Linearization in solid-solid phase transitions

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Joint work with Manuel Friedrich (Münster).

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The aim of the talk

Our goal 1.: to identify a model for solid-solid phase transitions which allows both for macroscopic phase transitions and for suitable compactness results in Sobolev spaces.

Our goal 2.: to prove convergence of the model in a suitable sense to an effective linearized sharp interface model.

The elastic energy

$\Omega =$ bounded domain in $\mathbb{R}^2$ with Lipschitz boundary.

Elastic energy $y \mapsto \int_\Omega W(\nabla y)\,dx$, where $W : \mathbb{M}^{3\times 3} \to [0, +\infty)$ satisfies:

H1. (Regularity) W is continuous;

H2. (Frame indifference) $W(RF) = W(F)$ for every $R \in SO(2)$ and $F \in \mathbb{M}^{2\times 2}$;

H3. (Two-well rigidity) $W(A) = W(B) = 0$, where

$$A = \mathrm{Id}, \text{ and } B = \begin{pmatrix} 1 & 0 \\ 0 & 1+\lambda \end{pmatrix}, \text{ for } \lambda > 0;$$

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Remark: after an affine change of variables one can always suppose that the two wells have the form given in H3.

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In our setting $\lambda > 0 \Rightarrow$ exactly one rank-one connection.

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$$QA - B = a \otimes \nu \text{ with } Q \in SO(2),\ a, \nu \in \mathbb{R}^2, \text{ and } |\nu| = 1$$
$$\Updownarrow$$
$$Q = \mathrm{Id},\ \nu = e_2, \text{ and } a = -\lambda e_2.$$

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$A = \mathrm{Id}$, and $B = \begin{pmatrix} 1 & 0 \\ 0 & 1+\lambda \end{pmatrix}$, for $\lambda > 0$;

H4. (Coercivity) there exists a constant $c_1 > 0$ such that

$$W(F) \geq c_1 \mathrm{dist}^2(F, SO(2)\{A,B\}) \quad \text{for every } F \in \mathbb{M}^{2\times 2};$$

H5. (Quadratic behavior around the two wells) there exists $\delta_W > 0$ such that W is of class C^2 in

$$\{F \in \mathbb{M}^{2\times 2} : \mathrm{dist}(F, SO(2)\{A,B\}) < \delta_W\}.$$

H6. (Growth conditions from above)

The theory of solid-solid phase transitions

$$E_\varepsilon^P(y) := \underbrace{\frac{1}{\varepsilon^2}\int_\Omega W(\nabla y)\,dx}_{\text{Elastic energy with a non-convex density}} + \underbrace{\int_\Omega P_\varepsilon(\nabla^2 y)\,dx}_{\text{An } \varepsilon\text{-dependent singular perturbation}}$$

The parameter ε in the expressions above is related to the size of transition layers
The first term favors deformations y whose gradient is close to the two **wells** of W, whereas the second term penalizes **transitions** between two different values of the gradient.

A sharp interface limit for solid-solid phase transitions

A standard singularly perturbed two-well problem takes the form

$$I_\varepsilon(y) := \frac{1}{\varepsilon^2}\int_\Omega W(\nabla y)\,dx + \varepsilon^2\int_\Omega |\nabla^2 y|^2\,dx$$

for every $y \in H^2(\Omega;\mathbb{R}^2)$. This corresponds to the choice

$$P_\varepsilon(G) = \varepsilon^2|G|^2 \quad \text{for} \quad G \in \mathbb{R}^{2\times 2}.$$

- S. Conti - I. Fonseca - G. Leoni (2002): Γ-convergence neglecting rotational invariance;
- S. Conti - B. Schweizer (2006): Γ-convergence via rotational invariance in the linearized setting;
- **S. Conti - B. Schweizer (2006): Γ-convergence via rotational invariance in the nonlinear setting**;
- S. Conti - B. Schweizer (2006): Γ-convergence via rotational invariance in the nonlinear setting with impenetrability constraints.

A sharp interface limit for solid-solid phase transitions

Denote by $\mathcal{Y}$ the class of admissible limiting deformations, defined as

$$\mathcal{Y} := \cup_{R \in SO(2)} \mathcal{Y}_R, \quad \text{where} \quad \mathcal{Y}_R := \left\{ y \in H^1(\Omega; \mathbb{R}^2) : \nabla y \in BV(\Omega; R\{A, B\}) \right\}.$$

Lemma (S. Conti - B. Schweizer (2006))

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Let W satisfy assumptions H1.–H4. Then, for all sequences $\{y^\varepsilon\}_\varepsilon \subset H^2(\Omega; \mathbb{R}^2)$ for which

$$\sup_{\varepsilon > 0} I_\varepsilon(y^\varepsilon) < +\infty$$

there exists a map $y \in \mathcal{Y}$ such that, up to the extraction of a (non-relabeled) subsequence, there holds

$$y^\varepsilon - \fint_\Omega y^\varepsilon(x)\, dx \to y \quad \text{strongly in } H^1(\Omega; \mathbb{R}^2).$$

The limit sharp interface energy: main ingredients

- Limiting deformations y are locally laminates [G. Dolzmann - S. Müller (1995)], that is

$$\mathcal{Y}_R := \Big\{ y : \partial\{x \in \Omega : \nabla y(x) \in RA\} \text{ consists of subsets of lines that intersect } \partial\Omega \text{ and are parallel to } \mathrm{e}_1, \text{ and } y \text{ is affine on each ball } B_r \in \Omega \text{ such that } \mathcal{H}^1\big(B_r \cap \partial\{x \in \Omega : \nabla y(x) \in RA\}\big) = 0 \Big\}.$$

- The limiting sharp interface energy (in the strong L^1-topology) is given by

$$I_0(y) := \begin{cases} k_0 \mathcal{H}^1(J_{\nabla y}) & \text{if } y \in \mathcal{Y} \\ +\infty & \text{otherwise in } L^1(\Omega; \mathbb{R}^2). \end{cases}$$

- The cell formula k_0 is the optimal profile between the two phases, defined as

$$k_0 := \inf \Big\{ \liminf_{\varepsilon \to 0} I_\varepsilon(y^\varepsilon, Q) : \lim_{\varepsilon \to 0} \|y^\varepsilon - y_0\|_{L^1(Q)} = 0 \Big\},$$

where y_0 is a continuous function with $\nabla y_0 = A\chi_{\{x_2>0\}} + B\chi_{\{x_2<0\}}$ and Q is the two-dimensional unit cube centered in the origin.

Linearization

Rescaled displacement $u := (y - id)/\varepsilon$.

$$L_\varepsilon(y) := \frac{1}{\varepsilon^2}\int_\Omega W(\nabla y)\,dx + 0 \cdot \int_\Omega |\nabla^2 y|^2\,dx$$

for every $y \in H^2(\Omega;\mathbb{R}^2)$. This corresponds to the choice

$$P_\varepsilon(G) = 0 \cdot |G|^2 \quad \text{for} \quad G \in \mathbb{R}^{2\times 2}.$$

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- G. Dal Maso - M. Negri - D. Percivale (2002): Γ-convergence for single-well elasticity, no perturbation;
- B. Schmidt (2008): Γ-convergence for multiwell energies, where the wells are ε-close to the identity, no perturbation;

Multiwell linearization for solid-solid phase transitions

[R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018)]

$$F_\varepsilon(y) := \frac{1}{\varepsilon^2}\int_\Omega W(\nabla y)\,dx + \varepsilon^{2-r}\int_\Omega |\nabla^2 y|^2\,dx$$

for $r \in [1,2]$ and $y \in H^2(\Omega;\mathbb{R}^2)$. This corresponds to the choice

$$P_\varepsilon(G) = \varepsilon^{2-r}|G|^2, \quad \text{for} \quad G \in \mathbb{R}^{2\times 2\times 2}.$$

Remark: here the singular higher order term penalizes transitions between different wells in a stronger way with respect to the functionals I_ε.

In [R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018)] arbitrary dimension for a finite number of different wells, more general growth conditions, external forces, different scalings of the singular perturbation.

Multiwell linearization for solid-solid phase transitions

Lemma (R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018))

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Let W satisfy assumptions H1.–H5. Then, for all sequences $\{y^\varepsilon\}_\varepsilon \subset H^2(\Omega;\mathbb{R}^2)$ satisfying $\sup_{\varepsilon>0} F_\varepsilon(y^\varepsilon) < +\infty$ we find rotations $R^\varepsilon \in SO(2)$, translations $t^\varepsilon \in \mathbb{R}^2$, and phases $M^\varepsilon \in \{A, B\}$ such that

$$\sup_{\varepsilon>0} \left\| \frac{y^\varepsilon - (R^\varepsilon M^\varepsilon x + t^\varepsilon)}{\varepsilon} \right\|_{W^{1,r}(\Omega)} < +\infty.$$

Crucial ingredient: the rigidity estimate in [G. Friesecke - R. James - S. Müller (2002)]

Remark: Geometric rigidity for sequences with bounded F_ε-energy + prescribed boundary conditions $y^\varepsilon = id + \varepsilon g$ ensure

$$\sup_{\varepsilon>0} \|u^\varepsilon\|_{W^{1,r}(\Omega)} < +\infty \quad \text{for} \quad u^\varepsilon := \frac{y^\varepsilon - id}{\varepsilon}.$$

Multiwell linearization for solid-solid phase transitions

- Write the nonlinear energy in terms of the displacement fields by setting

$$\hat{F}_\varepsilon(u) = F_\varepsilon(\mathrm{Id} + \varepsilon u) \quad \text{for} \quad u \in H^2(\Omega;\mathbb{R}^2).$$

- The effective linearized energy has the form

$$F_0(u) := \begin{cases} \int_\Omega Q(\mathrm{Id}, e(u)) & \text{if } u \in H^1(\Omega;\mathbb{R}^2), \\ +\infty & \text{otherwise.} \end{cases}$$

where

$$Q(\mathrm{Id}, F) := \frac{1}{2} D^2 W(\mathrm{Id}) F : F \quad \text{and} \quad e(u) := \frac{1}{2}((\nabla u)^T + \nabla u).$$

Theorem (R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018))

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain. Let W satisfy assumptions H1.–H5. Then

$$\Gamma - \lim_{\varepsilon \to 0} \hat{F}_\varepsilon = F_0$$

with respect to the weak $W^{1,r}$-topology.

Phase transition and linearization: Heuristics

- In [R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018)] imposing certain boundary conditions, one can always infer that the same phase, e.g. $A = \mathrm{Id}$, is active. Then it is indeed meaningful to perform a linearization around the identity.
- In [S. Conti - B. Schweizer (2006)]: laminate structure of the limiting configurations, different phases may be active and phase transitions between the different phase regions occur.

Why?

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Why?
In [R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018)], the second-order penalization is so strong that basically phase transitions are forbidden.

In particular, the B-phase region, i.e., the set where the deformation gradient ∇y^ε takes values in a neighborhood $SO(2)B$, denoted by T_B^ε in the following, has small $\mathcal{L}^2$-measure.

A heuristic argument for the smallness of T_B^ε

Boundedness of the energy + H4.

$$\Downarrow$$

$$\mathcal{H}^1(\partial T_B^\varepsilon) \leq \|\mathrm{dist}(\nabla y^\varepsilon, SO(2))\|_{L^2(\Omega)} \|\nabla^2 y^\varepsilon\|_{L^2(\Omega)} \leq C\varepsilon\varepsilon^{\frac{r}{2}-1} = \varepsilon^{\frac{r}{2}}.$$

Isoperimetric inequality in dimension two

$$\Downarrow$$

$$\min\{\mathcal{L}^2(T_B^\varepsilon), \mathcal{L}^2(\Omega \setminus T_B^\varepsilon)\} \leq C\varepsilon^r.$$

Assuming that T_B^ε is the **minority phase**, i.e. the minimum is attained for T_B^ε

$$\mathcal{L}^2(T_B^\varepsilon) \leq C\varepsilon^r.$$

Phase transition and linearization: challenges

- This scaling of the area of the minority phase excludes phase transitions where both $\mathcal{L}^2(T_B^\varepsilon)$ and $\mathcal{L}^2(\Omega \setminus T_B^\varepsilon)$ are bounded uniformly from below. The same calculation for the model in [S. Conti - B. Schweizer (2006)] would give

$$\mathcal{H}^1(\partial T_B^\varepsilon) \leq C.$$

This reflects the fact that (macroscopic) phase transitions are expected in that framework.

- For compactness of the displacement fields $u^\varepsilon = (y^\varepsilon - \mathrm{Id})/\varepsilon$ we necessarily need $\mathcal{L}^2(T_B^\varepsilon) \to 0$ as otherwise $|\nabla u^\varepsilon| \to +\infty$ on a set of positive measure. Since $|\nabla u^\varepsilon| \sim 1/\varepsilon$ on T_B^ε, it turns out that the bound $\mathcal{L}^2(T_B^\varepsilon) \leq C\varepsilon^r$ is sharp in order to derive the uniform estimate $\|\nabla u\|_{L^r(\Omega)} \leq C$.

Then, how to see phase transitions and linearization together?

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Key idea : to use a generalized definition of the rescaled displacement fields which measures the distance of the deformations y^ε from suitable rigid movements which may be different on the components of a partition of Ω which is induced by the A and B phase regions. This allows us to

- derive a linearization result for configurations where both phases are present, in particular where (macroscopic) phase transitions occur;
- obtain compactness results in a piecewise Sobolev setting.

The model

$$E_\varepsilon(y) := \frac{1}{\varepsilon^2}\int_\Omega W(\nabla y)\,dx + \varepsilon^2\int_\Omega |\nabla^2 y|^2\,dx + \underbrace{\eta_\varepsilon^2\int_\Omega (|\partial^2_{11}y|^2 + |\partial^2_{12}y|^2)\,dx}_{\text{higher-order penalization in direction } e_2}.$$

for every $y \in H^2(\Omega;\mathbb{R}^2)$, where $\{\eta_\varepsilon\}_\varepsilon \subset [0,+\infty)$ is an increasing sequence satisfying $\lim_{\varepsilon\to 0}\eta_\varepsilon = +\infty$. This corresponds to the choice

$$P_\varepsilon(G) = \varepsilon^2|G|^2 + \eta_\varepsilon^2\sum_{i=1,2}(|G_{i11}|^2 + |G_{i12}|^2), \quad \text{for} \quad G \in \mathbb{R}^{2\times 2\times 2}.$$

Remark:

- Without the assumption $\lim_{\varepsilon\to 0}\eta_\varepsilon = +\infty$ the limit model would be be defined in $GSBD^2(\Omega)$ and would exhibit branching. Price to pay: one rank-one connection.
- The additional penalization term does not affect the qualitative behavior of the sharp interface limit.

A two-well rigidity estimate

A crucial ingredient for the compactness result is the following

Theorem (E.D. - M. Friedrich)

Let Ω be a bounded simply connected Lipschitz domain in $\mathbb{R}^2$. Then there exists a constant $C = C(\Omega, A, B) > 0$ such that for every $y \in H^2(\Omega;\mathbb{R}^2)$ there exist a rotation $R \in SO(2)$ and a function $\mathcal{M} \in BV(\Omega;\{A,B\})$ satisfying

$$\|\nabla y - R\mathcal{M}\|_{L^2(\Omega)} \leq C\varepsilon\sqrt{F_\varepsilon(y)} + C\frac{\eta_\varepsilon}{\varepsilon}F_\varepsilon(y) \quad \textit{and} \quad |D\mathcal{M}|(\Omega) \leq CF_\varepsilon(y).$$

Remark: The analogous result holds true in arbitrary dimensions.

Main ideas for the proof

- **Strategy**: to replace the gradient ∇y, which satisfies $\nabla y \approx SO(2)\{A, B\}$, by an associated vector field $\gamma = \nabla y \chi_{\{\nabla y \approx SO(2)A\}} + \nabla y B^{-1} \chi_{\{\nabla y \approx SO(2)B\}}$.
- Usage of rigidity estimates for vector fields with nonzero curl established in [A. Chambolle - A. Giacomini - M. Ponsiglione (2007)], and [S. Müller - L. Scardia - C. Zeppieri (2014)].

Compactness result

Sequences of deformations $\{y^\varepsilon\}_\varepsilon$ with equibounded ε-energies can be decomposed into the sum of two parts:

(a) Piecewise rigid movements, where 'piecewise' refers to associated Caccioppoli partitions induced by the A and B phase region. These converge to the limit y of the original deformations.

(b) Elastic displacements of order ε whose strain is equibounded in L^2. These converge to a limiting displacement field, which is piecewise Sobolev, with possible jumps along horizontal lines.

Compactness result

- Denote by $\mathscr{P}$ the following collection of Caccioppoli partitions of Ω

$$\mathscr{P} := \Big\{\mathcal{P} = \{P_j\}_j \text{ partition of } \Omega : \bigcup_j \partial P_j \cap \Omega \text{ consists of subsets of lines}$$

$$\text{parallel to the } \mathrm{e}_1 - \text{axis which extend up to the boundary of } \Omega\Big\}.$$

- Let $\mathcal{U}$ be the set of elastic displacements whose jump sets are the union of countably many horizontal lines, namely

$$\mathcal{U} := \Big\{u \in SBV^2_{loc}(\Omega;\mathbb{R}^2) : \ \mathcal{H}^1(J_u) < +\infty,\ \nabla u \in L^2(\Omega;\mathbb{M}^{2\times 2}),$$

$$\text{and} \quad J_u \subset \bigcup_{i\in\mathbb{N}} (\mathbb{R}\times\{s_i\}) \cap \Omega\Big\}.$$

Compactness result

Theorem (E.D. - M. Friedrich)

Let $\{y^\varepsilon\}_\varepsilon \subset H^2(\Omega;\mathbb{R}^2)$ *be a sequence of deformations satisfying the uniform energy estimate*

$$\sup_{\varepsilon>0} E_\varepsilon(y^\varepsilon) < +\infty.$$

Then, up to the extraction of a non-relabeled subsequence, the following holds:
(a) There exists a constant $\tilde{C} > 0$*, and Caccioppoli partitions* $\mathcal{P}^\varepsilon := \{P_j^\varepsilon\}_j$ *of* Ω *such that*

$$\sup_{\varepsilon>0} \mathcal{H}^1\big(\bigcup_j \partial^* P_j^\varepsilon\big) < +\infty, \ \sup_{\varepsilon>0} \frac{\eta_\varepsilon}{\varepsilon} \int_{-\infty}^{+\infty} \mathcal{H}^0\big((\mathbb{R}\times\{t\}) \cap \bigcup_j \partial^* P_j^\varepsilon \cap \Omega\big)\, dt < +\infty.$$

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There exist associated rotations $R^\varepsilon \in SO(2)$, *as well as collections of matrices* $\mathcal{M}^\varepsilon := \{M_j^\varepsilon\}_j$, *with* $M_j^\varepsilon \in \{A, B\}$ *for every* j *and* ε, *such that*

$$\sup_{\varepsilon>0} \frac{1}{\varepsilon} \|\nabla y^\varepsilon - \sum\nolimits_j R^\varepsilon M_j^\varepsilon \chi_{P_j^\varepsilon}\|_{L^2(\Omega)} < +\infty.$$

Compactness result

Theorem (E.D. - M. Friedrich)

(b) There exist a limiting rotation $R \in SO(2)$, a limiting deformation $y \in \mathcal{Y}_R$, and a limiting partition $\mathcal{P} = \{P_j\}_j \in \mathscr{P}$ such that

$$\begin{aligned}
&R^\varepsilon \to R, \\
&P_j^\varepsilon \to P_j \quad \text{in measure for all } j \in \mathbb{N}, \\
&y^\varepsilon - \fint_\Omega y^\varepsilon(x)\,dx \to y \quad \text{strongly in } H^1(\Omega;\mathbb{R}^2), \\
&\sum_j R^\varepsilon M_j^\varepsilon \chi_{P_j^\varepsilon} \rightharpoonup^* \nabla y \quad \text{weakly* in } BV(\Omega;\mathbb{M}^{2\times 2}).
\end{aligned}$$

Compactness result

Theorem (E.D. - M. Friedrich)

(c) Defining the rescaled displacement fields associated to $\mathcal{P}^\varepsilon, \mathcal{M}^\varepsilon$, $\mathcal{T}^\varepsilon$, and R^ε by

$$u^\varepsilon := \sum_j \frac{y^\varepsilon - (R^\varepsilon M_j^\varepsilon x + t_j^\varepsilon)\chi_{P_j^\varepsilon}}{\varepsilon},$$

there exists $u \in \mathcal{U}$ such that

$$\begin{aligned} &u^\varepsilon \to u \quad \text{a.e. in } \Omega, \\ &\nabla u^\varepsilon \rightharpoonup \nabla u \quad \text{weakly in } L^2(\Omega; \mathbb{M}^{2\times 2}). \end{aligned}$$

The effective limiting model (E.D. - M. Friedrich)

- The asymptotic cell formula is given by

$$k_1 := \inf \Big\{ \liminf_{\varepsilon \to 0} E_\varepsilon(y^\varepsilon, Q) : \ \lim_{\varepsilon \to 0} \|y^\varepsilon - y_1\|_{L^1(Q)} = 0 \Big\},$$

  where y_1 is a continuous function with $\nabla y_1 = A\chi_{\{x_2>0\}} + B\chi_{\{x_2<0\}}$. The asymptotic cell formula represents the energy of an optimal profile transitioning from phase A to B, and satisfies $k_1 \geq k_0$.

- Our effective linearized energy is defined as

$$E_0(y,u,\mathcal{P}) := \int_\Omega Q(\nabla y(x), \nabla u(x))\, dx + k_1 \mathcal{H}^1(J_{\nabla y}) + 2k_1 \mathcal{H}^1\Big((J_u \cup (\bigcup_j \partial P_j \cap \Omega)) \setminus J_{\nabla y} \Big)$$

  for $(y,u,\mathcal{P})$ admissible limiting triple.

Some final remarks

1. Besides the elastic energy, the functional contains two surface terms: the jumps of ∇y represent the energy associated to single phase transitions between A and B. The second surface term corresponds to two consecutive phase transitions with a small intermediate layer. It enters the energy functional with double cost with respect to single phase transitions.

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2. Our effective energy reduces to the one in [S. Conti - B. Schweizer (2006)] for $u = 0$ and $\mathcal{P}$ coinciding with the collection of connected components of the two sets $\{x \in \Omega : \nabla y(x) = A\}$, and $\{x \in \Omega : \nabla y(x) = B\}$. In particular, our additional penalization does not affect the qualitative behavior of the sharp interface limit.

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2. Our effective energy reduces to the one in [S. Conti - B. Schweizer (2006)] for $u = 0$ and $\mathcal{P}$ coinciding with the collection of connected components of the two sets $\{x \in \Omega : \nabla y(x) = A\}$, and $\{x \in \Omega : \nabla y(x) = B\}$. In particular, our additional penalization does not affect the qualitative behavior of the sharp interface limit.
3. Our linearization result reduces to the one in [R. Alicandro - G. Dal Maso - G. Lazzaroni - M. Palombaro (2018)] for $u \in H^1(\Omega; \mathbb{R}^2)$, for the trivial partition $\mathcal{P}$ consisting only of Ω, and for a deformation $y \in \mathcal{Y}$ with $\nabla y = \mathrm{Id}$ in Ω.

Thank you for your attention!