FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
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PARABOLIC PROBLEMS ARISING IN REAL-WORLD APPLICATIONS

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Overview

Parabolic evolution equations are a cornerstone in the mathematical modelling of irreversible processes in the natural sciences and, in general, well understood. Still, there are many **real-world applications** with inherently **nonsmooth data** where classical methods basing on relatively smooth data fail to apply. Here, "nonsmooth data" may refer to the underlying spatial **domain** $\Omega \subset \mathbb{R}^3$, the **coefficients**, or the fact that (inhomogeneous) **mixed boundary conditions** are given. Usually the models also consist of **systems**.

These challenges can be overcome within the framework of analytic semigroups or **maximal parabolic regularity** by deriving **precise information about fractional powers** of the associated operators and **permanence principles** for **optimal elliptic regularity** as well as **interpolation identities** for function spaces in the context of mixed boundary conditions. We list three real-world examples for which one obtains satisfying wellposedness results using these techniques, and also optimal control considerations for one example.

Thermistor problem

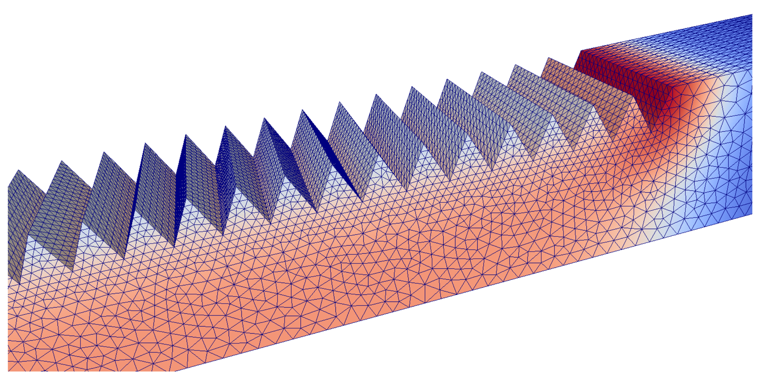
Here we are concerned with the heating of a workpiece $\Omega \subset \mathbb{R}^3$, made of a conducting material such as steel, by means of direct current, so-called **Joule heating**. The associated **quasilinear heat equation** with **Robin boundary conditions** describing the evolution of the temperature θ is given by

$$\theta' - \operatorname{div}(\eta(\theta)\kappa\nabla\theta) = (\sigma(\theta)\rho\nabla\varphi)\cdot\nabla\varphi,$$
$$\nu\cdot\eta(\theta)\kappa\nabla\theta + \alpha\theta = \alpha\theta_l.$$

The forcing corresponds to the strength of the electric field induced by the potential φ given by the potential equation with **inhomogeneous mixed boundary conditions**

$$-\operatorname{div}(\sigma(\theta)\rho\nabla\varphi) = 0, \qquad \begin{cases} \varphi = 0 & \text{on } \Gamma_D, \\ \nu\cdot\sigma(\theta)\rho\nabla\varphi = u & \text{on } \partial\Omega\setminus\Gamma_D \end{cases}$$

with $\varphi = 0$ on $\Gamma_D \subset \partial\Omega$ representing grounding and the current (control) u on $\partial\Omega\setminus\Gamma_D$. The thermistor problem is of importance e.g. in the process of **steel hardening** for **gear racks** which are nonsmooth and nonconvex.



A gear rack as used in numerical simulations of the thermistor problem.

The particular challenge in the thermistor system is the combination of inhomogeneous mixed boundary conditions with the quasilinear coupling of temperature and potential (**thermistor** effect). If Ω is a **Lipschitz manifold** compatible with Γ_D and η,σ are Lipschitz-continuous conductivity functions, and $q > 3$ is such that $-\operatorname{div}(\kappa\nabla)\colon W^{1,q}(\Omega) \to W_0^{-1,q}(\Omega)$ and $-\operatorname{div}(\kappa\nabla)\colon W^{1,q}_{\Gamma_D}(\Omega) \to W^{-1,q}_{\Gamma_D}(\Omega)$ are surjective (**optimal elliptic regularity**), then it is possible to eliminate the potential equation in terms of θ and to rely on **maximal parabolic regularity** techniques for the resulting **quasilinear** equation for θ to obtain: for every $u \in L^\infty(0,T;L^3(\partial\Omega\setminus\Gamma_D))$ and r large enough, there are unique local-in-time solutions

$$\varphi \in L^\infty(0,T;W^{1,q}_{\Gamma_D}(\Omega)), \quad \theta \in W^{1,r}(0,T;W_0^{-1,q}(\Omega)) \cap L^r(0,T;W^{1,q}(\Omega)).$$

This allows to consider an associated **optimal control problem** with a desired temperature θ_d on $\Omega_d \subseteq \Omega$ at time T and control u, subject to **control- and state constraints**

$$\min_{(\theta,u)} \frac{1}{2}\int_{\Omega_d} |\theta(T)-\theta_d|^2 + \frac{\beta}{2}\|u\|^2_{H^1(0,T;L^3(\partial\Omega\setminus\Gamma_D))} \quad \text{s.t.} \quad \begin{cases} u_{\mathsf{min}} \le u \le u_{\mathsf{max}}, \\ \theta \le \theta_{\mathsf{melt}}. \end{cases}$$

Keller-Segel model in chemotaxis

This model describes the evolution of the density u of cellular slime molds driven by a chemo-attractant of concentration v which induces movement of the slime molds towards higher concentrations of the attractant (**chemotaxis**). The attractant is degraded by an enzyme of concentration p produced by the slime molds, from which a complex of concentration w is created. This gives rise to a **reaction-diffusion system** for (v,p,w) coupled with a **Fokker-Planck type equation** for u with drift induced by v:

$$u' - k_u\Delta u = -\chi\operatorname{div}(u\nabla v), \qquad p' - k_p\Delta p = -r_1vp + (r_{-1}+r_2)w + r_pu,$$
$$v' - k_v\Delta v = -r_1vp + r_{-1}w + r_vu, \quad w' - k_w\Delta w = r_1vp - (r_{-1}+r_2)w,$$

subject to homogeneous Neumann conditions (experimental setting) and with given initial concentrations. Under the assumption that Ω is a **Lipschitz manifold** and that there is $q > 3$ such that $-\Delta + 1\colon W^{1,q}(\Omega) \to W^{-1,q}$ is surjective (**optimal elliptic regularity**), we obtain the previously unknown result that for all nonnegative initial concentrations smooth enough and r large, there exist unique nonnegative local-in-time solutions

$$u,v,p,w \in W^{1,r}(0,T;L^{q/2}(\Omega)) \cap L^r(0,T;\operatorname{dom}_{L^{q/2}}(\Delta)) \cap L^\infty(0,T;L^\infty(\Omega)).$$

The main idea is to solve for (v,p,w) in dependence of u, and to re-insert in the first equation, thereby obtaining a **single**, but **nonlocal-in-time** equation which can be dealt with via **maximal parabolic regularity**. This wellposedness result is a starting point for further investigations of the rich dynamics of this system.

Van Roosbroeck system of semiconductors

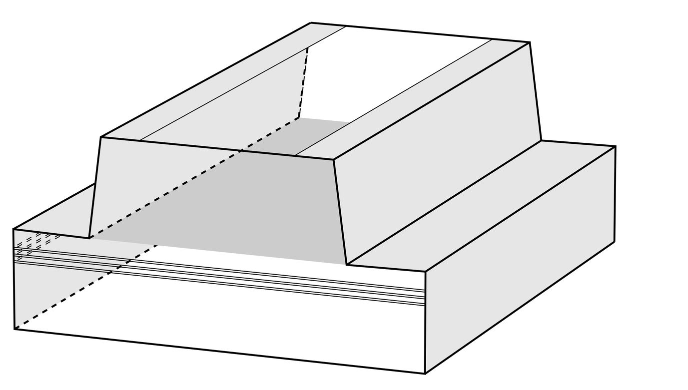
In the van Roosbroeck system for a **semiconductor** device $\Omega \subset \mathbb{R}^3$, negative and positive charge carriers, electrons and holes, move by diffusion and drift within a self-consistent electrical field. Thereby, they recombine to charge-neutral electron-hole pairs or, vice versa, split up from pairs to single charges. The evolution of the densities (u_1,u_2) of electrons and holes is given by the **current-continuity equations** which are **semilinear Fokker-Planck equations** with **inhomogeneous mixed boundary conditions**

$$u_k' - \operatorname{div} j_k = r^\Omega(u_1,u_2,\varphi), \qquad \begin{cases} u_k = U_k & \text{on } \Gamma_D, \\ \nu\cdot j_k = r^\Gamma(u_1,u_2,\varphi) & \text{on } \Gamma_N, \end{cases}$$
$$j_k = \mu_k\big(\nabla u_k + (-1)^k u_k\nabla\varphi\big)$$

for $k = 1,2$. The recombination functions r^Ω, r^Γ depend on the material and include the **quadratic gradient** case $r^\Omega(u_1,u_2,\phi) \sim |\nabla u|^2$. The associated electrostatic potential is subject to the potential equation with **inhomogeneous mixed boundary conditions**

$$-\operatorname{div}(\varepsilon\nabla\varphi) = \mathfrak{d} + u_1 - u_2 \qquad \begin{cases} \varphi = \varphi_{\Gamma_D} & \text{on } \Gamma_D, \\ \nu\cdot(\varepsilon\nabla\varphi) + \varepsilon_{\Gamma_N}\varphi = \varphi_{\Gamma_N} & \text{on } \Gamma_N, \end{cases}$$

A critical component here is the **doping** $\mathfrak{d}$ which lives on a **two-dimensional surface** embedded into the semiconductor device and which induces special charge flow properties.



⟵ Scheme of a ridge waveguide quantum well laser with two material layers divided by the dark plane. The top and bottom of the structure carry Dirichlet boundary conditions for the electrostatic potential, with Neumann boundary conditions for the rest (indicated by shading). At the bottom, a triple quantum well structure corresponds to the doping $\mathfrak{d}$.

If Ω is a **Lipschitz manifold** compatible with Γ_D, if there is $q > 3$ such that $-\operatorname{div}(\eta_k\nabla\cdot)$ and $-\operatorname{div}(\varepsilon\nabla\cdot)+\varepsilon_{\Gamma_N}\colon W^{1,q}_{\Gamma_D}(\Omega) \to W^{-1,q}_{\Gamma_D}(\Omega)$ are surjective (**optimal elliptic regularity**), r^Ω, r^Γ are Lipschitz, and $\mathfrak{d} \in H^{-3/q,q}(\Omega)$, then there exists a unique local-in-time solution

$$u_k \in C^{1-\tau/2}([0,T];H_D^{\tau-1,q}(\Omega)) \cap C([0,T];W_D^{1,q}(\Omega)) \cap C^1((0,T];H^{\tau-1,q}(\Omega))$$

for $k = 1,2$ and some $\tau > 0$. This follows from **extrapolating optimal elliptic regularity** to the Bessel scale and classical analytic semigroup theory using **fractional powers**.

Selected publications

[1] H. Meinlschmidt, C. Meyer, J. Rehberg: **Optimal control of the thermistor problem in three spatial dimensions, part 1: Existence of optimal controls**. SIAM J. Control Optim. 55 #5 (2017), 2876–2904.

[2] H. Meinlschmidt, C. Meyer, J. Rehberg: **Optimal control of the thermistor problem in three spatial dimensions, part 2: Optimality conditions**. SIAM J. Control Optim. 55 #4 (2017), 2368–2392.

[3] H. Meinlschmidt, J. Rehberg: **Extrapolated elliptic regularity and application to the van Roosbroeck system of semiconductors**. J. Differ. Equ. 280 (2021), 375–404.

[4] D. Horstmann, H. Meinlschmidt, J. Rehberg: **The full Keller-Segel model is well posed on nonsmooth domains**. Nonlinearity 31 #4 (2018), 1560–1592.

Department of DATA SCIENCE

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