Numerical algorithms for optimal control problems governed by Kobayashi–Warren–Carter type systems

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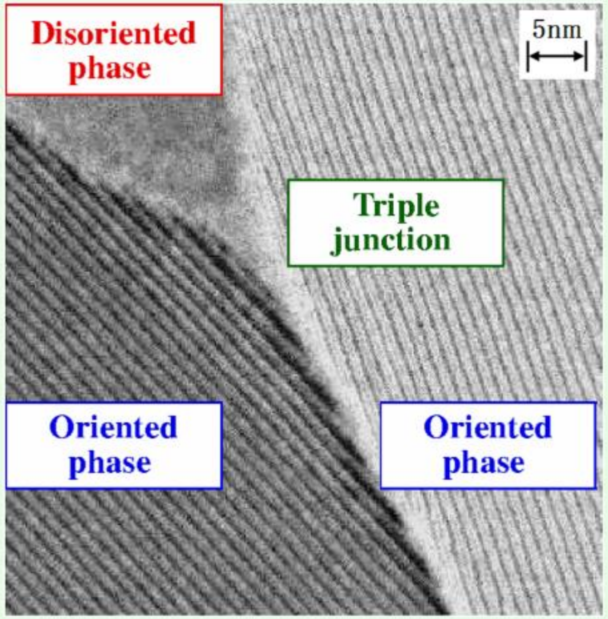
1. Kobayashi–Warren–Carter type system of grain boundary motion

$0 < T < \infty$, $\Omega := (0,1) \subset \mathbb{R}$: b.d.d. domain, $\Gamma = \partial\Omega := \{0,1\}$, $\varepsilon > 0$.

State system $(\mathrm{S})_\varepsilon$: cf. [Kobayashi–Warren–Carter](2000)

$$\begin{cases} \partial_t \eta - \partial_x^2 \eta + g(\eta) + \alpha'(\eta)\sqrt{\varepsilon^2 + |\partial_x \theta|^2} = M_u u(t,x), \ (t,x) \in Q := (0,T) \times \Omega, \\ \alpha_0(t,x)\partial_t \theta - \partial_x \left(\alpha(\eta) \dfrac{\partial_x \theta}{\sqrt{\varepsilon^2 + |\partial_x \theta|^2}} + \nu^2 \partial_x \theta \right) = M_v v(t,x), \ (t,x) \in Q, \\ \partial_x \eta = 0, \ \ \theta = 0 \text{ on } \Sigma := (0,T) \times \Gamma, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ x \in \Omega. \end{cases}$$

- $\eta = \eta(t,x)$: orientation order,
  $\theta = \theta(t,x)$: orientation angle of grain
- $u = u(t,x)$: temperature , $v = v(t,x)$: forcing for θ
- $g \in C^2(\mathbb{R})$: Lipschitz perturbation
- $\alpha_0 \in W^{1,\infty}(Q)$: fixed function
- $0 < \alpha \in C^2(\mathbb{R})$: convex mobility
- $\nu > 0$, $M_u > 0$, $M_v > 0$: fixed constants
- $[\eta_0, \theta_0] = [\eta_0(x), \theta_0(x)]$: fixed initial data of $[\eta, \theta]$



2. Optimal control problem

$\Omega := (0,1), \ \ Q = (0,T) \times \Omega, \ \ H := L^2(\Omega), \ \ \mathscr{H} := L^2(0,T;H), \ \ \varepsilon > 0.$

Problem (OP)$_\varepsilon$: find $[u^*, v^*] \in [\mathscr{H}]^2$, called optimal control, s.t.

$$[u^*, v^*] = \text{arg-min}\, \mathcal{J}_\varepsilon = \mathcal{J}_\varepsilon(u,v) \text{ on a class } [\mathscr{H}]^2,$$

with a cost functional $\mathcal{J}_\varepsilon : [u,v] \in [\mathscr{H}]^2 \mapsto \mathcal{J}_\varepsilon(u,v) \in [0,\infty)$, defined as

$$\mathcal{J}_\varepsilon(u,v) := \frac{M_\eta}{2} \int_0^T \left|(\eta - \eta_{\mathrm{ad}})(t)\right|_H^2 dt + \frac{M_\theta}{2} \int_0^T \left|(\theta - \theta_{\mathrm{ad}})(t)\right|_H^2 dt + \frac{a_u}{2} \int_0^T \left|u(t)\right|_H^2 dt + \frac{a_v}{2} \int_0^T \left|v(t)\right|_H^2 dt.$$

In the context,

- $u = u(t,x)$: the temperature control for η, $\ v = v(t,x)$: the control for θ
- $[\eta, \theta] \in [\mathscr{H}]^2$: the solution to the state system (S)$_\varepsilon$, for any $[u,v] \in [\mathscr{H}]^2$
- $[\eta_{\mathrm{ad}}, \theta_{\mathrm{ad}}] \in [\mathscr{H}]^2$: the admissible target profile for $[\eta, \theta]$
- $M_\eta > 0$, $M_\theta > 0$, $a_u > 0$, $a_v > 0$: positive constants.

Previous works (cf. [Antil, Ito, Kenmochi, K., Moll, Nakayashiki, Shirakawa, Yamazaki](2008–))

* The state system $(\mathrm{S})_\varepsilon$ admits a unique solution $[\eta, \theta]$ for $[u, v]$ and continuous dependence for the forcing term.
* The problem $(\mathrm{OP})_\varepsilon$ admits at least one optimal control $[u^*, v^*] \in [\mathscr{H}]^2$
* (Necessary condition for $(\mathrm{OP})_\varepsilon$) Let $[u^*, v^*] \in [\mathscr{H}]^2$ be the optimal control for $(\mathrm{OP})_\varepsilon$. Then, it holds that:

$$M_u p^* + a_u u^* = 0, \ M_v z^* + a_v v^* = 0 \ \text{ in } \ \mathscr{H}$$

In the context, $[\eta^*, \theta^*] := \mathcal{S}_\varepsilon[u^*, v^*]$ and $[p^*, z^*] \in [\mathscr{H}]^2$ is a unique solution of the following adjoint system $(\mathrm{A})_\varepsilon$:

$(\mathrm{A})_\varepsilon$

$$\begin{cases} -\partial_t p^* - \partial_x^2 p^* + \big(g'(\eta^*) + \alpha''(\eta^*) f_\varepsilon(\partial_x \theta^*)\big) p^* + \alpha'(\eta^*) f_\varepsilon'(\partial_x \theta^*) \partial_x z^* = M_\eta(\eta^* - \eta_{\mathrm{ad}}) \ \text{ in } Q, \\ -\partial_t(\alpha_0 z^*) - \partial_x \big(\alpha(\eta^*) f_\varepsilon''(\partial_x \theta^*) \partial_x z^* + \nu^2 \partial_x z^* + \alpha'(\eta^*) f_\varepsilon'(\partial_x \theta^*) p^*\big) = M_\theta(\theta^* - \theta_{\mathrm{ad}}) \ \text{ in } Q, \\ \partial_x p^* = z^* = 0 \ \text{ in } \Sigma, \\ p^*(T, x) = z^*(T, x) = 0, \ x \in \Omega \end{cases}$$

- $f_\varepsilon(\omega) := \sqrt{\varepsilon^2 + |\omega|^2}, \forall \omega \in \mathbb{R}, \varepsilon > 0 \ \big(f_\varepsilon \to |\cdot| \text{ in } L^\infty(\mathbb{R}) \text{ as } \varepsilon \downarrow 0\big)$
- $\mathcal{S}_\varepsilon : [u, v] \in [\mathscr{H}]^2 \mapsto [\eta, \theta] := \mathcal{S}_\varepsilon[u, v]$: the solution operator for $(\mathrm{S})_\varepsilon$

◇Key-Lemma for Numerical algorithm

Key-Lemma

Let $n \in \mathbb{N}$ be a fixed number, and let $\beta \in (0,1)$ and $\mu \in (0,1)$. Also, let $[u_n, v_n] \in [\mathscr{H}]^2$ be the optimal control for $(\mathrm{OP})_\varepsilon$ and, let $[\eta_n, \theta_n] := \mathcal{S}_\varepsilon[u_n, v_n]$ and $[p_n, z_n] \in [\mathscr{H}]^2$ be a unique solution of the adjoint system $(\mathrm{A})_\varepsilon$. Put

$$d_{0,n} := M_u p_n + a_u u_n \text{ and } d_{1,n} := M_v z_n + a_v v_n,$$

and assume that at least one of the following conditions is satisfied:

$$d_{0,n} \neq 0 \text{ in } \mathscr{H}, \; d_{1,n} \neq 0 \text{ in } \mathscr{H}.$$

Then, there is a minimal constant $\varsigma_n \in \mathbb{N}$ such that

$$\mathcal{J}_\varepsilon\left(u_n - \beta^{\varsigma_n} d_{0,n}, v_n - \beta^{\varsigma_n} d_{1,n}\right) - \mathcal{J}_\varepsilon(u_n, v_n) \leq -\mu\beta^{\varsigma_n} \left|[d_{0,n}, d_{1,n}]\right|^2_{[\mathscr{H}]^2}$$

Keypoint:

- The Gateaux differential of the cost guarantees that this Key-Lemma holds
- The constant $\rho_n := \beta^{\varsigma_n}$ plays the important role in numerical algorithm

3. Main results

Main results (Numerical algorithm for $(\mathrm{OP})_\varepsilon$)

Step 0 Give the stop parameter μ;

Step 1 Choose the pair of initial functions $[u, v] \in [\mathscr{H}]^2$, and put $[u_n, v_n] := [u, v]$;

Step 2 Solve the state system $(\mathrm{S})_\varepsilon$, and let $[\eta_n, \theta_n] := S_\varepsilon(u_n, v_n)$;

Step 3 Solve the adjoint system for n, and let $[p_n, z_n]$ be the solution to the adjoint system $(\mathrm{A})_\varepsilon$;

Step 4 Put

$$d_{0,n} := M_u p_n + a_u u_n \ \text{ and } \ d_{1,n} := M_v z_n + a_v v_n.$$

Test: If

$$|[d_{0,n}, d_{1,n}]|_{[\mathscr{H}]^2} < \mu,$$

then, STOP; Otherwise, go to Step 5;

Step 5 Put

$$u_{n+1} := u_n - \rho_n d_{0,n} \ \text{ and } \ v_{n+1} := v_n - \rho_n d_{1,n},$$

where ρ_n is some appropriate constant in Key-Lemma;

Step 6 Set $n = n + 1$, and go to Step 2.

Main results (Convergence of the numerical algorithm)

Let $\{[u_n, v_n]\}_{n\in\mathbb{N}} \subset [\mathscr{H}]^2$ be defined by the numerical algorithm. In addition, let $[p_n, z_n]$ be the solution to the adjoint system $(\mathrm{A})_\varepsilon$ for the focring term $[M_\eta(\eta_n - \eta_{\mathrm{ad}}), M_\theta(\theta_n - \theta_{\mathrm{ad}})]$ with $[\eta_n, \theta_n] = S_\varepsilon[u_n, v_n]$. Then, it holds:

(I)

$$\lim_{n\to\infty} \mathcal{J}_\varepsilon(u_n, v_n) \text{ exists;}$$

(II)

$$\lim_{n\to\infty}(M_u p_n + a_u u_n) = 0, \ \lim_{n\to\infty}(M_v z_n + a_v v_n) = 0 \text{ in } \mathscr{H};$$

(III) $\exists [u_*, v_*] \in [\mathscr{H}]^2$, $[p_*, z_*] \in [\mathscr{H}]^2$, and $\{n_k\}_{k\in\mathbb{N}} \subset \{n\}_{n\in\mathbb{N}}$ such that $p_* \in L^2(0,T; H^1(\Omega))$, $z_* \in L^2(0,T; H^1_0(\Omega))$, $[p_*, z_*]$ is a unique solution of the adjoint system $(\mathrm{A})_\varepsilon$, and

$$\begin{cases} [u_{n_k}, v_{n_k}] \to [u_*, v_*] \text{ weakly in } [\mathscr{H}]^2, \\ M_u p_* + a_u u_* = 0, \ M_v z_* + a_v v_* = 0 \text{ in } \mathscr{H}, \end{cases} \quad \text{as } k \to \infty.$$

Keypoint:

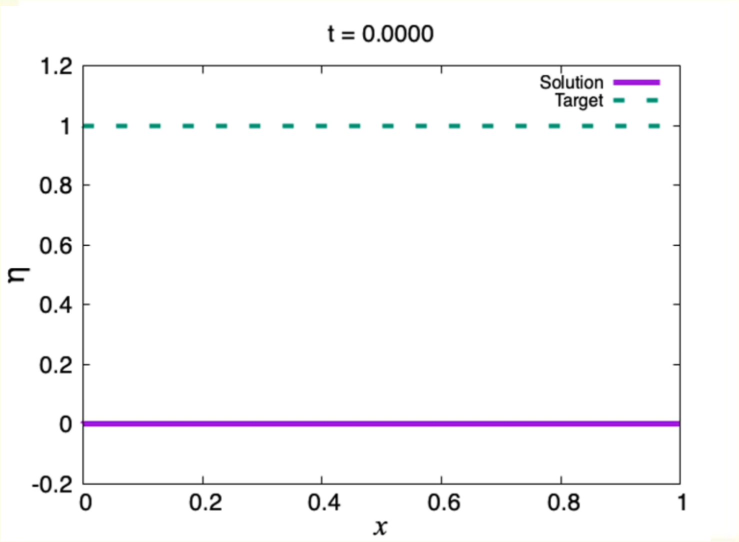
- This convergence is based on the linear programming

Main results (Numerical experiment)

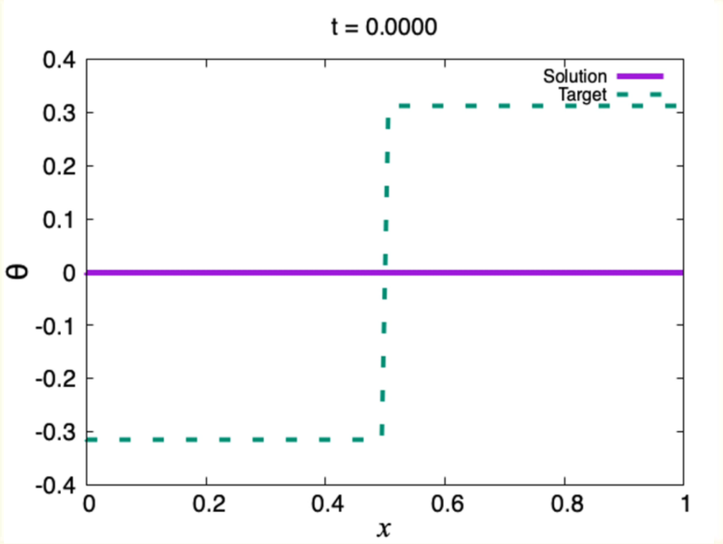
Setting

- $T = 0.5$, $Q = (0, T) \times \Omega = (0, 0.5) \times (0, 1)$, given initial data $[u_1, v_1] = [0, 0]$
- $\mu = 1.0 \times 10^{-3}$, $\beta = 0.5$, $\varepsilon = 0.01$, $\nu = 0.1$, $M_u = 1.0$, $M_v = 1.0$, $M_\eta = 1.0$, $M_\theta = 1.0$, $a_u = 1.0$, $a_v = 1.0$

Results of the solution η and θ



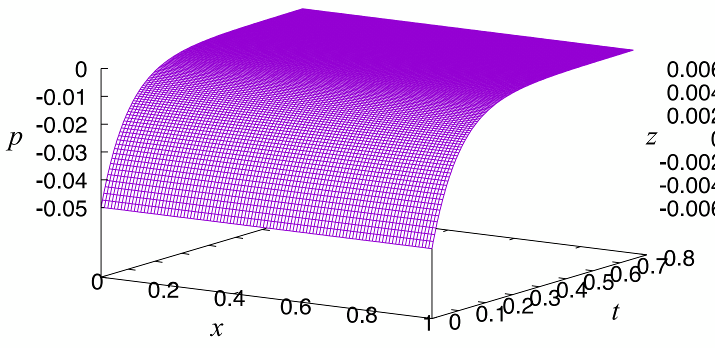
time development of η,



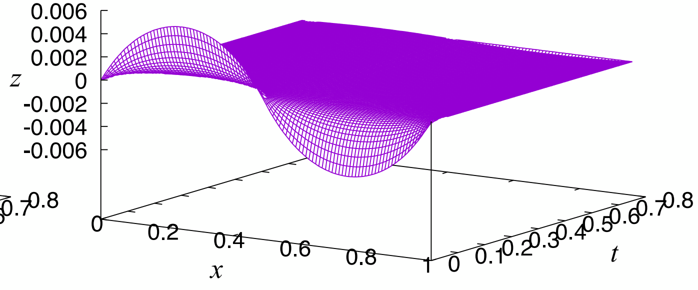
time development of θ

Main results (Numerical experiment)

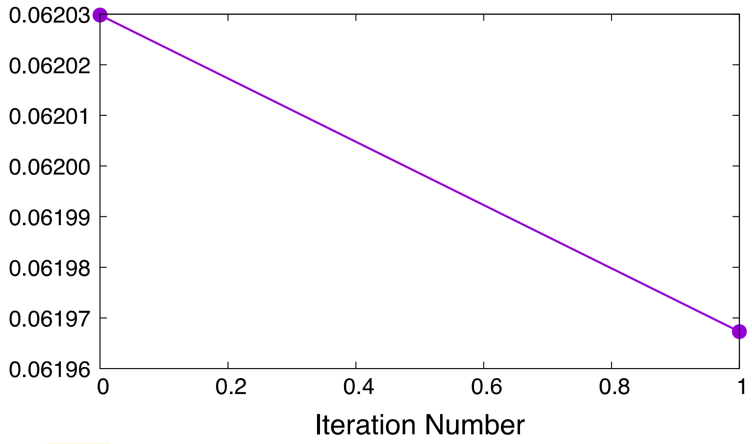
Graph of p, z and cost functional J_ε



time development of p



time development of z



time development of cost J_ε

- $M_u p + a_u u = 0$, $M_v z + a_v v = 0$ in $\mathscr{H}$
- the cost functional J_ε approaches to a stationary point

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$\Omega := (0,1)$, $Q = (0,T) \times \Omega$, $H := L^2(\Omega)$, $\mathscr{H} := L^2(0,T;H)$, $\varepsilon > 0$.

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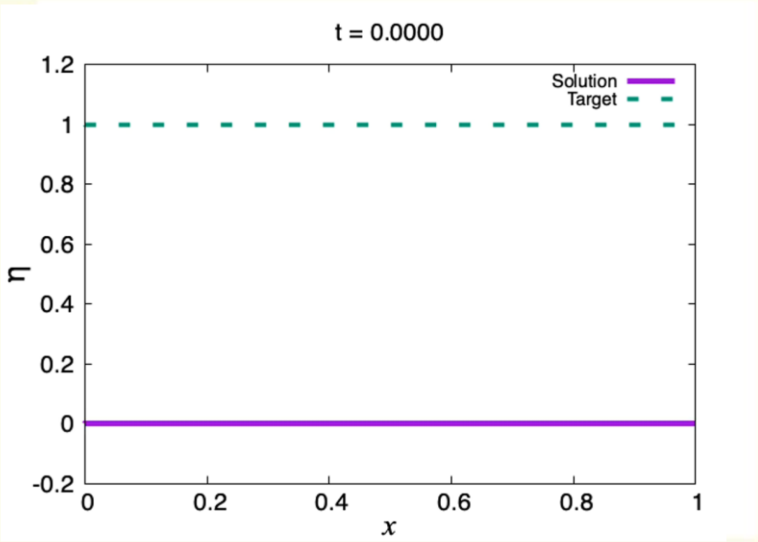
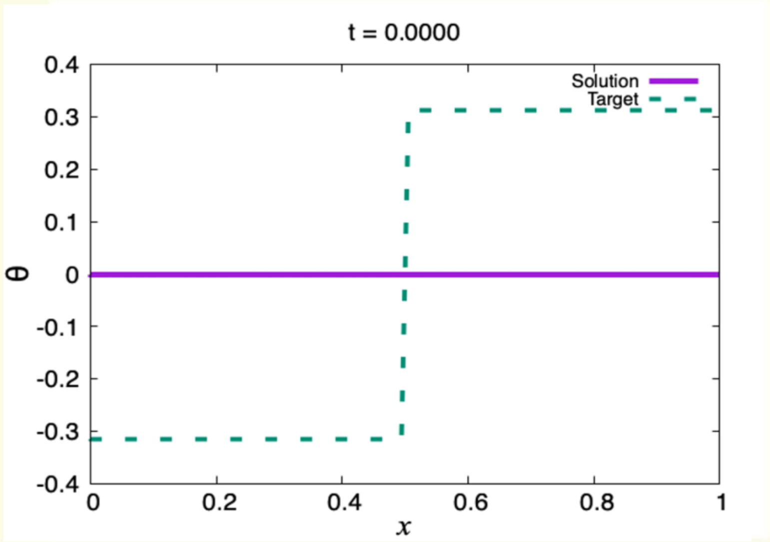


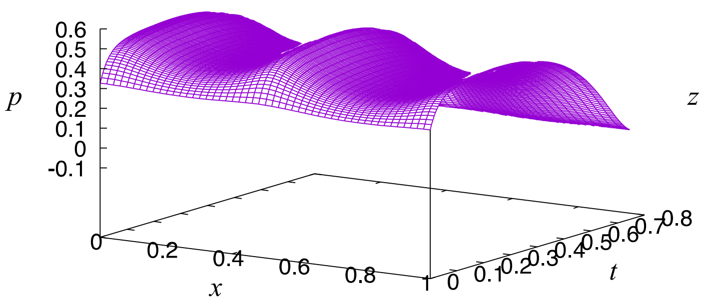
time development of η,



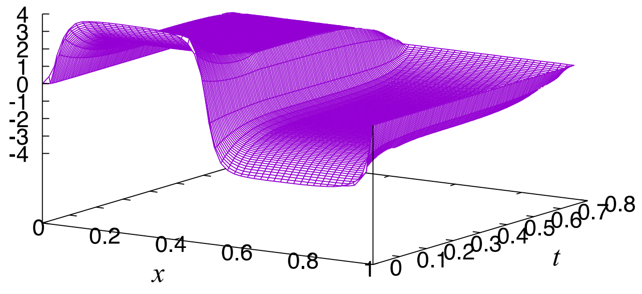
time development of θ

Main results (Numerical experiment)

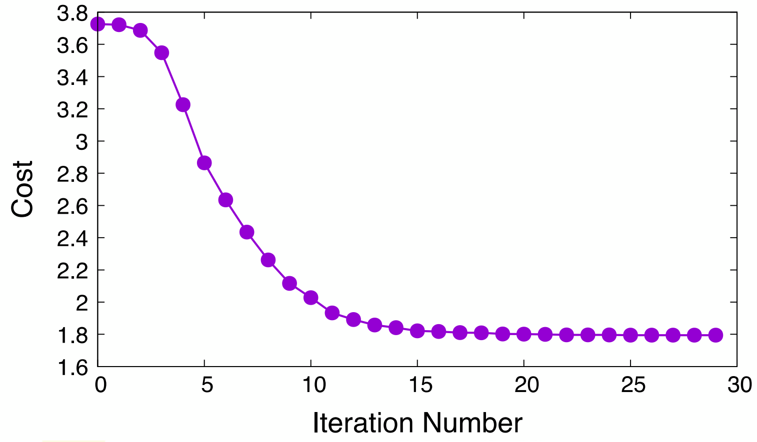
Graph of p, z and cost functional J_ε



time development of p



time development of z



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$$+ \frac{a_u}{2} \int_0^T \left|u(t)\right|_H^2 dt + \frac{a_v}{2} \int_0^T \left|v(t)\right|_H^2 dt.$$

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Setting

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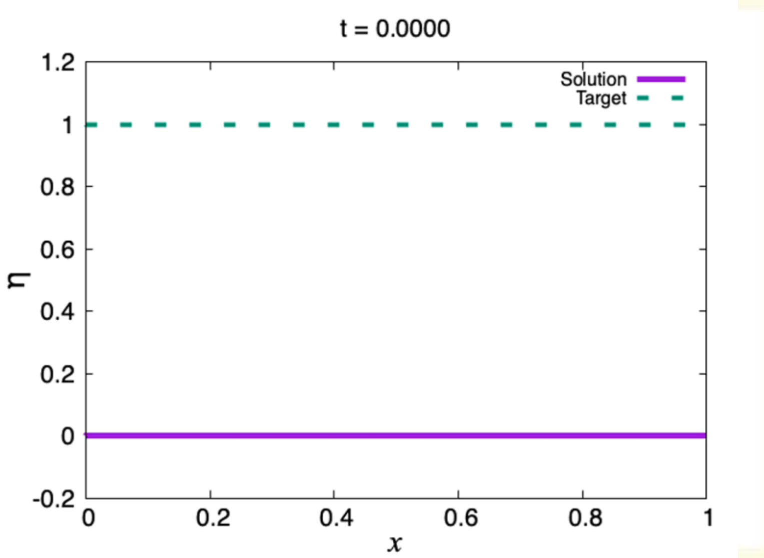
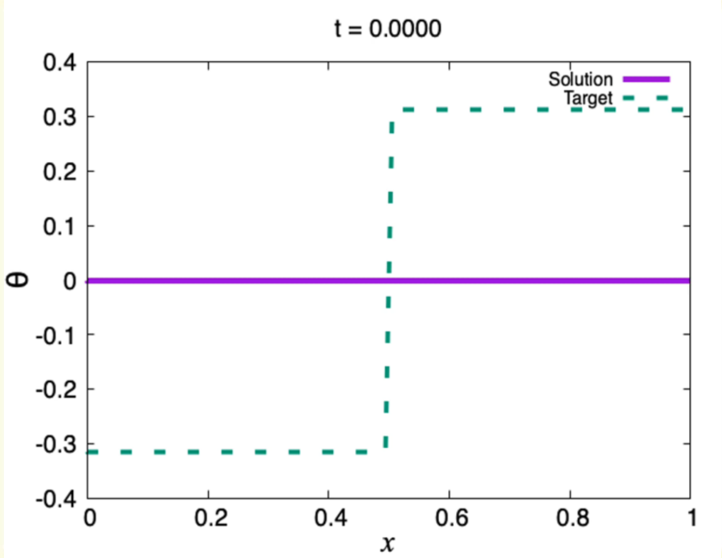


time development of η,



time development of θ

Main results (Numerical experiment)

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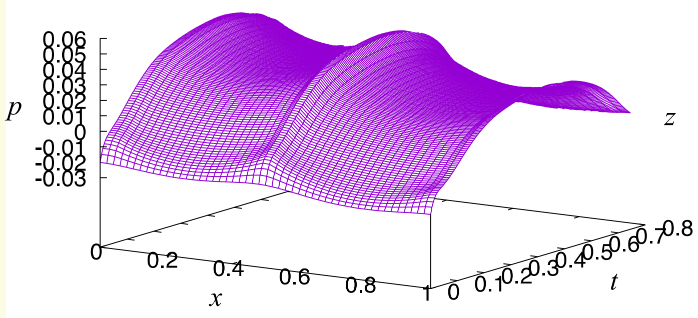

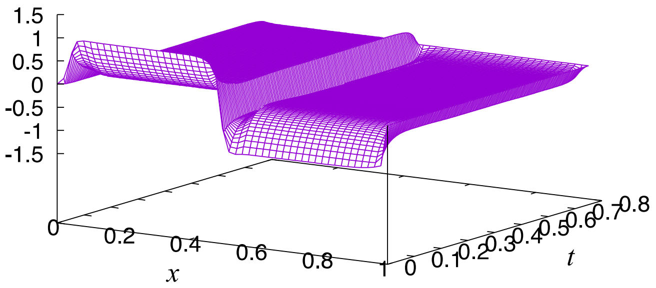

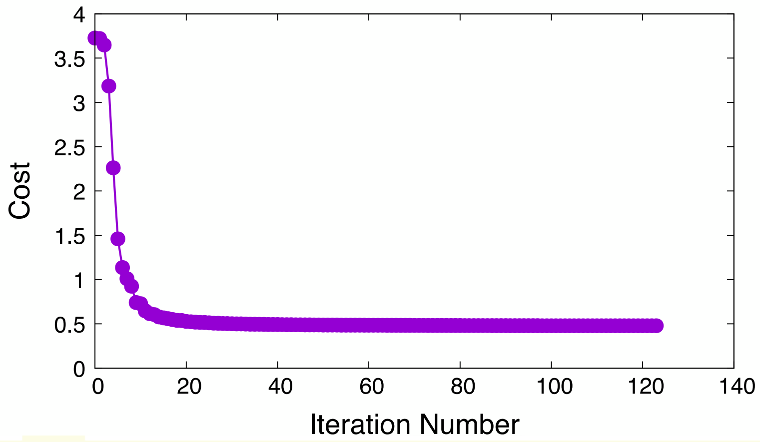

time development of p time development of z time development of cost J_ε

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Problems in future

(I) Consideration for numerical experiment

(II) Numerical algorithm and numerical experiment for multi-dimension

Keypoint :

- the domain of temperature controls is constrained in multi-dimension

$\Rightarrow$ neccesary condition for tamperature controls is the inequality $(p_n + u_n, h - u_n)_{\mathscr{H}} \geq 0$,

$h \in \{\text{constraint set}\} \subset \mathscr{H}$, when $M_u = M_v = a_u = a_v = 1.0$

- determination of the optimum search direction by means of projection onto the constraint set

Kobayashi–Warren–Carter type system of grain boundary motion

$0 < T < \infty$, $\Omega := (0,1) \subset \mathbb{R}$: b.d.d. domain, $\Gamma = \partial\Omega := \{0,1\}$.

State system (S): cf. [Kobayashi–Warren–Carter](2000)

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\begin{cases}
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\partial_x \eta = 0, \ \ \theta = 0 \text{ on } \Sigma := (0,T) \times \Gamma, \\
\eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ x \in \Omega.
\end{cases}
$$

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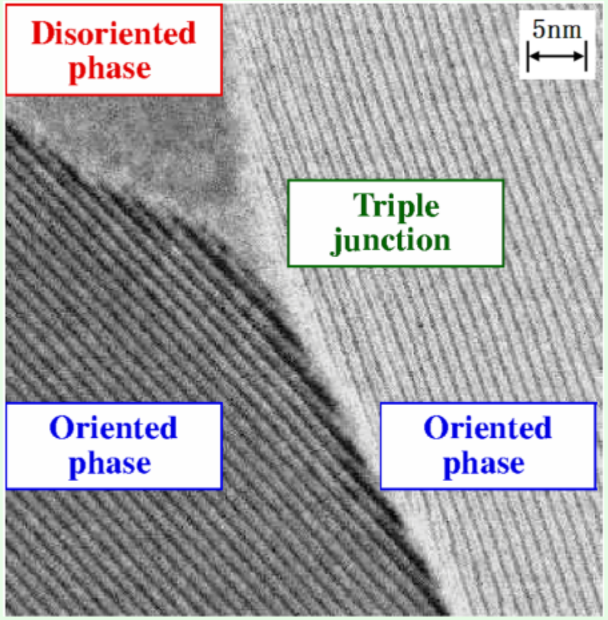

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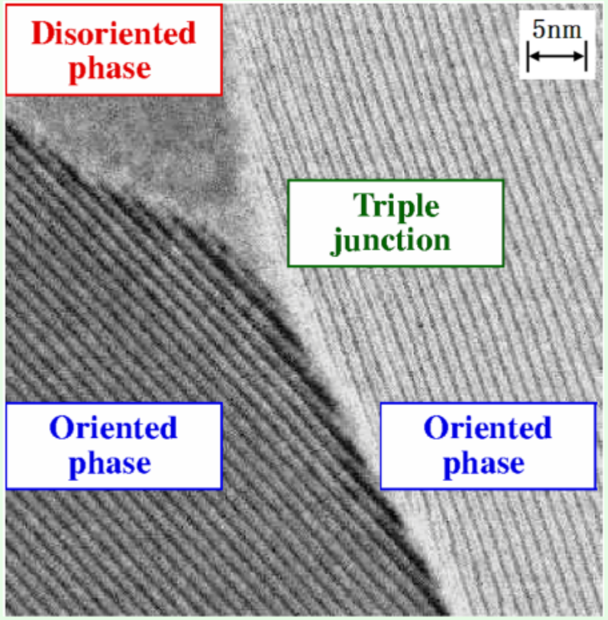

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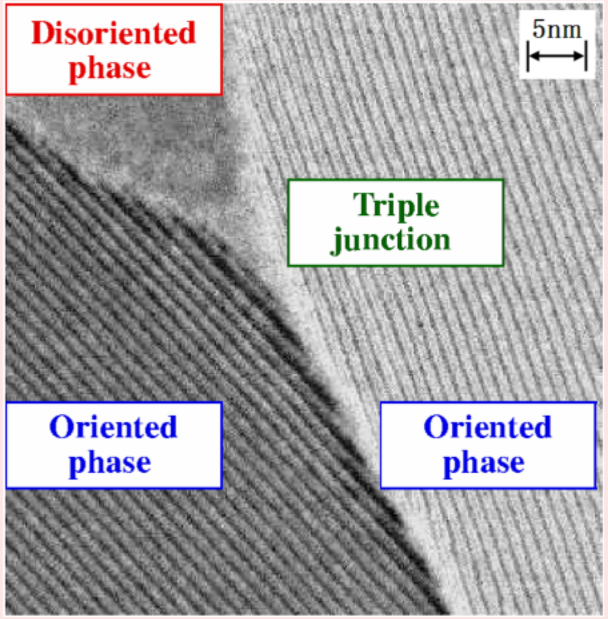
$0 < T < \infty$, $\Omega := (0,1) \subset \mathbb{R}$: b.d.d. domain, $\Gamma = \partial\Omega := \{0,1\}$, $\varepsilon > 0$.

State system $(\mathrm{S})_\varepsilon$: cf. [Kobayashi–Warren–Carter](2000)

$$\begin{cases} \partial_t \eta - \partial_x^2 \eta + g(\eta) + \alpha'(\eta) f_\varepsilon(\partial_x \theta) = M_u u(t,x), \ (t,x) \in Q := (0,T) \times \Omega, \\ \alpha_0(t,x)\partial_t \theta - \partial_x \big(\alpha(\eta) f'_\varepsilon(\partial_x \theta) + \nu^2 \partial_x \theta \big) = M_v v(t,x), \ (t,x) \in Q, \\ \partial_x \eta = 0, \ \ \theta = 0 \text{ on } \Sigma := (0,T) \times \Gamma, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ x \in \Omega. \end{cases}$$

- $\eta = \eta(t,x)$: orientation order,
  $\theta = \theta(t,x)$: orientation angle of grain
- $u = u(t,x)$: temperature , $v = v(t,x)$: forcing for θ
- $g \in C^2(\mathbb{R})$: Lipschitz perturbation
- $\alpha_0 \in W^{1,\infty}(Q)$: fixed function
- $0 < \alpha \in C^2(\mathbb{R})$: convex mobility
- $\nu > 0$, $M_u > 0$, $M_v > 0$: fixed constants
- $[\eta_0, \theta_0] = [\eta_0(x), \theta_0(x)]$: fixed initial data of $[\eta, \theta]$
- $f_\varepsilon(\omega) := \sqrt{\varepsilon^2 + |\omega|^2}$, $\forall \omega \in \mathbb{R}$ $\big(f_\varepsilon \to |\cdot| \text{ in } L^\infty(\mathbb{R}) \text{ as } \varepsilon \downarrow 0 \big)$



Main results

Main Results

Results. Numerical algorithm for $(\mathrm{OP})_\varepsilon$

- construction of the numerical algorithm
- convergence of the numerical algorithm
- numerical experiment

Assumption.

(A0) $\nu > 0$, $\varepsilon > 0$, $M_\eta > 0$, $M_\theta > 0$, $M_u > 0$, $M_v > 0$, $a_u > 0$, $a_v > 0$ are fixed constants.

(A1) $0 < \alpha_0 \in W^{1,\infty}(Q)$

(A2) $\alpha \in C^2(\mathbb{R})$: convex, s.t. α and $\alpha\alpha'$ are Lipschitz on $\mathbb{R}$,

$$\alpha'(0) = 0, \text{ and } \delta_\alpha := \inf \alpha(\mathbb{R}) \cup \alpha_0(\overline{Q}) > 0$$

(A3) $g \in C^2(\mathbb{R})$: Lipschitz, having a non-negative potential $G \in C^3(\mathbb{R})$.

(A4) $[\eta_0, \theta_0] \in H^1(\Omega) \times H^1_0(\Omega)$

Proposition 1 (cf. [Antil, Ito, Kenmochi, K., Moll, Nakayashiki, Shirakawa, Yamazaki](2008–))

Under (A0)–(A4) and $[u, v] \in [\mathscr{H}]^2$, the state system $(\mathrm{S})_\varepsilon$ admits a unique solution $[\eta, \theta]$, defined as follows.

(S0) $\eta \in W^{1,2}(0,T;H) \cap L^\infty(0,T;H^1(\Omega)) \subset C(\overline{Q})$

$\theta \in W^{1,2}(0,T;H) \cap L^\infty(0,T;H^1_0(\Omega)) \subset C(\overline{Q})$

(S1) $\partial_t \eta - \partial_x^2 \eta + g(\eta) + \alpha'(\eta) f_\varepsilon(\partial_x \theta) = M_u u$ in $\mathscr{H}$,

subject to $\partial_x \eta = 0$ a.e. in Σ, and $\eta(0) = \eta_0$ in H

(S2) $\alpha_0(t)\partial_t \theta(t) - \partial_x \big(\alpha(\eta(t)) f'_\varepsilon(\partial_x \theta(t)) + \nu^2 \partial_x \theta(t) \big) = M_v v(t)$ in H,

a.e. $t \in (0,T)$, subject to $\theta = 0$ a.e. in Σ, and $\theta(0) = \theta_0$ in H

* $f_\varepsilon(\omega) := \sqrt{\varepsilon^2 + |\omega|^2}$, $\forall \omega \in \mathbb{R}$, $\varepsilon > 0$ $\big(f_\varepsilon \to |\cdot|$ in $L^\infty(\mathbb{R})$ as $\varepsilon \downarrow 0 \big)$
* $\mathcal{S}_\varepsilon : [u, v] \in [\mathscr{H}]^2 \mapsto [\eta, \theta] := \mathcal{S}_\varepsilon[u, v]$: the solution to $(\mathrm{S})_\varepsilon$

Proposition 2 (Existence of optimal controls) (cf. [Antil, K., Nakayashiki, Shirakawa, Yamazaki](2020–))

Under (A0)–(A4),

The problem $(\mathrm{OP})_\varepsilon$ admits at least one optimal control $[u^*, v^*] \in [\mathscr{H}]^2$

Proposition 3 (Necessary condition for (OP)$_\varepsilon$) (cf. [Antil, K., Nakayashiki, Shirakawa, Yamazaki](2020–))

Under (A0)–(A4), and let $[u^*, v^*] \in [\mathscr{H}]^2$ be the optimal control for (OP)$_\varepsilon$. Then, it holds that:

$$M_u p^* + a_u u^* = 0, \ M_v z^* + a_v v^* = 0 \ \text{ in } \ \mathscr{H}$$

In the context, $[\eta^*, \theta^*] := \mathcal{S}_\varepsilon[u^*, v^*]$ and $[p^*, z^*] \in [\mathscr{H}]^2$ is a unique solution of the following adjoint system (A)$_\varepsilon$:

(A)$_\varepsilon$

$$\begin{cases} -\partial_t p^* - \partial_x^2 p^* + \big(g'(\eta^*) + \alpha''(\eta^*) f_\varepsilon(\partial_x \theta^*)\big) p^* + \alpha'(\eta^*) f'_\varepsilon(\partial_x \theta^*) \partial_x z^* = M_\eta(\eta^* - \eta_{\mathrm{ad}}) \ \text{ in } Q, \\ -\partial_t(\alpha_0 z^*) - \partial_x\big(\alpha(\eta^*) f''_\varepsilon(\partial_x \theta^*) \partial_x z^* + \nu^2 \partial_x z^* + \alpha'(\eta^*) f'_\varepsilon(\partial_x \theta^*) p^*\big) = M_\theta(\theta^* - \theta_{\mathrm{ad}}) \ \text{ in } Q, \\ \partial_x p^* = z^* = 0 \ \text{ in } \Sigma, \\ p^*(T, x) = z^*(T, x) = 0, \ x \in \Omega \end{cases}$$

Keypoint:

- This linear system corresponds to the adjoint of the linearized state system, and the coefficients and forcing terms are given by using the solution to the state system