1, \tag{68}$$

where J still has the form (62), this time with

$$F(y, g) := \frac{1}{2} \int_D (y - y_d)^2 \, \mathrm{d}x \,, \tag{69a}$$

$$y_d(x_1, x_2) := x_1^2 \, x_2^2. \tag{69b}$$

Note that y_d is different from the y_d in (65b) and, in contrast to (65a), the integration in (69a) is over all of D. Once again, $\varepsilon = 10^{-5}$ is fixed, and the employed descent direction is $w_{\mathrm{d}}(y, p) = -\frac{1}{\varepsilon} yp$ (see [9, (29)] for the corresponding adjoint equation).

In this case, the nonconvexity of the problem is much more visible in the numerical results than during previous examples. We observe a considerable dependence of the final shape not only on the initial shape function g_0, but also on the initial guess for λ during the line searches, see the results depicted in [9, Figs. 7–9]. In Example 3 of [9, Sec. 3.2], there is x_1-x_2-symmetry as well as symmetry with respect to the signs of x_1 and x_2, respectively, provided the initial shape function satisfies the same symmetry. These symmetries are visible in [9, Fig. 7], slightly broken in the final shape due to the discrete grid.

For convenience, the following list includes, once again, the bibliographic information for the included papers as well as the bibliographic information of further relevant references.

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