A constrained gradient system associated with 3D grain boundary motion

Hiroshi Watanabe

Faculty of Science and Technology, Oita University

Joint Work: Salvador Moll (Universitat de Valéncia)
Ken Shirakawa (Chiba University)

The 81th Fujihara seminar
Mathematical Aspects for Interfaces and Free Boundaries

Hilton Niseko Village, JAPAN
4/6/2024

Phase-field model of grain boundary (2D case)

Situation:

In a time-interval $(0,\infty)$, a spatial domain $\Omega \subset \mathbb{R}^2$ is occupied by a polycrystal (e.g. Ceramics).

Target:

The movement of grain boundaries.

Mathematical model

Kobayashi-Warren-Carter (2000) Phisica D

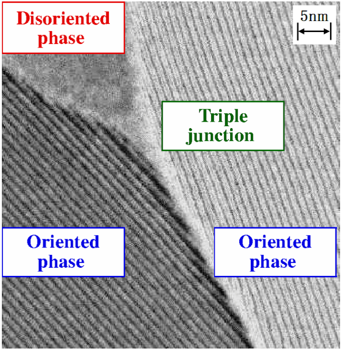
System of parabolic equations in $Q := (0,\infty) \times \Omega$

- $\eta = \eta(t,x)$, $(t,x) \in \Omega_T$, : orientation order,

$$0 \le \eta \le 1, \begin{cases} \eta = 1 \cdots \text{oriented}, \\ \eta = 0 \cdots \text{disoriented}. \end{cases}$$

- $\theta = \theta(t,x)$, $(t,x) \in Q$, : orientation angle.
- $\vec{v} = \begin{pmatrix} \eta \cos\theta \\ \eta \sin\theta \end{pmatrix}$: mean orientation in Q.

Micrograpf (Si_3N_4)
UBE Scientific Analysis Laboratory
http://www.ube-ind.co.jp/usal/



Phase-field model of grain boundary (2D case)

Situation:

In a time-interval $(0, \infty)$, a spatial domain $\Omega \subset \mathbb{R}^2$ is occupied by a polycrystal (e.g. Ceramics).

Target:

The movement of grain boundaries.

Mathematical model

Kobayashi-Warren-Carter (2000) Phisica D

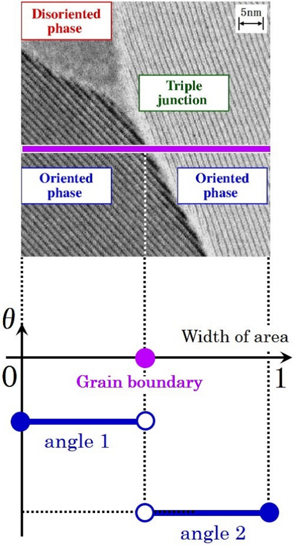
System of parabolic equations in $Q := (0, \infty) \times \Omega$

- $\eta = \eta(t, x)$, $(t, x) \in \Omega_T$, : orientation order,

$$0 \leq \eta \leq 1, \begin{cases} \eta = 1 \cdots \text{oriented}, \\ \eta = 0 \cdots \text{disoriented}. \end{cases}$$

- $\theta = \theta(t, x)$, $(t, x) \in Q$, : orientation angle.
- $\vec{v} = \begin{pmatrix} \eta \cos\theta \\ \eta \sin\theta \end{pmatrix}$: mean orientation in Q.

Micrograpf (Si_3N_4)
UBE Scientific Analysis Laboratory
http://www.ube-ind.co.jp/usal/



Derivation of the 2D model

Gradient flow of the free-energy

$$(\eta,\theta) \mapsto \mathscr{F}(\eta,\theta) := \frac{1}{2}\int_\Omega |\nabla\eta|^2\,dx + \int_\Omega G(\eta)\,dx + \Phi(\eta,\theta),$$

$$\Phi(\eta,\theta) := \int_\Omega \alpha(\eta)|\nabla\theta|\,dx, \qquad : \text{Interfacial energy}$$

$$D(\mathscr{F}) = H^1(\Omega) \times BV(\Omega) \cap L^2(\Omega).$$

- $\alpha : \mathbb{R} \longrightarrow (0,\infty)$: given function (mobility).

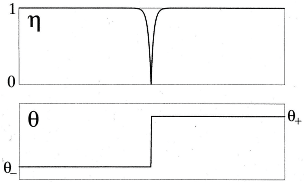
Kobayashi-Warren-Carter system:

$$\begin{cases} -\begin{bmatrix} \eta_t \\ \alpha_0(\eta)\theta_t \end{bmatrix} = \nabla_{(\eta,\theta)}\mathscr{F}(\eta,\theta) \quad \text{in } Q. \\ \text{(B.C.)} + \text{(I.C.)} \end{cases}$$

- $\alpha_0 : \mathbb{R} \longrightarrow (0,\infty)$: given function (mobility).

$$\alpha_0(\eta) = \alpha(\eta) := \frac{\eta^2}{2} + \delta_0, \quad \forall \eta \in \mathbb{R}, \text{ with } \delta_0 > 0.$$

Structural observation for sol.



[Kobayashi-Warren-Carter](2000)

$$G(\eta) = \frac{1}{2}(\eta-1)^2, \quad \forall \eta \in \mathbb{R}.$$

Free energy

$$\mathcal{F}_2(\eta,\theta) := \frac{1}{2}\int_\Omega |\nabla\eta|^2\,dx + \int_\Omega G(\eta)\,dx + \int_\Omega \alpha(\eta)|\nabla\theta|\,dx + \frac{\kappa^2}{2}\int_\Omega |\nabla\theta|^2\,dx \in [0,\infty].$$

orientations, misorieatations in 3D ($|\nabla\theta|$: the misorientation on a short scale)

1. Kobayashi–Warren (2005): dynamics of polycrystals, $|\nabla\theta| \sim |\nabla P|$, $(P \in SO(3))$
2. Pusztai et.al. (2005): polycrystalline solidification, $|\nabla\theta| \sim |\nabla q|$, $(q \in \mathbb{S}^3 \subset \mathbb{R}^4)$

Energy functional

$$[\eta,\mathbf{u}] \in L^2(\Omega)\times L^2(\Omega;\mathbb{R}^M) \mapsto \mathcal{F}(\eta,\mathbf{u})$$

$$:= \begin{cases} \frac{1}{2}\int_\Omega |\nabla\eta|^2\,dx + \int_\Omega G(\eta)\,dx + \int_\Omega \alpha(\eta)|\nabla\mathbf{u}|\,dx + \frac{\kappa^2}{2}\int_\Omega |\nabla\mathbf{u}|^2\,dx, \\ \qquad \text{if } \eta \in H^1(\Omega) \text{ and } \mathbf{u} \in H^1(\Omega;\mathbb{R}^M), \\ +\infty, \quad \text{otherwise.} \end{cases}$$

Constrained L^2-gradient flow

$$\frac{\partial\mathbf{u}}{\partial t} \in -\pi_{\mathbf{u}}\left(\frac{\delta\mathcal{F}}{\delta\mathbf{u}}(\eta,\mathbf{u})\right)$$

- $\mathbf{u} \in \mathbb{S}^{M-1}$: constraint condition
- $\pi_{\mathbf{u}} : \mathbb{R}^M \to T_{\mathbf{u}}\mathbb{S}^{M-1}$: orthogonal projection
- $T_{\mathbf{u}}\mathbb{S}^{M-1}$: tangent plane of $\mathbb{S}^{M-1}$ at $\mathbf{u} \in \mathbb{S}^{M-1}$

$\mathbb{S}^3_+ \leftarrow$ (uniquely identification using the quaternion representation) $\rightarrow$ $SO(3)$

Problem

3D model (P) $\kappa > 0$

$$\begin{cases} \partial_t \eta - \Delta\eta + g(\eta) + \alpha'(\eta)|\nabla \mathbf{u}| = 0 \text{ in } Q := (0,\infty)\times\Omega, \\ \nabla\eta\cdot\mathbf{n}_\Gamma = 0 \text{ on } \Sigma := (0,\infty)\times\partial\Omega, \\ \eta(0,x) = \eta_0(x),\ x\in\Omega; \end{cases}$$

$$\begin{cases} \partial_t \mathbf{u} - \mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\mathbf{u}}{|\nabla\mathbf{u}|} + \kappa^2\nabla\mathbf{u}\right) = \left(\alpha(\eta)|\nabla\mathbf{u}| + \kappa^2|\nabla\mathbf{u}|^2\right)\mathbf{u} \text{ in } Q, \\ \left(\alpha(\eta)\dfrac{\nabla\mathbf{u}}{|\nabla\mathbf{u}|} + \kappa^2\nabla\mathbf{u}\right)\mathbf{n}_\Gamma = 0 \text{ on } \Sigma, \\ \mathbf{u}(0,x) = \mathbf{u}_0(x),\ x\in\Omega. \end{cases}$$

- $\Omega \subset \mathbb{R}^N$: bounded domain $(1 < N \in \mathbb{N})$
- $\Gamma := \partial\Omega$: Lipschitz boundary
- $\mathbf{n}_\Gamma$: unit normal vector on Γ
- $\eta(t,x) \in \mathbb{R}$
- $\mathbf{u}(t,x) \in \mathbb{S}^{M-1}$ $(1 < M \in \mathbb{N})$

Representation of projection

$$-\pi_{\mathbf{u}}(\partial_{\mathbf{u}}\Phi(\eta,\mathbf{u})) \qquad \left(\Phi(\eta,\mathbf{u}) = \int_\Omega \alpha(\eta)|\nabla\mathbf{u}|dx\right)$$

$$= \mathrm{div}\left(\alpha(\eta)\frac{\nabla\mathbf{u}}{|\nabla\mathbf{u}|}\right) + \alpha(\eta)|\nabla\mathbf{u}|\mathbf{u}.$$

$$\forall\ \mathbf{w}\in\mathbb{R}^M;\ \pi_{\mathbf{u}}(\mathbf{w}) = \mathbf{w} - (\mathbf{w}\cdot\mathbf{u})\mathbf{u}$$

$\mathfrak{X} := L^2(\Omega) \times L^2(\Omega; \mathbb{R}^M)$, $\mathfrak{W} := H^1(\Omega) \times H^1(\Omega; \mathbb{R}^M)$

Definition (solution)

A pair of functions $U := [\eta, \mathbf{u}] \in L^2_{loc}([0, \infty); \mathfrak{X})$ is called a solution to the system (P), if

$$U = [\eta, \mathbf{u}] \in W^{1,2}_{loc}([0, \infty); \mathfrak{X}) \cap L^\infty_{loc}(0, \infty; \mathfrak{W}), \quad 0 \le \eta \le 1 \text{ and } \mathbf{u} \in \mathbb{S}^{M-1}, \text{ a.e. in } Q,$$

$$\big(\partial_t \eta(t) + g(\eta(t)) + \alpha'(\eta(t))|\nabla \mathbf{u}(t)|, \varphi\big)_{L^2(\Omega)} + \big(\nabla \eta(t), \nabla \varphi\big)_{L^2(\Omega)} = 0,$$

for any $\varphi \in H^1(\Omega)$, a.e. $t > 0$, subject to $\eta(0) = \eta_0$ in $L^2(\Omega)$,

and there exist functions $\mathcal{B} \in L^\infty(Q; \mathbb{R}^{MN})$ and $\mu \in L^1_{loc}([0, \infty); L^1(\Omega))$, such that

$$\mathcal{B} \in \mathrm{Sgn}^{M,N}(\nabla \mathbf{u}) \text{ in } \mathbb{R}^{MN}, \quad \mu := (\alpha(\eta)\mathcal{B} + \kappa^2 \nabla \mathbf{u}) : \nabla \mathbf{u}, \text{ a.e. in } Q,$$

$$\int_\Omega \partial_t \mathbf{u}(t) \cdot \boldsymbol{\psi} \, dx + \int_\Omega (\alpha(\eta(t))\mathcal{B}(t) + \kappa^2 \nabla \mathbf{u}(t)) : \nabla \boldsymbol{\psi} \, dx = \int_\Omega \mu(t) \mathbf{u}(t) \cdot \boldsymbol{\psi} \, dx,$$

for any $\boldsymbol{\psi} \in C^1(\overline{\Omega}; \mathbb{R}^M)$, a.e. $t > 0$, subject to $\mathbf{u}(0) = \mathbf{u}_0$ in $L^2(\Omega; \mathbb{R}^M)$,

Here, $\mathrm{Sgn}^{M,N} : \mathbb{R}^{MN} \to 2^{\mathbb{R}^{MN}}$ is the subdifferential of the Euclidian norm in $\mathbb{R}^{MN}$, $:$ is the inner product for $M \times N$ matrices.

Assumptions and Main Theorems

(A1) $g \in C^1(\mathbb{R})$ is a fixed Lipschitz function with a potential $0 \leq G \in C^2(\mathbb{R})$, i.e. $G'(s) = \frac{d}{ds}G(s) = g(s)$ on $\mathbb{R}$, satisfying $g(0) \leq 0, \ \ g(1) \geq 0$.

(A2) $0 < \alpha \in C^2(\mathbb{R})$ is such that

- $\alpha'(0) = 0, \quad \alpha'' \geqq 0$ on $\mathbb{R}$ and α and $\alpha\alpha'$ are Lipschitz continuous on $\mathbb{R}$.
- $\alpha^* := \inf \alpha(\mathbb{R}) > 0$.

(A3) $U_0 := [\eta_0, \mathbf{u}_0] \in L^\infty(\Omega) \times L^2(\Omega; \mathbb{R}^m) \cap \mathfrak{W}$ is a fixed pair of initial data satisfying

$$0 \leq \eta_0 \leq 1, \quad \mathbf{u}_0 \in \mathbb{S}^{M-1} \quad \text{a.e. in } \Omega$$

Summary of Main Theorems

(I) Existence of time-global solutions, invariance principle for $\mathbf{u}$

(II) ω-limit set is nonempty, any ω-limit points $[\eta^\infty, \mathbf{u}^\infty]$ are solutions to a stationary problem of (P)

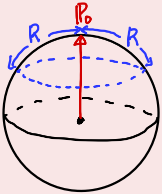
(III) For a small $\mathbf{u}_0$ in some sense, solutions $\mathbf{u}$ become constant vectors in finite time.

Global Existence of solutions, invariance principle

Main Theorem I (Moll–Shirakawa–W., submitted)

Let $U_0 = [\eta_0, \mathbf{u}_0] \in \mathfrak{W}$ with $0 \leq \eta_0 \leq 1$, $\mathbf{u}_0 \in \mathbb{S}^{M-1}$ a.e. in Ω. Then, the system (P) admits at least one solution $U = [\eta, \mathbf{u}] \in L^2_{loc}([0,\infty); \mathfrak{X})$, such that

$$\mathcal{F}(U(s)) + \int_0^T \|\partial_t U(t)\|^2_{\mathfrak{X}} dt \leq \mathcal{F}(U_0), \quad \text{for all } T > 0.$$



Also, concerning the function $\mathcal{B} \in L^\infty(Q; \mathbb{R}^{MN})$, it holds that

$$\begin{cases} \operatorname{div}\big(\alpha(\eta)\mathcal{B} + \kappa^2 \nabla \mathbf{u}\big) \in L^2_{\mathrm{loc}}([0,\infty); L^1(\Omega; \mathbb{R}^M)), \\ \operatorname{div}\big(\alpha(\eta)\mathcal{B} + \kappa^2 \nabla \mathbf{u}\big) \wedge \mathbf{u} \in L^2_{\mathrm{loc}}([0,\infty); L^2(\Omega; \Lambda_2(\mathbb{R}^M))). \end{cases}$$

Moreover, if

$$\exists\ \mathbf{p}_0 \in \mathbb{S}^{M-1} \ \text{ s.t. } \ \mathbf{u}_0 \in \overline{B_g(\mathbf{p}_0; R)} \text{ with } R \in \left(0, \frac{\pi}{2}\right),$$

then

$$\mathbf{u} \in \overline{B_g(\mathbf{p}_0; R)}, \quad \text{a.e. in } \Omega, \quad \text{for all } t \in [0, \infty).$$

- $B_g(\mathbf{p}_0; R)$: the open ball on $\mathbb{S}^{M-1}$ centered at $\mathbf{p}_0$ with radius R.

Large time behavior I

$$\omega(U) := \left\{ \bar{U} = [\bar{\eta}, \bar{\mathbf{u}}] \in \mathfrak{W} \;\middle|\; \begin{array}{l} \exists\ \{t_n\}_{n=1}^{\infty} \subset (0,\infty), \text{ s.t. } t_n \uparrow \infty, \text{ and } U(t_n) = \\ {[\eta(t_n), \mathbf{u}(t_n)]} \to \bar{U} = [\bar{\eta}, \bar{\mathbf{u}}] \text{ in } \mathfrak{X}, \text{ as } n \to \infty. \end{array} \right\}.$$

Main Theorem II

The ω-limit set $\omega(U)$ is nonempty and compact in $\mathfrak{X}$, and moreover, any *ω-limit point* $U^\infty = [\eta^\infty, \mathbf{u}^\infty] \in \omega$ solves the following variational system:

$$\big(g(\eta^\infty) + \alpha'(\eta^\infty)|\nabla \mathbf{u}^\infty|, \varphi\big)_H + \big(\nabla \eta^\infty, \nabla \varphi\big)_H = 0, \text{ for any } \varphi \in V;$$

$$\int_\Omega (\alpha(\eta^\infty)\mathcal{B}^\infty + \kappa^2 \nabla \mathbf{u}^\infty) : \nabla \boldsymbol{\psi}\, dx = \int_\Omega \mu^\infty \mathbf{u}^\infty \cdot \boldsymbol{\psi}\, dx, \text{ for any } \boldsymbol{\psi} \in C^1(\overline{\Omega}; \mathbb{R}^M),$$

with $\mathcal{B}^\infty \in L^\infty(\Omega; \mathbb{R}^{MN})$ and $\mu^\infty \in L^1(\Omega)$, fulfilling

$$\begin{cases} \mathcal{B}^\infty \in \mathrm{Sgn}^{M,N}(\nabla \mathbf{u}^\infty) \text{ in } \mathbb{R}^{MN}, \\ \mu^\infty := (\alpha(\eta)\mathcal{B}^\infty + \kappa^2 \nabla \mathbf{u}^\infty) : \nabla \mathbf{u}^\infty, \end{cases} \quad \text{a.e. in } \Omega.$$

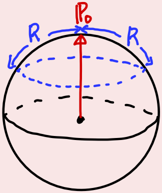
$$\mathcal{F}(U(s)) + \int_0^T \|\partial_t U(t)\|_{\mathfrak{X}}^2 dt \le \mathcal{F}(U_0), \quad \text{for all } T > 0.$$

Large time behavior II

Main Theorem III

In addition to the assumptions as in Main Theorem I, we assume that

$$\exists\ \mathbf{p}_0 \in \mathbb{S}^{M-1} \text{ s.t. } \mathbf{u}_0 \in \overline{B_g(\mathbf{p}_0; R)}, \text{ with } 0 \le R < \frac{\pi}{4}.$$



Then, it holds that, there exists $T^* \in [0, +\infty)$ such that

$$\int_\Omega \mathrm{dist}_g(\mathbf{u}(t,x), \mathbf{p}_c(t))^2\, dx \to 0, \text{ as } t \uparrow T^*,$$

where $\mathbf{p}_c(t)$ is the Barycenter of $\mu := \mathbf{u}(t)\sharp\mathcal{L}^N$, i.e. the minimizer of

$$\mathbf{p} \in \mathbb{S}^{M-1} \mapsto \Psi_\mu(\mathbf{p}) := \frac{1}{2}\int_{\mathbb{S}^{M-1}} \mathrm{dist}_g(\cdot, \mathbf{p})^2 d\mu = \frac{1}{2}\int_\Omega \mathrm{dist}_g(\mathbf{u}(t,x), \mathbf{p})^2 dx.$$

- $B_g(\mathbf{p}_0; R)$: the open ball on $\mathbb{S}^{M-1}$ centered at $\mathbf{p}_0$ with radius R.
- $\mathrm{dist}_g(\mathbf{u}(t,x), \mathbf{p}_c(t))$: the geodesic distance on the sphere from $\mathbf{u}(t,x)$ to $\mathbf{p}_c(t)$.
- $\mu := \mathbf{u}(t)\sharp\mathcal{L}^N$: the push-forward measure
- μ: any Radon measure on $\overline{B_g(\mathbf{p}_0, R)}$ for $R < \frac{\pi}{2}$; $\exists_!\ \mathbf{p}_c(t)$: barycenter [B. Afsari, Proc. Amer. Math. Soc., (2011)]

Approximating problems

Approximating problems $(\mathrm{P})^{\kappa}_{\varepsilon,\nu,\delta}$

$$\begin{cases} \partial_t \eta - \Delta \eta + g(\eta) + \alpha'(\eta)\gamma_\varepsilon(\nabla \mathbf{u}) = 0, \text{ in } Q, \\ \nabla \eta \cdot \mathbf{n}_\Gamma = 0 \text{ on } \Sigma, \\ \eta(0,x) = \eta_0(x), \ x \in \Omega; \end{cases}$$

$$\begin{cases} \partial_t \mathbf{u} - \mathrm{div}\bigl(\alpha(\eta)\partial\gamma_\varepsilon(\nabla \mathbf{u}) + \kappa^2 \nabla \mathbf{u} + \nu|\nu\nabla \mathbf{u}|^{N-1}\nu\nabla \mathbf{u}\bigr) + \varpi_\delta(\mathbf{u}) \ni \mathbf{0} \text{ in } Q, \\ \bigl(\alpha(\eta)\partial\gamma_\varepsilon(\nabla \mathbf{u}) + \kappa^2 \nabla \mathbf{u} + \nu|\nu\nabla \mathbf{u}|^{N-1}\nu\nabla \mathbf{u}\bigr)\mathbf{n}_\Gamma \ni \mathbf{0} \text{ on } \Sigma, \\ \mathbf{u}(0,x) = \mathbf{u}_0(x), \ x \in \Omega; \quad (\nu \mathbf{u}_0 \in W^{1,N+1}(\Omega;\mathbb{R}^M)) \end{cases}$$

(A5) For any $\varepsilon \geq 0$, $\gamma_\varepsilon : \mathbb{R}^{MN} \longrightarrow [0,\infty)$ is a continuous convex function, defined as

$$\gamma_\varepsilon : W = \bigl[w_k^\ell\bigr]_{\substack{1 \leq \ell \leq M \\ 1 \leq k \leq N}} \in \mathbb{R}^{MN} \mapsto \gamma_\varepsilon(W) := \sqrt{\varepsilon^2 + |W|^2} \in \mathbb{R}.$$

(A6) For any $\delta > 0$, $\Pi_\delta \in C^2(\mathbb{R}^M)$ is the following function:

$$\Pi_\delta : \mathbf{w} \in \mathbb{R}^M \mapsto \Pi_\delta(\mathbf{w}) := \frac{1}{4\delta}(|\mathbf{w}|^2 - 1)^2 \in \mathbb{R}.$$

We let $\varpi_\delta \in C^1(\mathbb{R}^M;\mathbb{R}^M)$ be the gradient of Π_δ, i.e.:

$$\varpi_\delta : \mathbf{w} \in \mathbb{R}^M \mapsto \varpi_\delta(\mathbf{w}) := \nabla \Pi_\delta(\mathbf{w}) = \frac{1}{\delta}\bigl(|\mathbf{w}|^2 - 1\bigr)\mathbf{w} \in \mathbb{R}^M.$$

Outline of Proof (1/2)

Ref: Barrett–Feng–Prohl

1. Well-posedness of $(\mathrm{P})^{\kappa}_{\varepsilon,\nu,\delta}$: theory of subdifferential, Mosco conv. $(\mathbf{u}_{\varepsilon,\nu,\delta} \in \mathbb{R}^M)$
2. Properties of approximating sol. $(\eta_{\varepsilon,\nu,\delta}, \mathbf{u}_{\varepsilon,\nu,\delta})$
   - Energy inequality $\quad ((\because)$ (1st-eq) $\times\, \partial_t \eta_{\varepsilon,\nu,\delta} +$ (2nd-eq) $\cdot\, \partial_t \mathbf{u}_{\varepsilon,\nu,\delta})$
   - $|\mathbf{u}_0| \leq 1$ a.e. in $\Omega \implies |\mathbf{u}_{\varepsilon,\nu,\delta}| \leq 1$ a.e. in Ω $\quad (\varpi_\delta = (1/\delta)(|\mathbf{w}|^2 - 1)\mathbf{w})$

     $(\because)$ (2nd-eq) $\cdot\, \mathbf{u}_{\varepsilon,\nu,\delta}\chi(|\mathbf{u}_{\varepsilon,\nu,\delta}|)$, $\chi(z) := \frac{(z-1)_+}{z}$
3. $\delta \to 0$
   - Energy inequality, $|\mathbf{u}_{\varepsilon,\nu,\delta}| \leq 1 \implies$ conv. of app. sol. $(\mathbf{u}_{\varepsilon,\nu} \in \mathbb{S}^{M-1})$

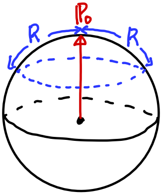
     $(\because)$ $\mathcal{F}_{\varepsilon,\nu,\delta}(U_0) = \mathcal{F}_{\varepsilon,\nu}(U_0) =: C < +\infty$. $(\because\ \mathbf{u}_0 \in \mathbb{S}^{M-1} \implies \Pi_\delta(\mathbf{u}_0) = 0)$
   - $\nabla \mathbf{u}_{\varepsilon,\nu,\delta} \to \nabla \mathbf{u}_{\varepsilon,\nu}$ in $L^q_{loc}(0,\infty; L^q(\Omega;\mathbb{R}^{MN}))$ for $\forall q \in [1,2)$

     : Compactness theorem (ref. Chen–Hong–Hungerbühler)
   - Characterization of limit functions: wedge product, theory of multi-vector

Outline of Proof (Main Theorem I) (2/2)

4. Convergence of approximating sol. $\nu \to 0$
   - Range constraint in $\overline{B_g(\mathbf{p}_0; R)}$ with $R \in \left(0, \frac{\pi}{2}\right)$

     : Invariance principle (ref. Giacomelli–Łasica–Moll [3])
   - Others are the same as $\delta \to 0$.
5. Convergence of approximating sol. $\varepsilon \to 0$: same as $\nu \to 0$



Theorem (Invariance principle)

If

$$\exists\, \mathbf{p}_0 \in \mathbb{S}^{M-1} \ \text{ s.t. } \ \mathbf{u}_0 \in \overline{B_g(\mathbf{p}_0; R)} \text{ with } R \in \left(0, \frac{\pi}{2}\right),$$

then

$$\mathbf{u} \in \overline{B_g(\mathbf{p}_0; R)}, \quad \text{a.e. in } \Omega, \quad \text{for all } t \in [0, \infty).$$

$(\because)$ Proof by contradiction. $(\mathbf{u} = \mathbf{u}_{\varepsilon,\nu})$

$$\exists\, T^* := \inf\{t \in [0, T) \ ; \ \mathbf{u}(t, \Omega) \not\subset \overline{B_g(\mathbf{p}_0; R)}\}.$$

Due to the continuity of $\mathbf{u}$,

$$\exists\, \delta > 0 \ \text{ s.t. } \ \mathbf{u}(t, \Omega) \subset B_g(\mathbf{p}_0; \frac{\pi}{2}) \quad \text{for } t \in [0, T^* + \delta).$$

Invariance Principle (1/2)

$\mathbf{p} \mapsto (p^r; p^{\theta_1}, \ldots, p^{\theta_{M-2}})$: a polar coordinate system centered at $\mathbf{p}_0$ on $B_g(\mathbf{p}_0; \frac{\pi}{2})$

Eells-Sampson (1964)

$$\pi_{\mathbf{u}}(\mathrm{div} Z)^i = \mathrm{div}\mathbf{Z}^i + \sum_{j,k,\ell} \Gamma^i_{j,k}(\mathbf{u})\mathbf{u}^j_{x^\ell}\mathbf{Z}^k_\ell\,,\ i = r, \theta_1, \ldots, \theta_{M-2}\,,$$

for any $Z \in W^{1,1}(\Omega; \mathbb{R}^{MN})$ such that $Z \in T_{\mathbf{u}}(\mathbb{S}^{M-1})$.

We take

$$Z := \alpha(\eta_{\varepsilon,\nu})\,[\nabla f_\varepsilon](\nabla \mathbf{u}_{\varepsilon,\nu}) + \kappa^2 \nabla \mathbf{u}_{\varepsilon,\nu} + \nu|\nu\nabla \mathbf{u}_{\varepsilon,\nu}|^{N-1}\nu\nabla \mathbf{u}_{\varepsilon,\nu}.$$

The Christoffel symbols of the 2nd kind for r:

$$\Gamma^r = -\frac{\sin(2r)}{2}\begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & \sin^2(\theta_1) & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \ldots & \sin^2(\theta_1)\cdot\ldots\cdot\sin^2(\theta_{M-3}) \end{pmatrix}.$$

Invariance Principle (2/2)

$$u_t^r = \mathrm{div}\mathbf{Z}^r - \frac{\sin 2u^r}{2}\left(\frac{\alpha(\eta)}{\sqrt{\varepsilon^2+|\nabla\mathbf{u}|^2}} + \kappa^2 + \nu^{N+1}|\nabla\mathbf{u}|^{N-1}\right)\times$$

$$\times\left(|\nabla u^{\theta_1}|^2 + \sum_{i=1}^{M-3}\sin^2(u^{\theta_1})\cdot\ldots\cdot\sin^2(u^{\theta_i})|\nabla u^{\theta_{i+1}}|^2\right)$$

$$\leq \mathrm{div}\mathbf{Z}^r. \quad \left(\because \quad u^r \in \left[0, \frac{\pi}{2}\right]\right)$$

Thus,

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (u^r - R)_+^2 = \int_\Omega u_t^r (u^r - R)_+ \leq \int_\Omega \mathrm{div}\mathbf{Z}^r (u^r - R)_+$$

$$= -\int_{\Omega\cap\{u^r>R\}} \mathbf{Z}^r : \nabla u^r$$

$$= -\int_{\Omega\cap\{u^r>R\}} |\nabla u^r|^2 \left(\frac{\alpha(\eta)}{\sqrt{\varepsilon^2+|\nabla\mathbf{u}|^2}} + \kappa^2 + \nu^{N+1}|\nabla\mathbf{u}|^{N-1}\right) \leq 0.$$

Outline of proof (Main Theorem II)

Tools: the method for 2D-model + wedge product

$\mathbf{u}_n := \mathbf{u}(s_n + \cdot),\ \eta_n := \eta(s_n + \cdot),\ s_n \to \infty\ (n \to \infty)$

1. Convergence of solutions ($n \to \infty$): definitions of sol., energy ineq.
   - $\begin{cases} \mathbf{u}_n \to \mathbf{u}^\infty & \text{in } C([0,1];L^2(\Omega)) \text{ and weakly in } L^\infty(0,1;H^1(\Omega;\mathbb{R}^M)) \\ \partial_t \mathbf{u}_n \to 0 & \text{in } L^2(0,1;L^2(\Omega;\mathbb{R}^M)) \end{cases}$
   - $\begin{cases} \eta_n \to \eta^\infty & \text{in } C([0,1];L^2(\Omega)) \text{ and weakly in } L^\infty(0,1;H^1(\Omega)) \\ \partial_t \eta_n \to 0 & \text{in } L^2(0,1;L^2(\Omega)) \end{cases}$
2. Convergence of $\nabla \mathbf{u}$
   - $\nabla \mathbf{u}_n \to \nabla \mathbf{u}^\infty$ strongly in $L^1(0,1;L^1(\Omega;\mathbb{R}^M))$
3. Characterization of limit functions: wedge product ($\wedge \mathbf{u}_n$)

$$\partial_t \mathbf{u}_n - \mathrm{div}(\alpha(\eta_n)\mathcal{B}_n + k^2 \nabla \mathbf{u}_n) = (\mu_n - \mathbf{f}_n \cdot \mathbf{u}_n)\mathbf{u}_n + \mathbf{f}_n.$$

$$\Downarrow$$

$$-\mathrm{div}(\alpha(\eta^\infty)\mathcal{B}^\infty + \kappa^2 \nabla \mathbf{u}^\infty) - ((\alpha(\eta^\infty)\mathcal{B}^\infty + \kappa^2 \nabla \mathbf{u}^\infty) : \nabla \mathbf{u}^\infty)\mathbf{u}^\infty$$
$$= -(\mathbf{f}^\infty \cdot \mathbf{u}^\infty)\mathbf{u}^\infty + \mathbf{f}^\infty$$

Outline of proof (Main Theorem III)

Ref: Giacomelli–Łasica–Moll

1. Range constraint for solutions:

$$\mathbf{u}_0 \in \overline{B_g(\mathbf{p_0}, R)} \quad (R \in (0, \tfrac{\pi}{4})) \implies \mathbf{u}(\mathbf{t}) \in \overline{B_g(\mathbf{p}_c(t), 2R)}, \text{ a.e. in } \Omega$$

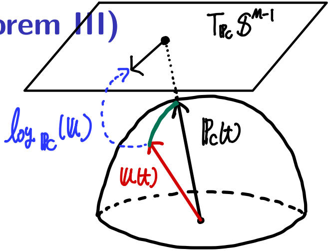
2. Geometric representation of equation:

$(u^r, u^{\theta_1}, \dots, u^{\theta_{M-2}})$: polar coordinates centered at $\mathbf{p}_c(t)$

$$\begin{aligned} u^r_t =& \mathrm{div}\mathbf{Z}^r - \alpha(\eta)\frac{\sin 2u^r}{2}\left(\mathcal{B}^{\theta_1}\cdot\nabla u^{\theta_1} + \sum_{i=1}^{M-3}\sin^2(u^{\theta_1})\cdot\ldots\cdot\sin^2(u^{\theta_i})\mathcal{B}^{\theta_{i+1}}\cdot\nabla u^{\theta_{i+1}}\right) \\ &- \kappa^2\frac{\sin 2u^r}{2}\left(|\nabla u^{\theta_1}|^2 + \sum_{i=1}^{M-3}\sin^2(u^{\theta_1})\cdot\ldots\cdot\sin^2(u^{\theta_i})|\nabla u^{\theta_{i+1}}|^2\right) \\ \le& \mathrm{div}\mathbf{Z}^r - \alpha^*\frac{\sin(2u^r)}{2}\left(\mathcal{B}^{\theta_1}\cdot\nabla u^{\theta_1} + \sum_{i=1}^{M-3}\sin^2(u^{\theta_1})\cdot\ldots\cdot\sin^2(u^{\theta_i})\mathcal{B}^{\theta_{i+1}}\cdot\nabla u^{\theta_{i+1}}\right). \end{aligned}$$

- $\mathbf{Z}^r := \alpha(\eta)\mathcal{B}^r + \kappa^2\nabla u^r$
- $\tilde{B}^\theta := \mathcal{B}^{\theta_1}\cdot\nabla u^{\theta_1} + \sum_{i=1}^{M-3}\sin^2(u^{\theta_1})\cdot\ldots\cdot\sin^2(u^{\theta_i})\mathcal{B}^{\theta_{i+1}}\cdot\nabla u^{\theta_{i+1}}$

Outline of proof (Main Theorem III)



3. Computation for $\Psi_{\mu(t)}(\mathbf{p}_c(t))$

$$
\begin{aligned}
\frac{d}{dt}\Psi_{\mu(t)}(\mathbf{p}_c(t)) &= \frac{1}{2}\frac{d}{dt}\int_\Omega \mathrm{dist}_g(\mathbf{u}(t,x),\mathbf{p}_c(t))^2 dx \\
&= \frac{1}{2}\frac{d}{dt}\int_\Omega u^r(t,x)^2 dx \\
&\le -\alpha^*\int_\Omega \left(\mathcal{B}^r\cdot\nabla u^r + \frac{u^r\sin(2u^r)}{2}\tilde{B}^\theta\right) \\
&\le -\alpha^*\int_\Omega \left(\mathcal{B}^r\cdot\nabla u^r + \cos u^r\sin^2(u^r)\tilde{B}^\theta\right) \\
&\le -\alpha^*\cos(2R)\int_\Omega \left(\mathcal{B}^r\cdot\nabla u^r + \sin^2(u^r)\tilde{B}^\theta\right) \\
&= -\alpha^*\cos(2R)\int_\Omega |D\mathbf{u}|_g \\
&\le -C(\alpha^*,R,N,\Omega)\|u^r\|_{L^{\frac{N}{N-1}}} \\
&\le -(2R)^{\frac{N-2}{N}}C(\alpha^*,R,N,\Omega)(\Psi_{\mu(t)}(\mathbf{p}_c(t)))^{\frac{N-1}{N}}.
\end{aligned}
$$

Hence,

$$
\Psi_{\mu(t)}(\mathbf{p}_c(t)) \le \left(\Psi_{\mu(0)}(\mathbf{p}_c(0))^{\frac{1}{N}} - \frac{\tilde{C}}{N}t\right)_+^N.
$$

$$
u^r_t \le \mathrm{div}\mathbf{Z}^r - \alpha^*\frac{\sin(2u^r)}{2}\tilde{B}^\theta
$$

$\mathbf{u}(\mathbf{t}) \in \overline{B_g(\mathbf{p}_c(t),2R)}$, a.e. in Ω

$$
\begin{aligned}
\|u^r\|_{L^{\frac{N}{N-1}}} &= \|\log_{\mathbf{p}_c}(\mathbf{u})\|_{L^{\frac{N}{N-1}}} \\
&\le C(R,N,\Omega)\int_\Omega |D\log_{\mathbf{p}_c}\mathbf{u}| \\
&\le C(R,N,\Omega)\frac{u^r}{\sin u^r}\int_\Omega |D\mathbf{u}|_g
\end{aligned}
$$

([Jost, (2017), Cor. 5.6.1])

Remark and Future works

$$
\begin{cases}
\partial_t \eta - \Delta \eta + g(\eta) + \alpha'(\eta)|\nabla \mathbf{u}| = 0 \text{ in } Q := (0,\infty)\times\Omega, \\
\partial_t \mathbf{u} - \operatorname{div}\left(\alpha(\eta)\dfrac{\nabla \mathbf{u}}{|\nabla \mathbf{u}|} + \kappa^2 \nabla \mathbf{u}\right) = \left(\alpha(\eta)|\nabla \mathbf{u}| + \kappa^2 |\nabla \mathbf{u}|^2\right)\mathbf{u} \ \text{ in } Q, \\
\nabla \eta \cdot \mathbf{n}_\Gamma = 0, \quad \left(\alpha(\eta)\dfrac{\nabla \mathbf{u}}{|\nabla \mathbf{u}|} + \kappa^2 \nabla \mathbf{u}\right)\mathbf{n}_\Gamma = 0 \text{ on } (0,\infty)\times\partial\Omega,
\end{cases}
$$

Remark

- If $M = 2$, (P) is equivalent to 2D model (without time mobility)
  $(\because)$ $\mathbf{u} = (u_1, u_2)^t = (\cos\theta, \sin\theta)^t$ (ref. Giacomelli-Mazón-Moll (2013)).
- If $M = 4$, comparison with other models (ex. Kobayashi-Warren) is open.

Related results

1. Time mobility: $\alpha_0(\eta)\partial_t \mathbf{u}$
   ($\exists$ sol., Main Theorem II: OK)
2. The invariance principle and Main Theorem III only hold for 2-D models with constant time mobility.

Future works

1. Uniqueness of sol.:
   ref. Giacomelli–Łasica–Moll [3]
2. Time discritization:
   under consideration
3. $\kappa \to 0$: challenging problem