# State-constrained optimal control problem with radiation interface conditions

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A state-constrained optimal control problem arising in the context of sublimation crystal growth is considered. The presence of pointwise state-constraints and nonlocal radiation interface conditions constitutes the major issue of this problem. A regularity result of the state is presented that allows to derive the optimality condition.

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# 1 Introduction

We discuss an optimal control problem arising in the context of sublimation crystal growth. To be more precise, the physical vapor transport (PVT) method is considered where polycrystalline powder is placed under a low-pressure inert gas atmosphere at the bottom of a cavity inside a crucible. The crucible is heated up to 2000 till 3000 K by induction. Due to the high temperatures and the low pressure, the powder sublimates and crystallizes at a single-crystalline seed located at the cooled top of the cavity such that the desired single crystal grows into the reaction chamber (see [1] and the references therein for more details). Here, we focus on the control of the conductive-radiative heat transfer in the reaction chamber which is denoted by  $\Omega_g \subset \mathbb{R}^N$ ,  $N \in \{2,3\}$ . More precisely, we aim at optimizing the temperature gradient in  $\Omega_g$  by directly controlling the heat source u in  $\Omega_s := \Omega \setminus \Omega_g$  where  $\Omega \subset \mathbb{R}^N$  denotes the domain of the entire crucible including the gas phase; see Figure 1 for an exemplary two-dimensional domain. Thus, the objective functional that we focus on reads as follows:

minimize 
$$J(u, y) := \frac{1}{2} \int_{\Omega_a} |\nabla y - z|^2 dx + \frac{\beta}{2} \int_{\Omega_s} u^2 dx$$

where y denotes the temperature,  $z \in L^2(\Omega_g)^N$  is the desired temperature gradient, and  $\beta$  is a given positive real number. Because of the high temperatures, it is essential to account for radiation on the outer boundary  $\Gamma_0 := \partial \Omega$ and on the interface  $\Gamma_r := \overline{\Omega}_s \cap \overline{\Omega}_g$ ; they are assumed to be sufficiently smooth. Thus, y is given by the solution of the stationary heat equation with radiation interface and boundary conditions on  $\Gamma_r$  and  $\Gamma_0$ , respectively:

(SL) 
$$\begin{cases} -\operatorname{div}(\kappa_s \nabla y) = u & \text{in } \Omega_s \\ -\operatorname{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \\ \kappa_g \left(\frac{\partial y}{\partial n_r}\right)_g - \kappa_s \left(\frac{\partial y}{\partial n_r}\right)_s = G\sigma |y|^3 y & \text{on } \Gamma_r \\ \kappa_s \frac{\partial y}{\partial n_0} + \varepsilon\sigma |y|^3 y = \varepsilon\sigma y_0^4 & \text{on } \Gamma_0. \end{cases}$$
 Figure 1.

The description  $n_0$  denotes the outward unit normal on  $\Gamma_0$  and  $n_r$  is the unit normal on  $\Gamma_r$  facing outward with respect to  $\Omega_s$ . Furthermore,  $\sigma \in \mathbb{R}^+$  represents the Boltzmann radiation constant;  $\varepsilon \in L^{\infty}(\Gamma_0 \cup \Gamma_r)$  with  $\varepsilon \geq \varepsilon_0 > 0$ is the emissivity;  $y_0 \in L^{\infty}(\Gamma_0)$  represents the external temperature which is assume to be positive and  $\kappa_s \in \mathcal{C}(\Omega_s)$ ,  $\kappa_g \in \mathcal{C}(\Omega_g)$  denote the thermal conductivities in  $\Omega_s$  and  $\Omega_g$ , respectively. The operator  $G : L^p(\Gamma_r) \to L^p(\Gamma_r)$  is linear and continuous for all  $1 \leq p \leq \infty$ . For the detailed definition on the operator G, we refer the reader to [1]. In addition to the stationary semilinear heat equation, the optimization is subject to the following pointwise stateand control-constraints:

(1) 
$$y(x) \le y_{\max}(x)$$
 a.e. in  $\Omega_s$ ,  $y_a(x) \le y(x) \le y_b(x)$  a.e. in  $\Omega_g$ ,  $u_a(x) \le u(x) \le u_b(x)$  a.e. in  $\Omega_s$ .

Here,  $u_a \in L^{\infty}(\Omega_s)$  and  $u_b \in L^{\infty}(\Omega_s)$  reflect the minimum and maximum heating power. Furthermore,  $y|_{\Omega_s}$  has to be bounded by  $y_{\max} \in \mathcal{C}(\Omega_s)$  to avoid melting of the solid components of crucible in  $\Omega_s$ . Finally, the state-constraints in  $\Omega_g$  are required to ensure sublimation of the polycrystalline powder and crystallization at the seed; notice that boundaries  $y_a, y_b \in \mathcal{C}(\Omega_g)$  satisfy  $y_a < y_b$ . The analysis of the control problem (P) turns out to be extremely delicate and at least there are two substantial reasons for this. Firstly, the pointwise state constraints in the set of explicit

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constraints (1) certainly constitute major difficulties in the corresponding first- and second-order analysis. Secondly, the involved nonlinearity in the state equation (SL) is in general not monotone so that standard techniques such as the Browder-Minty theorem are not applicable. The analysis of the purely control-constrained counterpart to (P) was recently performed in [1] which, however, cannot be transferred to the control problem (P) due to the presence of pointwise state constraints. One needs to significantly extend the analysis of the aforementioned references in order to gain a deeper insight into the solution structure of (SL).

#### 2 Existence and Uniqueness of the weak solution to (SL) in $W^{1,q}(\Omega)$

In the following, let us define the weak formulation of the state equation (SL) which is obtained by formal integration of (SL) by parts over the boundaries  $\Gamma_r$  and  $\Gamma_0$ ; cf. [2].

**Definition 1** Let q > N and q' > 0 such that  $\frac{1}{q} + \frac{1}{q'} = 1$ . A function  $y \in W^{1,q}(\Omega)$  is called a weak solution to (SL), if it satisfies

$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_r} (G\sigma |y|^3 y) v \, ds + \int_{\Gamma_0} \varepsilon \sigma |y|^3 y v \, ds = \int_{\Omega_s} u v + \int_{\Gamma_0} \varepsilon \sigma y_0^4 v \, ds \quad \forall v \in W^{1,q'}(\Omega).$$

The existence and uniqueness of the weak solution to (SL) in the sense of Definition 1 was verified in [2].

**Theorem 1** There exists  $q = q_0 \in (N, 6)$  such that for every  $u \in L^2(\Omega_s)$  the state equation (SL) admits a unique weak solution  $y = y(u) \in W^{1,q}(\Omega)$ . Furthermore, there exists a constant c > 0 depending only on  $\Omega$  such that

(2) 
$$\|y\|_{W^{1,q}(\Omega)} \le c \left(1 + \|u\|_{L^2(\Omega_s)} + \|y_0\|_{L^{\infty}(\Gamma_0)}^4 + \|u\|_{L^2(\Omega_s)}^4 + \|y_0\|_{L^{\infty}(\Gamma_0)}^{16}\right)$$

#### 3 First-order necessary optimality condition

Let us fix  $q = q_0 > N$  obtained from Theorem 1 and define  $\mathcal{U} := \{u \in L^2(\Omega_s) \mid u_a \leq u \leq u_b \text{ a.e. in } \Omega_s\}$ . We consider further an arbitrarily fixed  $\bar{u} \in \mathcal{U}$  and its corresponding state is denoted by  $\bar{y}$ . The linear operators  $F(\bar{y}): L^{\infty}(\Gamma_r) \to W^{1,q'}(\Omega)^*$  and  $B(\bar{y}): W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$  are defined by

$$< F(\bar{y})y, v>:= 4 \int_{\Gamma_r} (G\sigma |\bar{y}|^3 y) v ds \ \forall v \in W^{1,q'}(\Omega), \quad < B(\bar{y})y, v>:= \int_{\Omega} \kappa \nabla y \cdot \nabla v dx + \int_{\Gamma_0} 4\varepsilon \sigma \, |\bar{y}|^3 y v ds \ \forall v \in W^{1,q'}(\Omega)$$

In [2, Lemma 2.1], it is shown that  $B(\bar{y})$  is continuously invertible. Further, by  $\tau_r: W^{1,q}(\Omega) \to L^{\infty}(\Gamma_r)$ , we denote the trace operator on  $\Gamma_r$ . Thus,  $\mathcal{F}(\bar{y}) := \tau_r B(\bar{y})^{-1} F(\bar{y})$  is well defined as an operator from  $L^{\infty}(\Gamma_r)$  to  $L^{\infty}(\Gamma_r)$ .

**Definition 2** We say that  $\bar{u} \in \mathcal{U}$  satisfies the "eigenvalue restriction" if  $\lambda = -1$  is not an eigenvalue of  $\mathcal{F}(\bar{y})$ .

Relying on the eigenvalue restriction and assuming a Slater-type assumption in the sense of [2, Definition 5.2], the existence of Lagrange multipliers and an adjoint state associated with (P) was established in [2] which immediately leads to the following necessary optimality condition:

**Theorem 2 (First-order necessary optimality condition)** Let  $\bar{u} \in L^2(\Omega_s)$  be an optimal solution to (P) satis fying the linearized slater condition. Suppose further that  $\bar{u}$  satisfies the eigenvalue restriction. Then, there exist an adjoint state  $\bar{p} \in W^{1,q'}(\Omega)$ ,  $q' < \frac{N}{N-1}$ , and a triple of Lagrange multipliers  $(\mu_s, \mu_q^a, \mu_q^b) \in \mathcal{M}(\overline{\Omega}_s) \times \mathcal{M}(\overline{\Omega}_g) \times \mathcal{M}(\overline{\Omega}_g)$ such that

$$\begin{cases} -\operatorname{div}(\kappa_s \nabla \bar{y}) = \bar{u} & \operatorname{in} \Omega_s \\ -\operatorname{div}(\kappa_g \nabla \bar{y}) = 0 & \operatorname{in} \Omega_g \\ \kappa_g \left(\frac{\partial \bar{y}}{\partial n_r}\right)_g - \kappa_s \left(\frac{\partial \bar{y}}{\partial n_r}\right)_s = G\sigma |\bar{y}|^3 \bar{y} \quad \operatorname{on} \Gamma_r \\ \kappa_s \frac{\partial \bar{y}}{\partial n_r} + \varepsilon\sigma |\bar{y}|^3 \bar{y} = \varepsilon\sigma y_0^4 \quad \operatorname{on} \Gamma_0, \end{cases} \begin{cases} -\operatorname{div}(\kappa_g \nabla \bar{p}) = -\Delta \bar{y} + \operatorname{div} z + (\mu_g^b - \mu_g^a)_{|\Omega_g|} & \operatorname{in} \Omega_g \\ -\operatorname{div}(\kappa_s \nabla \bar{p}) = \mu_{s|\Omega_s} & \operatorname{in} \Omega_s \\ \kappa_g \left(\frac{\partial \bar{p}}{\partial n_r}\right)_g - \kappa_s \left(\frac{\partial \bar{p}}{\partial n_r}\right)_s = 4\sigma |\bar{y}|^3 G^* \bar{p} - \frac{\partial \bar{y}}{\partial n_r} + z \cdot n_r \\ + (\mu_g^b - \mu_g^a + \mu_s)_{|\Gamma_r|} & \operatorname{on} \Gamma_r \\ \kappa_s \frac{\partial \bar{p}}{\partial n_r} + 4\varepsilon \sigma |\bar{y}|^3 \bar{y} = \varepsilon \eta \nabla_{\theta} & \operatorname{on} \Gamma_{\theta} \end{cases}$$

$$\mu_s \ge 0, \ \mu_g^a \ge 0, \ \mu_g^b \ge 0, \qquad \int_{\overline{\Omega}_s} \mathcal{G}(\bar{u}) - y_{\max} \ d\mu_s = \int_{\overline{\Omega}_g} y_a - \mathcal{G}(\bar{u}) \ d\mu_g^a = \int_{\overline{\Omega}_g} \mathcal{G}(\bar{u}) - y_b \ d\mu_g^b = 0, \qquad \bar{u} = \mathbb{P}_{ad} \Big\{ -\frac{1}{\beta} \bar{p} \Big\}.$$

where  $\mathbb{P}_{ad}: L^2(\Omega_s) \to L^2(\Omega_s)$  denotes the pointwise projection operator on the admissible set  $\mathcal{U}$ .

### References

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