On the control of some systems modelling solidification processes and related phenomena

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Outline

1. Phase field models
   - Existence and uniqueness
   - Optimal control results
   - Controllability analysis
2. Binary alloy Carman-Kozeny models
   - Existence
   - Optimal control results
   - Other problems and questions
3. An additional controllability problem

The models

- Can be OK for phase change analysis
- Incorporate complex phenomena
- Appropriate for numerics
- For solidification and melting: Fix[1983], followed by Cagnalp, Hoffman-Jiong, etc.
- The variables:
  $\tau = \tau(x, t)$ (temperature)
  $u = u(x, t)$, $v = v(x, t)$ (solid fractions)
  $w = w(x, t)$ (liquid fraction)
  We expect: $u + v + w \equiv 1$, $u, v, w \geq 0$
- Motion is neglected!

Phase field models

The considered model

$$\tau_t - b\Delta\tau = \ell_1 u_t + \ell_2 v_t + \ell_3 w_t + f$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} - k\Delta \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}$$

$$g_i = \text{ cubic in } u, v, w, \text{ linear in } \tau$$
$$g_1 + g_2 + g_3 \equiv 0$$

+ Neumann conditions + initial conditions

Hypotheses:

- $0 < T < +\infty$, $\Omega \subset \mathbf{R}^3$ open, connected, bounded, C^2
- $\tau_0, u_0, \ldots$ in $H^2(\Omega)$, nonnegative, compatible, with $u_0 + v_0 + w_0 = 1$
- $f \in L^q(\Omega \times (0, T))$, $q > 5/2$

Theorem (Existence and uniqueness)

$\exists!$ *(strong) solution* $(\tau, u, v, w) \in W_2^{2,1}(Omega \times (0, T))^4$ *with* $u, v, w \geq 0$, $u + v + w \equiv 1$ $(\tau \in L^2(0, T; H^2(\Omega))$, $\tau_t \in L^2(\Omega \times (0, T))$, *etc.)*

Comments:

- Estimates
- Well-posedness, regularity, etc.
- OK with other boundary conditions, nonlinear terms, etc.
- Essential: the same diffusion coefficient k for u, v, w

$$\tau_t - b\Delta\tau = \ell_1 u_t + \ell_2 v_t + \ell_3 w_t + f$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} - \begin{pmatrix} k_1 \Delta u \\ k_2 \Delta v \\ k_3 \Delta w \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}$$

Global existence?

Formulation:

- $f \in \mathcal{U}_{ad} \subset L^q(\Omega \times (0, T))$ is the control
- (τ, u, v) is the state, $\tau \in \Theta_{ad} \subset L^q(\Omega \times (0, T))$
- The cost function:

$$J((\tau, u, v, f) = \frac{\alpha_0}{2} \iint |\tau - \tau_d|^2 + \frac{\alpha_1}{2} \iint |u - u_d|^2$$
$$\frac{\alpha_2}{2} \iint |v - v_d|^2 + \frac{N}{q} \iint |f|^q$$

- The problem:

$$\begin{cases} \text{Minimize} \quad J(\tau, u, v, f) \\ \text{Subject to} \quad f \in \mathcal{U}_{ad}, \quad \tau \in \Theta_{ad}, \quad M(\tau, u, v, f) = 0 \end{cases}$$

$M(\tau, u, v, f) = 0$: (τ, u, v) is the state associated to f

Hypotheses:

- $\alpha_i \geq 0$, $N > 0$
- $\mathcal{U}_{ad}$, Θ_{ad} are nonempty, closed and convex
- The admissible set E_{ad} is nonempty

$$E_{ad} = \{(\tau, u, v, f) : f \in \mathcal{U}_{ad}, \;\; \tau \in \Theta_{ad}, \;\; M(tau, u, v, f) = 0\}$$

Theorem (Existence of optimal controls)

$\exists(\hat{\tau}, \hat{u}, \hat{v}, \hat{f}) \in E_{ad}$ *with*
$J(\hat{\tau}, \hat{u}, \hat{v}, \hat{f}) \leq J(\tau, u, v, f) \;\; \forall(\tau, u, v, f) \in E_{ad}$

Characterization (Dubovitskii-Milyoutin formalism):

$$\begin{cases} \text{Minimize} \quad J(\tau, u, v, f) \\ \text{Subject to} \quad f \in \mathcal{U}_{ad}, \;\; \tau \in \Theta_{ad}, \;\; M(\tau, u, v, f) = 0 \end{cases}$$

The main idea: if (τ, u, v, f) is optimal,

$$DC(J) \cap TC(M) \cap FC(\mathcal{U}_{ad}) \cap FC(\Theta_{ad}) = \emptyset$$

Consequence: $\exists G_i$, not all zero, with

$$G_0 \in DC(J)^*, \;\; G_1 \in TC(M)^*, \;\; G_2 \in FC(\mathcal{U}_{ad})^*, \;\; G_3 \in FC(\Theta_{ad})^*$$

and

$$G_0 + G_1 + G_2 + G_3 = 0$$

The adjoint state (θ, p, q)

(associated to the linearized system at (τ, u, v, f))

$$-\theta_t - b\Delta\theta = H_1 p + H_2 q + \alpha_0(\tau - \tau_d)$$

$$-\begin{pmatrix} p \\ q \end{pmatrix}_t - b\Delta \begin{pmatrix} p \\ q \end{pmatrix} = -\begin{pmatrix} \ell_1' \\ \ell_2' \end{pmatrix} \theta_t + K \begin{pmatrix} p \\ q \end{pmatrix} + \begin{pmatrix} \alpha_1(u-u_d) \\ \alpha_2(v-v_d) \end{pmatrix}$$

"starting" from zero at $t = T$, etc.

Then, after some computations:

$\exists g_2, g_3$ such that

$$\iint \left(N|f|^{q-2}f + \theta\right) h = \iint g_2 h + \iint g_3 \psi$$
$$\forall h \in L^q(\Omega \times (0,T)), \quad M'(\tau, u, v, f)(\psi, , \lambda, \eta, h) = 0$$
$$\iint g_2(h - f) \geq 0 \quad \forall h \in \mathcal{U}_{ad}$$
$$\iint g_3(\psi - \tau) \geq 0 \quad \forall \psi \in \Theta_{ad}$$

Pointwise constraints on f and τ:

- $\mathcal{U}_{ad} = \{f \in L^q(\Omega \times (0,T)) : |f| \leq C_0\}$
- $\Theta_{ad} = \{\tau \in L^2(\Omega \times (0,T)) : 0 < C_1 \leq \tau \leq C_2\}$

For appropriate (large) C_0:

- $E_{ad} \neq \emptyset$ and existence holds
- Dubovitskii-Milyoutin's formalism can be applied

The optimality system:

$$\iint \left(N|f|^{q-2}f + \theta\right) h = \iint g_2 h + \iint g_3 \psi$$

$$\forall h \in L^q(\Omega \times (0,T)), \quad M'(\tau, u, v, f)(\psi, , \lambda, \eta, h) = 0$$

$$g_2 = \begin{cases} \leq 0 & f = C_0 \\ = 0 & |f| < C_0 \\ \geq 0 & f = -C_0 \end{cases} \qquad g_3 = \begin{cases} \leq 0 & \tau = C_2 \\ = 0 & C_1 < \tau < C_2 \\ \geq 0 & \tau = C_1 \end{cases}$$

Exact controllability to the trajectories:

- Locally supported distributed controls:
  $f 1_\omega$, with $\omega \subset\subset \Omega$, $f \in L^q(\omega \times (0,T))$
- The controllability problem: Fix τ_0, u_0, v_0 and find
  $f \in L^q(\omega \times (0,T))$ with

$$\tau_t - b\Delta\tau = \ell_1' u_t + \ell_2' v_t + f 1_\omega$$
$$\begin{pmatrix} u \\ v \end{pmatrix}_t - k\Delta \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \quad \text{etc.}$$

$$\tau(T) = \hat\tau(T) \quad \left(\text{and } \begin{pmatrix} u \\ v \end{pmatrix}(T) = \begin{pmatrix} \hat u \\ \hat v \end{pmatrix}(T) \right)$$

  $(\hat\tau, \hat u, \hat v)$ is an uncontrolled trajectory
- The aim: solve this problem at least for small
  dist. $((\tau_0, u_0, v_0), (\hat\tau(0), \hat u(0), \hat v(0)))$

Set $(\tau, u, v) = (\hat{\tau}, \hat{u}, \hat{v}) + (\varphi, y, z)$ and find f with

$$\begin{aligned} &\varphi_t - b\Delta\varphi = \ell_1' y_t + \ell_2' z_t + f 1_\omega \\ &\begin{pmatrix} y \\ z \end{pmatrix}_t - k\Delta \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} g_1' \\ g_2' \end{pmatrix} \qquad \text{etc.} \\ &\varphi(T) = 0 \quad \left(\text{and } \begin{pmatrix} y \\ z \end{pmatrix}(T) = 0 \right) \end{aligned}$$

After linearization at $(\tilde{\varphi}, \tilde{y}, \tilde{z})$:

$$\begin{aligned} &\varphi_t - b\Delta\varphi = \ell_1' y_t + \ell_2' z_t + f 1_\omega \\ &\begin{pmatrix} y \\ z \end{pmatrix}_t - k\Delta \begin{pmatrix} y \\ z \end{pmatrix} = M \begin{pmatrix} y \\ z \end{pmatrix} + \varphi \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \qquad \text{etc.} \\ &\varphi(T) = 0 \quad \left(\text{and } \begin{pmatrix} y \\ z \end{pmatrix}(T) = 0 \right) \end{aligned}$$

The strategy:

- Prove $\exists$ for this LNC problem
- Find a fixed point of $(\tilde{\varphi}, \tilde{y}, \tilde{z}) \mapsto (M, h_1, h_2) \mapsto (\varphi, y, z)$

- We introduce the adjoint state

$$\theta_t - b\Delta\theta = h_1 p + h_2 q$$
$$-\begin{pmatrix} p \\ q \end{pmatrix}_t - k\Delta \begin{pmatrix} p \\ q \end{pmatrix} = M^* \begin{pmatrix} p \\ q \end{pmatrix} - \theta_t \begin{pmatrix} \ell_1' \\ \ell_2' \end{pmatrix}$$

- We try to prove a Carleman estimate

$$\begin{cases} \iint \rho^{-2}\theta^2 \le \iint_{\omega\times(0,T)} \rho^{-2}\theta^2 \\ \forall \text{ solution } (\theta, p, q) \end{cases}$$

- Even better

$$\begin{cases} \iint \rho^{-2}(\theta^2 + p^2 + q^2) \le \iint_{\omega\times(0,T)} \rho^{-2}\theta^2 \\ \forall \text{ solution } (\theta, p, q) \end{cases}$$

This would imply observability for (θ, p, q) and thus null controllability for (φ, y, z)

Unfortunately it is unknown whether Carleman holds

$$-\theta_t - b\Delta\theta = h_1 p + h_2 q$$
$$-\begin{pmatrix} p \\ q \end{pmatrix}_t - k\Delta\begin{pmatrix} p \\ q \end{pmatrix} = M^*\begin{pmatrix} p \\ q \end{pmatrix} - \theta_t\begin{pmatrix} \ell_1' \\ \ell_2' \end{pmatrix}$$

What is known:

$$\begin{cases} \iint \rho^{-2}(\theta^2 + p^2 + q^2) \leq \iint_{\omega\times(0,T)} \rho^{-2}(\theta^2 + q^2) \\ \forall \text{ solution } (\theta, p, q) \end{cases}$$

A consequence of the results of Fursikov-Imanuvilov[1996]

This provides partial null controllability for (φ, y, z)
(with an additional control in the z-equation; realistic?)

A weaker question - unique continuation:

Assume that

$$\left\{ \begin{array}{l} -\theta_t - b\Delta\theta = h_1 p + h_2 q \\ -\begin{pmatrix} p \\ q \end{pmatrix}_t - k\Delta \begin{pmatrix} p \\ q \end{pmatrix} = M^* \begin{pmatrix} p \\ q \end{pmatrix} - \theta_t \begin{pmatrix} \ell_1' \\ \ell_2' \end{pmatrix} \end{array} \right.$$

$$\theta = 0 \quad \text{in} \quad \omega \times (0, T)$$

Do we have $\theta \equiv 0$?

Unfortunately, this is also unknown

This would lead to (local) approximate controllability results ...

The models

- Appropriate to describe seggregation phenomena in binary alloys
- Again suitable for numerical analysis (shown below)
- First introduced by Carman[1939], modified by Kozeny[1970], Scheidegger[1974]
- The variables:
  $\tau = \tau(x, t)$ (temperature)
  $c = c(x, t)$ (solute concentration)
  $\mathbf{u} = \mathbf{u}(x, t)$, $p = p(x, t)$ (velocity field and pressure)
  We expect: $c \geq c_\ell \geq 0$, c_ℓ: liquid conc. of the solute
- Motion effects are crucial!

The equations:

$$\tau_t + \mathbf{u}\cdot\nabla\tau - b\Delta\tau = f$$
$$c_t + \mathbf{u}\cdot\nabla c_\ell(c,\tau) - k\Delta c = 0$$
$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\tau + a_\varepsilon(c,\tau)\mathbf{u} + \nabla p = B(c,\tau)$$
$$\nabla\cdot\mathbf{u} = 0$$

Additional relations:

$$c_\ell = \psi(f_s)c, \quad f_s = f_s(c,\tau)\text{: solid fraction, } 0 \le f_s \le 1$$
$$a_\varepsilon = \alpha\, f_s^2\,(1+\varepsilon - f_s)^{-3} \quad \text{(Carman-Kozeny)}$$
$$B = b_0 + b_1\tau + b_2 c_\ell(c,\tau) \quad \text{(Boussinesq approximation)}$$

+ Neumann conditions + initial conditions

Formally, the case $\varepsilon = 0$ corresponds to a free-boundary model: $f_s = 1$ in the solid, $0 \le f_s < 1$ in the rest

Hypotheses:

- $0 < T < +\infty$, $\Omega \subset \mathbf{R}^3$ open, connected, bounded, C^2
- $\tau_0, c_0, \mathbf{u}_0$ in $H^1(\Omega)$, compatible
- $f \in L^2(\Omega \times (0,T))$

Theorem (Existence)

$\exists$ *weak solution* $(\tau, c, \mathbf{u})$
($\tau \in L^2(0,T;H^1(\Omega))$, $\tau_t \in L^2(0,T;H^{-1}(\Omega))$, *etc.)*

Comments:

- The interesting question: what happens as $\varepsilon \to 0$?
- There are results for $\Omega \subset \mathbf{R}^2$ Boldrini-Planas[2005]

Formulation:

- The cost function:

$$J(\tau, c, \mathbf{u}, f) = \frac{\alpha_0}{2} \iint |\tau - \tau_d|^2 + \frac{\alpha_1}{2} \iint |c - c_d|^2$$
$$\frac{\alpha_2}{2} \iint |\mathbf{u} - \mathbf{u}_d|^2 + \frac{N}{2} \iint |f|^2$$

- The problem:

$$\begin{cases} \text{Minimize} \quad J(\tau, c, \mathbf{u}, f) \\ \text{Subject to} \quad f \in \mathcal{U}_{ad}, \quad \tau \in \Theta_{ad}, \quad M(\tau, c, \mathbf{u}, f) = 0 \end{cases}$$

Hypotheses:

- $\alpha_i \geq 0$, $N > 0$
- $\mathcal{U}_{ad}$, Θ_{ad} are nonempty, closed and convex
- The admissible set E_{ad} is nonempty

$$E_{ad} = \{(\tau, c, \mathbf{u}, f) : f \in \mathcal{U}_{ad},\ \ \tau \in \Theta_{ad},\ \ M(\tau, c, \mathbf{u}, f) = 0\}$$

Theorem (Existence of optimal controls)

$\exists(\hat{\tau}, \hat{c}, \hat{\mathbf{u}}, \hat{f}) \in E_{ad}$ *with*
$J(\hat{\tau}, \hat{c}, \hat{\mathbf{u}}, \hat{f}) \leq J(\tau, c, \mathbf{u}, f)\ \ \forall(\tau, c, \mathbf{u}, f) \in E_{ad}$

Again: what happens as $\varepsilon \to 0$?

Characterization

- The adjoint state $(\theta, \psi, \mathbf{w})$

$$
\begin{aligned}
&-\theta_t - \mathbf{u}\cdot\nabla\theta - b\Delta\theta - \tfrac{\partial c_\ell}{\partial \tau}\mathbf{u}\cdot\nabla\psi = \alpha_0(\tau - \tau_d) + \dots \\
&-\psi_t - \tfrac{\partial c_\ell}{\partial c}\mathbf{u}\cdot\nabla\psi - k\Delta\psi = \alpha_1(c - c_d) + \dots \\
&-\mathbf{w}_t - (\mathbf{u}\cdot\nabla)\mathbf{w} - \nu\Delta\mathbf{w} + a_\varepsilon\mathbf{w} + \nabla q = \alpha_2(\mathbf{w} - \mathbf{w}_d) + \dots \\
&\nabla\cdot\mathbf{w} = 0
\end{aligned}
$$

"starting" from zero at $t = T$, etc.

- After some computations: $\exists g_2, g_3$ such that

$$
\begin{aligned}
&\textstyle\iint (Nf + \theta)\, h = \iint g_2 h + \iint g_3\psi \\
&\quad \forall h \in L^2(\Omega\times(0,T)), \quad M'(\tau, u, v, f)(\psi, , \lambda, \eta, h) = 0 \\
&\textstyle\iint g_2(h - f) \geq 0 \quad \forall h \in \mathcal{U}_{ad} \\
&\textstyle\iint g_3(\psi - \tau) \geq 0 \quad \forall \psi \in \Theta_{ad}
\end{aligned}
$$

Formulation (motivations in industrial problems):

- A second cost function:

$$J(\tau, c, \mathbf{u}, f) = T^*(f, c_e; \delta) + \frac{N}{q} \iint |f|^q$$

with $T^*(f, c_e; \delta) = \inf\{T > 0 : \|c(T) - c_e\|_{L^2} \leq \delta\}$

- The problem:

$$\begin{cases} \text{Minimize} \quad J(\tau, c, \mathbf{u}, f) \\ \text{Subject to} \quad f \in \mathcal{U}_{ad}, \quad \tau \in \Theta_{ad}, \quad M(\tau, u, v, f) = 0 \end{cases}$$

Some questions:

- Existence?
- Optimality conditions for $\hat{f}$, $\hat{T}$?

More comments and questions:

- Characterization leads to algorithms (as usual; work in progress . . .)
- Controllability results can also be considered
  For instance: for $N = 2$, local null controllability of τ and $\mathbf{u}$
  Also: large time null controllability of τ and $\mathbf{u}$
  EFC-Guerrero-Imanuvilov-Puel[2005]

The approximate controllability problem:

- Fix $u_0, u_T, \varepsilon > 0$. Find $f \in L^2(\omega \times (0, T))$ with

$$\begin{aligned} & u_t - k\Delta u + v + \alpha(x,t)u = f 1_\omega, \quad u(0) = u_0 \\ & v_t - \sigma u + \gamma v = 0, \quad v(0) = 0 \end{aligned} \qquad \text{etc.}$$

$$\|u(T) - u_T\|_{L^2} \leq \varepsilon$$

- Describes excitability and bistability phenomena, Hodgkin-Huxley[1952], Hastings[1975]. Also related to solidification.
- Memory effects:

$$\begin{aligned} & u_t - k\Delta u + \sigma \int_0^t e^{-\gamma(t-s)} u(s)\, ds + \alpha(x,t)u = f 1_\omega \\ & u(0) = u_0 \end{aligned} \qquad \text{etc.}$$

Fix $u_0, u_T, \varepsilon > 0$. Find $f \in L^2(\omega \times (0,T))$ with

$$\begin{aligned} u_t - k\Delta u + v + \alpha(x,t)u &= f1_\omega, \quad u(0) = u_0 \\ v_t - \sigma u + \gamma v &= 0, \quad v(0) = 0 \end{aligned} \qquad \text{etc.}$$

$$\|u(T) - u_T\|_{L^2} \leq \varepsilon$$

This is unknown

What is known:

- OK if $\sigma = 0$
- OK if v satisfies $v_t - \kappa\Delta v + \sigma u + \gamma v = 0, \quad v(0) = 0$
  Uniformly bounded controls $f_{\varepsilon,\kappa}$ as $\kappa \to 0$?

Approximate controllability also holds if $\alpha = \alpha(x)$

The proof:

- Consider the adjoint $h = h(x,t)$ with

$$-h_t - k\Delta h + \sigma \int_t^T e^{-\gamma(s-t)} h(s)\,ds + \alpha(x,t)h = 0$$
$$h(0) = h_T$$

- We prove unique continuation:

$$h = 0 \ \text{ in } \ \omega \times (0,T) \Rightarrow h \equiv 0$$

- This relies on the properties of h ...

THANK YOU VERY MUCH . . .