Approximation of dynamic boundary condition: The Allen–Cahn equation

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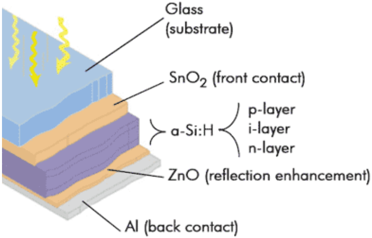
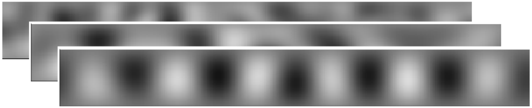
Interfacial dynamics in semiconductor models



Schematic cross-section of thin film a-Si:H photovoltaic cell

Interaction with domain walls in spinodal decomposition



Cahn–Hilliard equation

AC Equation with Dynamic Boundary Condition

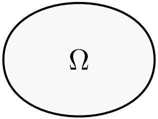
Sprekels and Wu [2010]: $\Omega \subset \mathbb{R}^d$, $d \geq 2$, with C^2 boundary

$$
\begin{aligned}
\partial_t u - \Delta u + F_{\mathrm{b}}'(u) &= 0, && \text{in } \Omega \times [0,T] \\
\partial_t \phi - \Delta_{\|} \phi + \partial_\nu u + \phi + F_{\mathrm{s}}'(\phi) &= 0, && \text{on } \partial\Omega \times [0,T] \\
u &= \phi, && \text{on } \partial\Omega \times [0,T]
\end{aligned}
$$

$$
u(0,\cdot) = u_0, \qquad \phi(0,\cdot) = \phi_0
$$

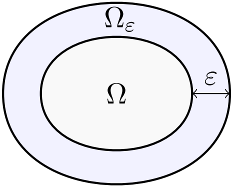
$\Delta_{\|}$ Laplace–Beltrami operator on $\partial\Omega$

- Cahn–Hilliard equation (R. Kenzler et al. [2001])
- Caginalp system (R. Chill, E. Fasangova and J. Pruess [2006])
- Nonisothermal Allen–Cahn equation (C. Gal and M. Grasselli, A. Miranville [2008])



$$r_{\mathrm{b}} \partial_t u - a_{\mathrm{b}} \Delta u + F_{\mathrm{b}}'(u) = 0, \qquad \text{in } \Omega \times [0,T]$$

$$\Omega_\varepsilon \overset{\text{def}}{=} \{x \in \mathbb{R}^d : \; \exists(y,\eta) \in \partial\Omega \times (0,\varepsilon), \quad x = y + \eta\nu(y)\}$$



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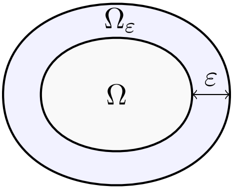
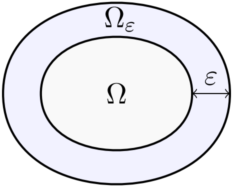


$$\begin{aligned}
r_{\mathrm{b}}\partial_t u - a_{\mathrm{b}}\Delta u + F_{\mathrm{b}}'(u) &= 0, && \text{in } \Omega \times [0,T] \\
r_{\mathrm{s}}\varepsilon^{\delta}\partial_t \phi - a_{\mathrm{s}}\varepsilon^{\alpha}\Delta\phi + \varepsilon^{\beta} F_{\mathrm{s}}'(\phi) &= 0, && \text{in } \Omega_\varepsilon \times [0,T] \\
u &= \phi && \text{on } \partial\Omega \times [0,T] \\
a_{\mathrm{b}}\partial_\nu u - a_{\mathrm{s}}\varepsilon^{\alpha}\partial_\nu\phi &= 0, && \text{on } \partial\Omega \times [0,T] \\
a_{\mathrm{s}}\varepsilon^{\alpha}\partial_\nu\phi &= 0, && \text{on } \partial\Omega_\varepsilon \backslash \partial\Omega \times [0,T]
\end{aligned}$$

$$\Omega_\varepsilon \stackrel{\text{def}}{=} \{x \in \mathbb{R}^d : \ \exists (y,\eta) \in \partial\Omega \times (0,\varepsilon), \quad x = y + \eta\nu(y)\}$$



$$\begin{aligned}
r_\mathrm{b}\partial_t u - a_\mathrm{b}\Delta u + F_\mathrm{b}'(u) &= 0, && \text{in } \Omega \times [0,T] \\
r_\mathrm{s}\varepsilon^{-1}\partial_t\phi - a_\mathrm{s}\varepsilon^{\alpha}\Delta\phi + \varepsilon^{-1}F_\mathrm{s}'(\phi) &= 0, && \text{in } \Omega_\varepsilon \times [0,T] \\
u &= \phi && \text{on } \partial\Omega \times [0,T] \\
a_\mathrm{b}\partial_\nu u - a_\mathrm{s}\varepsilon^{\alpha}\partial_\nu\phi &= 0, && \text{on } \partial\Omega \times [0,T] \\
a_\mathrm{s}\varepsilon^{\alpha}\partial_\nu\phi &= 0, && \text{on } \partial\Omega_\varepsilon \backslash \partial\Omega \times [0,T]
\end{aligned}$$

Today: $\delta = -1$, $\beta = -1$, $\alpha \in (-\infty, 1)$

Setting

$$r_{\mathrm{b}}\partial_t u - a_{\mathrm{b}}\Delta u + F_{\mathrm{b}}'(u) = 0, \quad \tfrac{r_{\mathrm{s}}}{\varepsilon}\partial_t\phi - a_{\mathrm{s}}\varepsilon^{\alpha}\Delta\phi + \tfrac{1}{\varepsilon}F_{\mathrm{s}}'(\phi) = 0$$

- Spaces

$$\widetilde{V}_\varepsilon = \left\{(u,\phi) \in \mathrm{H}^1(\Omega) \times \mathrm{H}^1(\Omega_\varepsilon) : \; u|_{\partial\Omega} = \phi|_{\partial\Omega}\right\}$$
$$\widetilde{H}_\varepsilon = \mathrm{L}^2(\Omega) \times \mathrm{L}^2(\Omega_\varepsilon)$$

- Energy functionals

$$\widetilde{\mathcal{E}}_\varepsilon(u,\phi) = \int_\Omega \frac{a_{\mathrm{b}}}{2}|\nabla u|^2 + F_{\mathrm{b}}(u)\mathrm{d}x + \int_{\Omega_\varepsilon} \frac{a_{\mathrm{s}}\varepsilon^{\alpha}}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F_{\mathrm{s}}(\phi)\mathrm{d}x$$

- Dissipation functionals

$$\widetilde{\mathcal{R}}_\varepsilon(\dot{u},\dot{\phi}) = \int_\Omega \frac{r_{\mathrm{b}}}{2}|\dot{u}|^2\mathrm{d}x + \frac{1}{\varepsilon}\int_{\Omega_\varepsilon} \frac{r_{\mathrm{s}}}{2}|\dot{\phi}|^2\mathrm{d}x$$

In this setting

$$r_{\mathrm{b}}\partial_t u - a_{\mathrm{b}}\Delta u + F_{\mathrm{b}}'(u) = 0, \quad \frac{r_{\mathrm{s}}}{\varepsilon}\partial_t \phi - a_{\mathrm{s}}\varepsilon^{\alpha}\Delta\phi + \frac{1}{\varepsilon}F_{\mathrm{s}}'(\phi) = 0$$

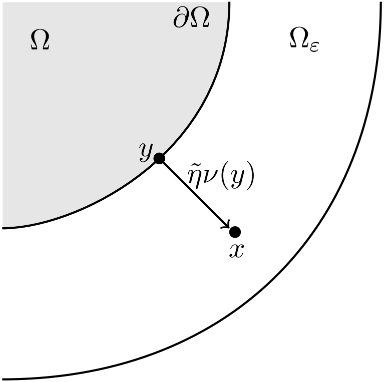
is formally equivalent to

$$0 = \mathrm{D}\widetilde{\mathcal{R}}_{\varepsilon}\big(\dot{u}, \dot{\phi}\big) + \mathrm{D}\widetilde{\mathcal{E}}_{\varepsilon}(u, \phi) \quad \text{(Force balance)}$$

Basic existence theory yields solutions

$$(u_{\varepsilon}, \phi_{\varepsilon}) \in \mathrm{L}^{\infty}(0, T; \widetilde{V}_{\varepsilon}) \cap \mathrm{H}^{1}(0, T; \widetilde{H}_{\varepsilon})$$

Transformation



- Change of coordinates
  $x = y + \tilde{\eta}\nu(y)$

$$x \mapsto (y, \tilde{\eta}) \in \partial\Omega \times (0, \varepsilon)$$

- Scaling

$$\tilde{\eta} = \varepsilon\eta, \ \ \eta \in (0, 1)$$

- Mapping

$$\mathrm{L}^2(\Omega_\varepsilon) \longrightarrow \mathrm{L}^2(\partial\Omega{\times}(0, 1))$$

- Spaces

$$\widetilde{V}_\varepsilon \longrightarrow V = \{(u, \phi) \in \mathrm{H}^1(\Omega) \times \mathrm{H}^1(\partial\Omega{\times}(0, 1)) : \ u|_{\partial\Omega} = \phi|_{\eta=0}\}$$

$$\widetilde{H}_\varepsilon \longrightarrow H = \mathrm{L}^2(\Omega) \times \mathrm{L}^2(\partial\Omega{\times}(0, 1))$$

- Energy functionals

$$\mathcal{E}_\varepsilon(u,\phi) = \int_\Omega \frac{a_\mathrm{b}}{2}|\nabla u|^2 + F_\mathrm{b}(u)\mathrm{d}x + \iint\limits_{\partial\Omega}\int_0^1 \left[\tfrac{a_\mathrm{s}\varepsilon^{\alpha+1}}{2}(|B_\varepsilon \nabla_\| \phi|^2 + \tfrac{1}{\varepsilon^2}|\partial_\eta \phi|^2) + F_\mathrm{s}(\phi)\right] J_\varepsilon \mathrm{d}\eta \mathrm{da}$$

- Dissipation functionals

$$\mathcal{R}_\varepsilon(\dot u, \dot\phi) = \int\limits_\Omega \tfrac{r_\mathrm{b}}{2}|\dot u|^2 \mathrm{d}x + \int\limits_{\partial\Omega}\int_0^1 \tfrac{r_\mathrm{s}}{2}|\dot\phi|^2 J_\varepsilon \mathrm{d}\eta\mathrm{da}$$

- Transformed solutions solve

$$\mathrm{D}\mathcal{E}_\varepsilon(u_\varepsilon,\phi_\varepsilon) + \mathrm{D}\mathcal{R}_\varepsilon(\dot u_\varepsilon, \dot\phi_\varepsilon) = 0$$

- Energy functionals

$$\mathcal{E}_\varepsilon(u,\phi) = \quad \mathcal{E}_\mathrm{b}(u) + \int\limits_{\partial\Omega}\int_0^1 \Big[\tfrac{a_\mathrm{s}\varepsilon^{\alpha+1}}{2}(|B_\varepsilon\nabla_\|\phi|^2 + \tfrac{1}{\varepsilon^2}|\partial_\eta\phi|^2) + F_\mathrm{s}(\phi)\Big] J_\varepsilon \mathrm{d}\eta \mathrm{da}$$

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- Transformed solutions solve

$$\mathrm{D}\mathcal{E}_\varepsilon(u_\varepsilon,\phi_\varepsilon) + \mathrm{D}\mathcal{R}_\varepsilon(\dot{u}_\varepsilon,\dot{\phi}_\varepsilon) = 0$$

$$\mathcal{E}_\varepsilon(u_\varepsilon(t),\phi_\varepsilon(t)) + \int_0^t \mathcal{R}_\varepsilon(\dot u_\varepsilon,\dot\phi_\varepsilon)\mathrm{d}\tau \le \mathcal{E}_\varepsilon(u_\varepsilon(0),\phi_\varepsilon(0))$$

- Case $\alpha \le -1$:
$$\|(u_\varepsilon,\phi_\varepsilon)\|_{\mathrm{L}^\infty(0,T;V)} \le C$$
- Case $\alpha \in (-1,1)$:
$$\|(u_\varepsilon,\phi_\varepsilon)\|_{\mathrm{L}^\infty(0,T;\overline{V})} \le C$$

  with

$$\overline{V} := \{(u,\phi) \in \mathrm{H}^1(\Omega) \times \mathrm{L}^2(\partial\Omega\times(0,1)) : \\ \partial_\eta\phi \in \mathrm{L}^2(\partial\Omega\times(0,1)),\ u|_{\partial\Omega} = \phi|_{\eta=0}\}$$

- Bounded dissipation functional
$$\|(\dot u_\varepsilon,\dot\phi_\varepsilon)\|_{\mathrm{L}^2(0,T;H)} \le C$$

We have

$$(u_\varepsilon, \phi_\varepsilon) \overset{*}{\rightharpoonup} (u, \phi) \text{ in } \mathrm{L}^\infty(0,T;V) \text{ (resp. in } \mathrm{L}^\infty(0,T;\overline{V}))$$
$$(u_\varepsilon, \phi_\varepsilon) \rightharpoonup (u, \phi) \text{ in } \mathrm{H}^1(0,T;H)$$

In particular

$$\Longrightarrow \quad \forall t \in [0,T]: \quad z_\varepsilon(t) \rightharpoonup z(t) \;\text{ in } H$$

Moreover, $z_\varepsilon \in \mathrm{C}_w([0,T], \widehat{V})$

$$\Longrightarrow \quad \forall t \in [0,T]: \quad z_\varepsilon(t) \rightharpoonup z(t) \;\text{ in } \widehat{V}$$

with $\widehat{V} = V$ for $\alpha \leq -1$ or $\widetilde{V} = \overline{V}$ for $\alpha \in (-1,1)$

$F_{\rm b}$ and $F_{\rm s}$ are λ-convex, i.e., $\exists\lambda \in \mathbb{R}$

$$u \mapsto F_{\rm b}(u) + \lambda|u|^2, \quad \phi \mapsto F_{\rm s}(\phi) + \lambda|\phi|^2 \quad \text{are convex,}$$

e.g. $\mathrm{C}^{1,1}$-perturbation of a convex function, double well potential $\mathbb{W}(u) = \frac{1}{4}(1-u^2)^2$

$$F_{\rm b}(u-v) \geq F_{\rm b}(u) - F_{\rm b}'(u)v - \lambda|v|^2, \quad \forall u, v \in \mathbb{R}$$

Consequence: For $z_\varepsilon = (u_\varepsilon, \phi_\varepsilon)$

$$\mathcal{E}_\varepsilon(z_\varepsilon - \widehat{z}_\varepsilon) + \lambda\|\widehat{z}_\varepsilon\|_H^2 \geq \mathcal{E}_\varepsilon(z_\varepsilon) - \langle \mathrm{D}\mathcal{E}_\varepsilon(z_\varepsilon), \widehat{z}_\varepsilon\rangle, \quad \forall \widehat{z}_\varepsilon \in V$$

Hence force balance equivalent to

$$\mathcal{E}_\varepsilon(z_\varepsilon(t) - \widehat{z}_\varepsilon) + \lambda\|\widehat{z}_\varepsilon\|_H^2 \geq \mathcal{E}_\varepsilon(z_\varepsilon(t)) + \langle G_\varepsilon \dot{z}_\varepsilon(t), \widehat{z}_\varepsilon\rangle, \quad \forall \widehat{z}_\varepsilon \in V$$

with $G_\varepsilon = \mathrm{D}\mathcal{R}_\varepsilon$

Definition: (Attouch [1984], Braides [2002], Dal Maso [1993])
$\mathcal{I}_0 : \mathcal{Y} \to \mathbb{R}_\infty$ **Γ-limit** of sequence $(\mathcal{I}_\varepsilon)_{\varepsilon>0}$ w.r.t. topology τ iff

(i) **liminf estimate:**

$$y_\varepsilon \xrightarrow{\tau} y \quad \Longrightarrow \quad \mathcal{I}_0(y) \leq \liminf_{\varepsilon\to 0} \mathcal{I}_\varepsilon(y_\varepsilon)$$

(ii) **limsup estimate** (existence of recovery sequence)**:**

$$\forall y \in \mathcal{Y}\, \exists (\widehat{y}_\varepsilon)_{\varepsilon>0} : \quad y_\varepsilon \xrightarrow{\tau} y \ \text{ and } \ \mathcal{I}_0(y) \geq \limsup_{\varepsilon\to 0} \mathcal{I}_\varepsilon(\widehat{y}_\varepsilon).$$

Theorem: $(\mathcal{I}_\varepsilon)_{\varepsilon>0}$ equi-coercive ($\bigcup_{\varepsilon>0}\{\mathcal{I}_\varepsilon \leq E\}$ precompact) and $\mathcal{I}_\varepsilon \xrightarrow{\Gamma} \mathcal{I}_0$; then

$$\min_{\mathcal{Y}} \mathcal{I}_0 = \lim_{\varepsilon\to 0} \min_{\mathcal{Y}} \mathcal{I}_\varepsilon.$$

$(y_\varepsilon)_{\varepsilon>0}$ minimizers of $\mathcal{I}_\varepsilon \Longrightarrow$ cluster points y are minimizers of $\mathcal{I}_0$

Minimization problems:

- Homogenization, Two-scale convergence
- Singular limits (Cahn–Hilliard $\longrightarrow$ Sharp interface)
- Young measure relaxation, penalization

Rate independent systems (Mielke, Roubíček, Stefanelli [2008])

- Two-scale Homogenization (Mielke & Timofte [2007], Hanke [2009])
- Damage to Delamination (Mielke, Thomas, Roubíček *in preparation*)
- Dimension reduction in linearized elastoplasticity (Mielke & L. *in preparation*)

Hamiltonian systems (Mielke [2008])
Gradient flows (Sandier & Serfaty [2004])

Γ-convergence of the Energies

$$\mathcal{E}_\varepsilon(u,\phi) = \mathcal{E}_\mathrm{b}(u) + \iint\limits_{\partial\Omega}\int_0^1 \left[\frac{a_\mathrm{s}\varepsilon^{\alpha+1}}{2}\left(|B_\varepsilon \nabla_\| \phi|^2 + \frac{1}{\varepsilon^2}|\partial_\eta\phi|^2\right) + F_\mathrm{s}(\phi)\right] J_\varepsilon \mathrm{d}\eta \mathrm{da}$$

(i) Case $\alpha = -1$

$$\mathcal{E}_0 : \begin{cases} V & \to \quad \mathbb{R}_\infty, \\ (u,\phi) & \mapsto \quad \begin{cases} \mathcal{E}_b(u) + \int_{\partial\Omega} \frac{a_\mathrm{s}}{2}|\nabla_\|\phi|^2 + F_\mathrm{s}(\phi)\mathrm{da} & \partial_\eta\phi = 0, \\ \infty & \text{otherwise} \end{cases} \end{cases}$$

(ii) Case $\alpha < -1$

$$\mathcal{E}_0 : \begin{cases} V & \to \quad \mathbb{R}_\infty, \\ (u,\phi) & \mapsto \quad \begin{cases} \mathcal{E}_b(u) + \mathcal{H}^{d-1}(\partial\Omega) F_\mathrm{s}(\phi)\mathrm{da} & \phi \text{ constant}, \\ \infty & \text{otherwise} \end{cases} \end{cases}$$

$$\mathcal{E}_\varepsilon(u,\phi) = \mathcal{E}_\mathrm{b}(u) + \iint_{\partial\Omega}\int_0^1 \left[\frac{a_\mathrm{s}\varepsilon^{\alpha+1}}{2}\left(|B_\varepsilon \nabla_\| \phi|^2 + \frac{1}{\varepsilon^2}|\partial_\eta \phi|^2\right) + F_\mathrm{s}(\phi)\right] J_\varepsilon \mathrm{d}\eta \mathrm{da}$$

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(ii) Case $\alpha < -1$

$$\mathcal{E}_0 : \begin{cases} V & \to \quad \mathbb{R}_\infty, \\ (u,\phi) & \mapsto \quad \begin{cases} \mathcal{E}_b(u) + \mathcal{H}^{d-1}(\partial\Omega) F_\mathrm{s}(\phi)\mathrm{da} & (u,\phi) \in V_c, \\ \infty & \text{otherwise} \end{cases} \end{cases}$$

(iii) Case $\alpha \in (-1,1)$

$$\overline{V} := \{(u,\phi) \in \mathrm{H}^1(\Omega) \times \mathrm{L}^2(\partial\Omega\times(0,1)) : \\ \partial_\eta \phi \in \mathrm{L}^2(\partial\Omega\times(0,1)),\ u|_{\partial\Omega} = \phi|_{\eta=0}\}$$

$$\mathcal{E}_0 : \begin{cases} \overline{V} & \rightarrow \quad \mathbb{R}_\infty, \\ (u,\phi) & \mapsto \quad \begin{cases} \mathcal{E}_b(u) + \int_{\partial\Omega} F_\mathrm{s}^{**}(\phi)\mathrm{da} & \partial_\eta \phi = 0, \\ \infty & \text{otherwise} \end{cases} \end{cases}$$

In the following: F_s convex

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$$\overline{V} := \{(u,\phi) \in \mathrm{H}^1(\Omega) \times \mathrm{L}^2(\partial\Omega\times(0,1)) : \partial_\eta \phi \in \mathrm{L}^2(\partial\Omega\times(0,1)),\ u|_{\partial\Omega} = \phi|_{\eta=0}\}$$

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In the following: F_{s} convex

Theorem

Let $z_\varepsilon = (u_\varepsilon, \phi_\varepsilon)$ *be solutions w.r.t.* $(\mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ *with*

$$(u_\varepsilon, \phi_\varepsilon) \overset{*}{\rightharpoonup} (u, \phi) \text{ in } \mathrm{L}^\infty(0,T;V) \text{ (resp. in } \mathrm{L}^\infty(0,T;\overline{V}))$$
$$(u_\varepsilon, \phi_\varepsilon) \rightharpoonup (u, \phi) \text{ in } \mathrm{H}^1(0,T;H)$$

then $z = (u, \phi)$ *is a solution w.r.t.* $(\mathcal{E}_0, \mathcal{R}_0)$, *i.e.*

$$\mathcal{E}_0(z(t) - \widehat{z}) + \lambda \|\widehat{z}\|_H^2 \geq \mathcal{E}_0(z(t)) + \langle G_0 \dot{z}(t), \widehat{z} \rangle, \quad \forall \widehat{z}_\varepsilon \in V \text{ (resp. } \overline{V})$$

with $G_0 = \mathrm{D}\mathcal{R}_0$. *In particular,* z *solves*

$$G_0(\dot{z}) + \mathrm{D}\mathcal{E}_0(u, \phi) = 0$$

Formally equivalent to

$$r_{\mathrm{b}}\partial_t u - a_{\mathrm{b}}\Delta u + F_{\mathrm{b}}'(u) = 0, \quad \text{in } \Omega \times [0,T]$$

- Case $\alpha = -1$

$$r_{\mathrm{s}}\partial_t \phi - a_{\mathrm{b}}\Delta_{\|}\phi + F_{\mathrm{s}}'(\phi) + a_{\mathrm{b}}\partial_\nu u = 0, \quad \text{on } \partial\Omega \times [0,T]$$

- Case $\alpha < -1$

$$\begin{aligned} r_{\mathrm{s}}\partial_t \phi + a_{\mathrm{b}}[\partial_\nu u] + F_{\mathrm{s}}'(\phi) = 0, &\quad \text{in } [0,T] \\ u = \phi = \text{const}, &\quad \text{on } \partial\Omega \times [0,T] \end{aligned}$$

- $\alpha \in (-1,1)$

$$r_{\mathrm{s}}\partial_t \phi + a_{\mathrm{b}}\partial_\nu u + F_{\mathrm{s}}'(\phi) = 0, \quad \text{on } \partial\Omega \times [0,T]$$

Set $\widehat{z}_\varepsilon = z_\varepsilon - \overline{z}_\varepsilon$, with $\overline{z}_\varepsilon(t)$ recovery sequence for $z(t) - \overline{z}(t)$.

$$\int_0^T \mathcal{E}_\varepsilon(\overline{z}_\varepsilon) + \lambda\|z_\varepsilon - \overline{z}_\varepsilon\|_H^2 \mathrm{d}t \geq \int_0^T \mathcal{E}_\varepsilon(z_\varepsilon) + \langle G_\varepsilon \dot{z}_\varepsilon, z_\varepsilon - \overline{z}_\varepsilon\rangle \mathrm{d}t$$

2. Integration by parts

$$\int_0^T \langle G_\varepsilon \dot{z}_\varepsilon, z_\varepsilon - \overline{z}_\varepsilon\rangle \mathrm{d}t = -\int_0^T \langle G_\varepsilon z_\varepsilon, \dot{\overline{z}}_\varepsilon\rangle \mathrm{d}t + \mathcal{R}_\varepsilon(z_\varepsilon(T)) - \mathcal{R}_\varepsilon(z_\varepsilon(0))$$

3. Passing to the limit + Integration by parts

$$\int_0^T \mathcal{E}_0(\overline{z}) + \lambda\|z - \overline{z}\|_H^2 \mathrm{d}t \geq \int_0^T \mathcal{E}_0(z) - \langle G_0 \dot{z}, z - \overline{z}\rangle \mathrm{d}t$$

4. Sequence $\overline{z}^\delta \to z - \widehat{z}$ in $\mathrm{L}^2(0,T;V_0)$. By arbitrariness of $\widehat{z}$

$$\mathcal{E}_0(z(t) - \widehat{z}) + \lambda\|\widehat{z}\|_H^2 \geq \mathcal{E}_0(z(t)) + \langle G_0 \dot{z}(t), \widehat{z}\rangle, \quad \forall \widehat{z} \in V/\overline{V}$$

Outlook

- Different scalings in dissipation potential
- More complex dissipation potentials (Heat equation with entropy as driving potential)
- Interfaces

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Thank You