Weierstrass Institute for
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Some problems associated with the second order optimal shape of a crystallisation interface

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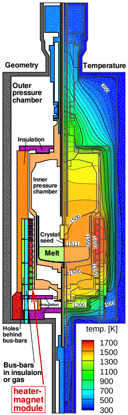
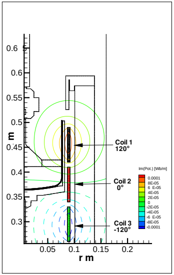
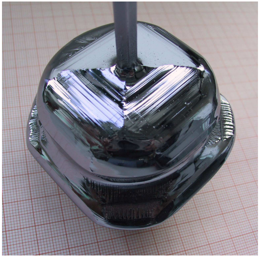
Topic: **Crystal growth from the melt (Czochralski method) in traveling magnetic fields**

Project heads: J. Sprekels, O. Klein (Weierstrass-Institute Berlin), F. Tröltzsch (TU Berlin).



- Modeling, simulation, optimal control.
- Investigation of a convection damping method based on traveling magnetic fields: **H**eater **M**agnet **M**odule, project KRIST$\widetilde{MAG}$® of Leibniz Institute of crystal growth Berlin (2008).
- **Recently**: modeling and control of effects associated with the crystallization interface (free boundary).

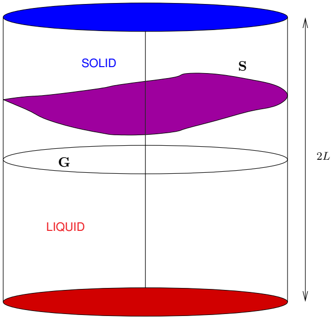




Content

Model

Geometry for the analysis in the system crystal–melt. Model the local (near to) equilibria in time (process is very slow).



Heat equation for the temperature in the domain $\Omega := G \times]-L,\, L[$

$$-\operatorname{div}(k_S(\theta)\,\nabla\theta) = f(x) \text{ in } \Omega \setminus S\,.$$

Transmission conditions for the heat flux

$$[-k_S\,\nabla\theta \cdot \nu] = \lambda(x) \text{ on } S\,.$$

Stefan condition (without or with surface tension) on S

$$\theta - \theta_{\text{eq}} = 0\,, \qquad \theta - \theta_{\text{eq}} = \operatorname{div}_S \sigma_q(x,\,\nu) + \sigma_x(x,\,\nu)\cdot\nu\,.$$

Minimization principle for the free energy

$$\Psi(S,\,\theta) := \int_S \sigma(x,\,\nu)\,dH_2 + \int_{\partial G \times]-L,L[} \kappa(x)\,\chi_S\,dH_2 - \int_\Omega (\theta - \theta_{\text{eq}})\,\chi_S\,dx\,.$$

A general remark on weak formulation

Quoting: Giaquinta, Modica, Souček, *Cartesian currents in the calculus of variations* about the problem of minimal surfaces:

> *Geometric measure theory provides in some sense the right setting for that.*
> *However, the result will be a kind of collection of problems, the precise formulation of each problem depending on the definitions one adopts for "surface", "boundary" and "area"*

$\Rightarrow$ There is a part of **freedom** in how to interpret a geometric equation. **Geometric measure theory** introduces notions of a *surface* sufficiently general/weak to allow for topological changes, compactness, lower s.c. of typical free energies.

Surface := boundary of a Caccioppoli set ($\chi \in BV(\Omega)$, $|\chi| = 1$ a. e. in Ω). Free-energy:

$$\Psi(\chi,\, \theta) := \int_\Omega \sigma(x,\, \frac{D\chi}{|D\chi|})\, d|D\chi| + \int_{\partial G \times]-L,L[} \kappa(x)\, \chi\, dH_2 - \int_\Omega (\theta - \theta_{\text{eq}})\, \chi\, dx\,.$$

Parametric minimization problem for the free energy Ψ:

$$\text{Min}\, \Psi(\chi,\, \theta), \quad \chi \in BV(\Omega),\, |\chi| = 1 \text{ almost everywhere},\, \theta \text{ fixed}.$$

Special features of the application in crystal growth:

- Industrial crystal growth is a *controled process*. In particular, there is a control on the topology of the interface.
- There is a *fixed crystallization direction* imposed by the *applied temperature gradient*.

No topological change is expected if the system is properly controled. Moreover:

- Defect formation in crystal growth: interest for the *optimal shape* of S.
- Need to control the shape up to *second order quantities* (convexity, curvature).

All this *cannot be expressed for too general a notion of surface*.

Non-parametric minimization problem for the surface free-energy $\Psi(S,\, \theta)$. Minimization in a class of graphs in a fixed coordinate system $S = \mathrm{graph}(\psi; G)$

$$\Psi(\psi,\, \theta) := \int_G \bar{\sigma}(\bar{x},\, \psi,\, \nabla\psi)\, d\bar{x} + \int_{\partial G} (\int_{-L}^{L} \mathrm{sign}(t - \psi(\bar{x}))\, \kappa(\bar{x},\, \psi(\bar{x}),\, t)\, dt)\, dH_1 - \int_G (\int_{-L}^{L} \mathrm{sign}(t - \psi(\bar{x}))\, \theta(\bar{x},\, \psi(\bar{x}),\, t)\, dt)\, d\bar{x}\,.$$

Here $\bar{\sigma}(x,\, q) = \sigma(x,\, -q,\, 1)$ ($q \in \mathbb{R}^2$) satisfies $\lambda_0\, \sqrt{1+q^2} \leq \bar{\sigma}(x,q) \leq \mu_0\, \sqrt{1+q^2}$.

Under what kind of assumption can we apply the classical approach ?

Consider data σ and κ independent on the $z-$variable: $\sigma = \sigma(\bar{x}, q)$, $\kappa = \kappa(\bar{x})$, $\bar{x} \in G$.

Assume that $q \mapsto \sigma(\bar{x}, q)$ is convex.

For the temperature gradient assume the strong sign condition

$$\sup_{G\times\mathbb{R}} \partial_z \theta < 0.$$

These conditions garanty that the non-parametric free energy Ψ is **convex**!

- The equation associated with the Stefan condition ($\sigma = 0$):

  $$\theta(\bar{x},\, \psi(\bar{x})) = 0 \text{ for } \bar{x} \in G\,,$$

  has a unique solution $\psi \in C^2(\overline{G})$ provided that $\theta \in C^2(\overline{G} \times \mathbb{R})$ (Implicit function theorem).
- The contact angle problem for the generalized mean curvature equation

  $$-\operatorname{div} \bar{\sigma}_q(\bar{x},\, \nabla\psi) = \theta(\bar{x},\, \psi) \text{ in } G, \quad -\bar{\sigma}_q(\bar{x},\, \nabla\psi)\cdot n(\bar{x}) = \kappa(\bar{x}) \text{ on } \partial G\,,$$

  has a unique solution in $C^{2,\alpha}(\overline{G})$ provided that $\theta \in C^{1,\alpha}(\overline{G} \times \mathbb{R})$ [results by Uraltseva, L. Simon, Spruck, Trudinger (1970s, 1980s)].

The non-parametric approach of the geometric problem is justified for monotone temperature profiles along the $z-$direction.

Problem for the mathematical method: the sign condition $\partial_z\theta < 0$ in Ω is not to expect for the solution of a general heat equation and *explicit classes of data*.
Heat sources, liquid convection, anisotropic heat diffusion, transmission conditions can deviate the applied temperature gradient.
$\Longrightarrow$ Difficulties to couple the mean curvature eq. approach to the heat equation in mathematical analysis.

The legitimacy of the classical problem formulation relies on control theoretical assumptions:
We postulate that the crystallization process can be controled in such a way:

- That $\partial_z\theta < 0$ pointwise in Ω (pointwise state constraint for $\partial_z\theta$);
- That there is $0 < L' < L$ such that $-L' < \psi(\bar{x}) < L'$ for all $\bar{x} \in G$ (pointwise state constraint on ψ).

Our approach in control theory

- Solve the heat equation $-\operatorname{div}(k\nabla\theta) = f$ in Ω with the radiation boundary condition

$$-k\nabla\theta \cdot n = \beta\,(\theta^4 - \theta_{\text{Ext}}^4) \text{ on } \partial\Omega\,.$$

  Control the external temperature in θ_{Ext}.

- Solve a **regularized mean curvature equation**

$$-\operatorname{div}\bar{\sigma}(\bar{x},\,\nabla\psi) = E(\theta)(\bar{x},\,\psi) \text{ in } G, \quad -\bar{\sigma}(\bar{x},\,\nabla\psi)\cdot n(\bar{x}) = \kappa(\bar{x}) \text{ on } \partial G\,,$$

  with a monotonization operator, for instance

$$E(\theta)(\bar{x}, z) = \theta(\bar{x}, z) - \|[\partial_z\theta - \gamma]^+\|_{L^\infty(\Omega)}\, z\,, \quad \gamma < 0\,.$$

- Impose pointwise state constraints

$$\partial_z\theta \leq \gamma < 0 \text{ in } \Omega, \quad -L' \leq \psi \leq L' \text{ in } G\,.$$

Def: Call feasible a control θ_{Ext} if solution(s) $(\theta,\,\psi)$ satisfy the pointwise state constraints.
Note: $E(\theta) = \theta$ for a feasible control.

A smooth problem

We first study the situation that the heat equation **decouples** from the geometric equation, and can be solved independently. That means:

- One-phase problem: $k_{\text{liquid}} = k_{\text{solid}}$, where $k =$ heat-conductivity;
- No release of latent heat, purely static equilibrium: $[-k\nabla\theta \cdot \nu] = \lambda = 0$ on S.

Results:

- Existence of a (continuously differentiable) control to state mapping

$$\theta_{\text{Ext}} \in W^{1,q}(\Omega)\,(q > 3) \longmapsto (\psi,\, \theta) \in C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)\,.$$

- Existence of an optimal control for the relevant second order objective functionals:

$$J(\psi,\, \theta) := \frac{1}{2}\,\|\psi - \psi_d\|^2_{W^{2,2}(G)} + \frac{1}{2}\,\|\theta - \theta_d\|^2_{W^{1,2}(S)}\,.$$

- Lagrange multipliers, adjoint equation, first order optimality system.

Lemma

Assume that $\Omega = G\times]-L,\, L[$, *with* $G \subset \mathbb{R}^2$ *a bounded domain of class* $\mathcal{C}^2$. *Assume that* $f \in L^q(\Omega)$, $q > 3$. *Let* k *be uniformly elliptic and satisfy*

$$k = \begin{pmatrix} \tilde{k} & 0 \\ 0 & 1 \end{pmatrix}, \quad \tilde{k} \in C^1(\overline{\Omega};\, \mathbb{R}^{2\times 2})\,.$$

Let $u \in W^{1,q}(\Omega)$. *Then, there is a unique* $\theta \in W^{2,q}(\Omega)$ *satisfying*

$$-\operatorname{div}(k\,\nabla\theta) = f \text{ in } \Omega, \quad -k\,\nabla\theta\cdot n = \beta\,(|\theta|^3\,\theta - |u|^3\,u) \text{ on } \partial\Omega\,.$$

Proof: $\Gamma_1 := \partial G\times]-L, L[, \Gamma_2 := G\times\{-L, L\}$.
Look at the PDEs and boundary conditions satisfied by the derivatives of θ, in particular by the functions θ_z, $kn_{\Gamma_1}\cdot\nabla\theta$ and $(n_{\Gamma_1}\times e_z)\cdot\nabla\theta$ (distributional sense).
Relying on the structure of k and the fact that Γ_1 and Γ_2 meet at right angle, the claim follows from the $W^{1,q}-$theory for elliptic equations with mixed boundary conditions on Lipschitz domains.

Lemma

$G \subset \mathbb{R}^2$, a bounded domain of class $\mathcal{C}^{2,\alpha}$, $\alpha \in]0,1]$; $\sigma \in C^3(\overline{G} \times \mathbb{R}^3 \setminus \{0\})$, convex and one-homogeneous in the $q-$variable; $\kappa \in C^{1,\alpha}(\partial G)$ satisfies the assumption $\|\kappa\|_\infty < \lambda_0$ ($\lambda_0 =$ largest constant such that $\sigma(\bar{x}, q) \geq \lambda_0\, |q|$).
$\theta \in C^{1,\alpha}(\overline{G} \times \mathbb{R})$ satisfies the condition $\gamma_0 := \sup_{G\times\mathbb{R}} \theta_z < 0$ in $G \times \mathbb{R}$.
Then there is a unique $\psi \in C^{2,\alpha}(\overline{G})$ solution to

$$-\operatorname{div} \bar{\sigma}_q(\bar{x},\, \nabla\psi) = \theta(\bar{x},\, \psi) \text{ in } G, \quad -\bar{\sigma}_q(\bar{x},\, \nabla\psi)\cdot n(\bar{x}) = \kappa(\bar{x}) \text{ on } \partial G\,.$$

Proof: Uraltseva in

- (1971) $\sigma = \sigma(q)$, $\kappa = 0$, G convex. *A priori* estimates.
- (1973) $\sigma = \sigma(q)$, $\kappa =$ const, G convex. Gradient estimate.
- (1975) $\sigma = |q|$, $\kappa =$ const. Gradient estimate.
- (1984) $\sigma = \sigma(\bar{x}, q)$, $\kappa = \kappa(x)$. Gradient estimate.

[Survey and some extensions on existence, uniqueness and *a priori* estimates in Druet, Port. Mat., to appear].

The composition of both solution-operators is not well defined! The solution of the heat equation:

- Does not necessarily satisfy $\theta_z < 0$;
- Is defined only in a bounded cylinder $G\times]-L, L[$.

Lemma

Let $\gamma < 0$, and $0 < L' < L$. Then, there is a continuously differentiable operator $E = E_{\gamma,\,L'} : W^{2,q}(\Omega) \to C^{1,\alpha}(\overline{G} \times \mathbb{R})$ such that

$$\sup_{G\times\mathbb{R}} \partial_z E(\theta) < 0 \text{ for all } \theta \in W^{2,q}(\Omega)\,.$$

Moreover, $E(\theta) = \theta$ in $\Omega_{L'}$ for all $\theta \in W^{2,q}(\Omega)$ such that $\sup_\Omega \partial_z\theta \leq \gamma$.

Proof: Denote $c_0 =$ embedding constant for $W^{1,q}(\Omega) \to C(\overline{\Omega})$. Let $g(t) \approx [t-\gamma]^+$. For $\theta \in W^{2,q}(\Omega)$

$$P(\theta)(\bar{x}, z) = \theta(\bar{x}, z) - c_0^{-1}\, \|g(\theta_z)\|_{W^{1,q}(\Omega)}\, z\,, \quad (\bar{x}, z) \in \Omega\,.$$

Let $f(t) \approx \text{sign}(t)\, \min\{|t|,\, L\}$, $f' > 0$, $f(t) = t$ for $|t| \leq L'$. Define

$$E(\theta)(\bar{x}, z) := P(\theta)(\bar{x},\, f(z)) \quad (\bar{x}, z) \in G \times \mathbb{R}\,.$$

Control space $U = W^{1,q}(\Omega)$. State space $Y := C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)$.

Control to state mapping $\mathcal{S} : U \to Y$, $u \mapsto y = (\psi, \theta)$ unique solution to

$$
\begin{aligned}
-\operatorname{div}(k\,\nabla\theta) &= f \quad \text{in } \Omega, & -k\,\nabla\theta\cdot n &= \beta\,(|\theta|^3\theta - |u|^3 u) \quad \text{on } \partial\Omega \\
-\operatorname{div}\bar{\sigma}_q(\bar{x},\,\nabla\psi) &= E(\theta)(\bar{x},\,\psi) \quad \text{in } G, & -\bar{\sigma}_q(\bar{x},\,\nabla\psi)\cdot n(\bar{x}) &= \kappa(\bar{x}) \quad \text{on } \partial G\,.
\end{aligned}
$$

Objective functional $J : Y \to \mathbb{R}^+$; Denote also $J : Y \times U \to \mathbb{R}^+$ the regularization

$$J(y,\,u) := J(y) + \frac{\rho}{q}\,\|u\|_U^q\,, \quad \rho > 0\,.$$

Set of admissible controls

$$U_{\text{ad}} := \left\{ u \in U \;:\; \begin{cases} \theta_{\min} \le u \le \theta_{\max} & \text{on } \partial\Omega \\ u \ge 0 & \text{on } G \times \{-L\} \\ u \le 0 & \text{on } G \times \{L\} \end{cases} \right\}.$$

Optimal control problem

$$(P_{\text{opt}}) = \min_{u \in U_{\text{ad}}} \{ f(u) := J(\mathcal{S}(u),\, u) \}$$

subject to the state constraints

$$\begin{aligned} -L' \ &\leq\ \psi(\bar{x})\ \leq\ L' \quad \text{for } \bar{x} \in G\,, \\ \theta_{\text{min}}\ &\leq\ \theta(\bar{x}, z)\ \leq\ \theta_{\text{max}} \text{ for } (\bar{x}, z) \in \Omega\,, \\ \partial_z \theta(\bar{x}, z)\ &\leq \gamma \qquad\quad \text{for } (\bar{x}, z) \in \Omega\,. \end{aligned}$$

Lemma

Assume that the functional J is nonnegative and lower-semicontinuous in the topology of $C^2(\overline{G}) \times C^1(\overline{\Omega})$. If there is at least one feasible control in U_{ad}, then the problem (P_{opt}) admits a (possibly not unique) optimal feasible solution $u \in \overline{U_{\text{ad}}}$.

Proof: By assumption, there is a least one minimal sequence of feasible controls $\{u_n\} \subset U_{\text{ad}}$. Since $\{f(u_n)\}$ is bounded, also $\|u_n\|_U \leq C$, and $\{(\psi_n,\, \theta_n)\} = \{\mathcal{S}(u_n)\}$ is bounded in $C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)$.

Differentiability of $\mathcal{S}$/ Solvability of the linearized problem.

Recall $y = (\psi,\, \theta) \in Y$. Introduce an operator $T:\ Y \times U \to Z$

$$Z := C^{\alpha}(\overline{G}) \times C^{1,\alpha}(\partial G) \times L^{q}(\Omega) \times W^{1,q}(\Omega)$$

$$T(y,\, u) = (\text{Mean curvature eq},\ \text{Contact-angle b. c.},\ \text{Heat eq.},\ \text{Rad. b. c.})$$

Note: all coefficients and functions involved in T are continuously differentiable.

Lemma

Let $u^* \in U$, and denote $(\psi^*,\, \theta^*) = y^* = \mathcal{S}(u^*)$. Consider
Then, the equation $\partial_y T(y^*,\, u^*)\, y = F$ has a unique solution $y = (\psi,\, \theta) \in Y$ such that

$$-\frac{d}{dx_i}(\bar\sigma_{q_i,\,q_j}(\bar x,\, \nabla\psi^*)\, \partial_{x_j}\psi) - \partial_z E(\theta^*)(\bar x,\, \psi^*)\, \psi = E'(\theta^*)\, \theta(\bar x,\, \psi^*) + F_1 \quad \text{in } G\,,$$

$$-n_i\, \bar\sigma_{q_i,\,q_j}(\bar x,\, \nabla\psi^*)\, \partial_{x_j}\psi = F_2 \quad \text{on } \partial G\,,$$

$$-\operatorname{div}(k\nabla\theta) = F_3 \quad \text{in } \Omega,$$

$$-k\nabla\theta \cdot n = 4\,\beta\, |\theta^*|^3\theta + F_4 \quad \text{on } \partial\Omega\,.$$

Corollary: Formula $\mathcal{S}'(u^*)\, u = -[\partial_y T(\mathcal{S}(u^*),\, u^*)]^{-1}\, \partial_u T(\mathcal{S}(u^*),\, u^*)\, u$.

Coupled system

Let us now consider a bilateral coupling between the heat equation and the geometric equation:

- Two-phases problem: $k_{\text{liquid}} \neq k_{\text{solid}}$, where $k =$ heat-conductivity;
- No release of latent heat, purely static equilibrium: $[-k\nabla\theta \cdot \nu] = \lambda = 0$ on S.

Thus, we consider the system of equations

$$-\operatorname{div}(k_S\,\nabla\theta) = f \text{ in } \Omega \setminus S, \quad -[k_S\,\nabla\theta \cdot \nu] = 0 \text{ on } S$$
$$-\operatorname{div}\bar{\sigma}_q(\bar{x},\,\nabla\psi) = \theta(\bar{x},\,\psi) \text{ in } G\,.$$

New problems in analysis:

- Regularity of the temperature: $C^{1,\alpha}$ regularity is excluded by the transmission conditions.
- Gradient estimate in the mean curvature equation is not clear.
- Existence and uniqueness (operator E requires Lispchitz continuous temperature).

New problem in optimal control:

- Temperature gradient discontinuous at interfaces implies that the nonlinear differential operator

  $$-\operatorname{div}\bar{\sigma}_q(\bar{x},\,\nabla\psi) - \theta(\bar{x},\,\psi)\,,$$

  has no continuous ψ derivative.

Results: *a priori* estimates. For $(\psi,\ \theta)$ a sufficiently smooth solution to the problem:

- The principal curvatures on the surface $S = \mathrm{graph}(\psi;\ G)$ are bounded *a priori* [Local results by L. Simon, Trudinger; Our contribution are estimates up to the boundary of S].
- Bounds for the temperature in $W^{2,r}(\Omega_i)$ $(r < 2)$, in $W^{2,2}(\Omega_i)$ and $W^{1,\infty}(\Omega)$ spaces under compatibility conditions for the junction of the surfaces S and $\partial\Omega$, the boundary data, and the coefficient matrices k_{liquid} and k_{solid}.
- Existence with a regularization operator E.

Results: Control theory

- Existence of an optimal feasible control.
- Weaker first order necessary conditions (directional derivatives).

Curvature estimate

Assume that $S = \mathrm{graph}(\psi;\, G)$ is a $\mathcal{C}^2$ graph-solution to the problem

$$\mathrm{div}_S\, \sigma_q(x,\, \nu) + \sigma_x(x,\, \nu) \cdot \nu = \theta(x) \text{ on } S, \quad \sigma_q(x,\, \nu) \cdot n(x) = \kappa(x) \text{ on } \partial S\,.$$

For $x \in \partial S$, assume that the function

$$p \mapsto \sigma_q(x,\, \sqrt{1-p^2}\, n(x) + p_1\, \tau(x) + p_2\, e_z) \cdot n(x)$$

is concave on $B_1(0;\, \mathbb{R}^2)$.

Then for $\alpha \in]0, 1]$ arbitrary

$$|\,\delta\,\nu| \leq C_\alpha\, (\|\theta\|_{C^\alpha(\overline{\Omega})} + \|\kappa\|_{C^{1,\alpha}(\partial\Omega)})\,.$$

Note: Hoelder bounds for the solution θ to the heat equation depend on the eigenvalues of the matrices k_{liquid} and k_{solid}, but not on the structure of S!

Setting for the regularity statement on the temperature:
$\Omega = G \times]-L,\ L[$, with $G \subset \mathbb{R}^2$ a bounded domain of class $\mathcal{C}^2$.

Let S be a *given surface* of class $\mathcal{C}^2$ of the relevant topology: $S \subset G \times]-L', L'[$, with $L' < L$, and the intersection $S \cap \partial G \times]-L, L[$ is a *single closed curve*.

Contact-angle α between S and $\Gamma_1 := \partial G \times]-L, L[$ defined via $\cos\alpha = \nu \cdot n$.

For the simplicity of the statement, assume that $k_{\text{liquid}} \neq k_{\text{solid}}$ are positive constants.

Compatibility function at triple point: $f_d = f_d(\alpha) := \cos\alpha$.

Neumann problem

Consider the Neumann-problem:

$$-\operatorname{div}(k_S\, \nabla\theta) = f \text{ in } \Omega, \quad [-k_S\, \nabla\theta \cdot \nu] = 0 \text{ on } S$$
$$-k\, \nabla\theta \cdot n = Q \text{ on } \partial\Omega\,.$$

Lemma

Assume that $f \in L^q(\Omega)$, $q > 3$. Let $Q \in W^{1,q}(\Omega)$. Assume that:

1. *The compatibility function satisfies $f_d = \cos\alpha \geq 0$ on ∂S;*
2. *The function Q has a representation $Q = f_d\, Q_1 + Q_2$ with $Q_1 \in W^{1/q',q}(\Gamma_1)$ and $Q_2 \in W_S^{1/q',q}(\Gamma_1)$.*

Then, every solution to the Neumann-problem belongs to $W^{1,\infty}(\Omega)$, and to $W^{2,2}(\Omega_{\mathit{liquid}})$ and $W^{2,2}(\Omega_{\mathit{solid}})$.
If only the condition 2. holds, then $\theta \in W^{2,r}(\Omega_{\mathit{liquid}})$, $\theta \in W^{2,r}(\Omega_{\mathit{solid}})$ for a $r > 6/5$.
In these statements the relevant norm of $\|\theta\|$ is continuously controled in terms of the data f, Q and $|\,\delta\,\nu|$.

Dirichlet-problem

Consider the Dirichlet-problem

$$-\operatorname{div}(k_S\,\nabla\theta) = f \text{ in } \Omega, \quad [-k_S\,\nabla\theta\cdot\nu] = 0 \text{ on } S$$
$$\theta = \theta_{\text{Ext}} \text{ on } \partial\Omega\,.$$

Lemma

Assume that $f \in L^q(\Omega)$, $q > 3$. Let $\theta_{\text{Ext}} \in W^{2,q}(\Omega)$. Assume that:

1. *The compatibility function satisfies $f_d \leq 0$ on ∂S (opposite sign of the inequality!);*
2. *The representation $n'\cdot\nabla\theta_{\text{Ext}} = f_d\,U_1 + U_2$ with $U_1 \in W^{1/q',q}(\Gamma_1)$ and $U_2 \in W_S^{1/q',q}(\Gamma_1)$.*

Then, the unique solution to the Dirichlet-problem belongs to $W^{1,\infty}(\Omega)$ and to $W^{2,2}(\Omega_{\text{liquid}})$ and $W^{2,2}(\Omega_{\text{solid}})$.
If only the condition 2. holds, then $\theta \in W^{2,r}(\Omega_{\text{liquid}})$, $\theta \in W^{2,r}(\Omega_{\text{solid}})$ for a $r > 6/5$.
In these statements the relevant norm of $\|\theta\|$ is continuously controled in terms of the data f, Q and $|\,\delta\,\nu|$.

Proofs: Druet, Math. Bohem. to appear. General case $f_d = f_d(k,\,S)$.

Application: Consider the isotropic surface problem

$$\mathrm{div}_S\, \nu = \theta \text{ on } S, \quad \nu \cdot n = \kappa \text{ on } \partial S\,.$$

The contact angle $\cos\alpha$ is given!

If $|\kappa| > 0$ on $\partial\Omega$ or $\kappa \equiv 0$, either the Dirichlet problem or the Neumann problem is solvable with θ in a bounded set of $W^{1,\infty}(\Omega)$.

The regularized mean curvature equation is uniquely solvable.

Fixed-point procedure for existence of solution.