Towards a sharper phase-field method for microstructure evolution problems

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joint work with Jędrzej Dobrzański

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Modelling, PDE analysis and computational mathematics in materials science
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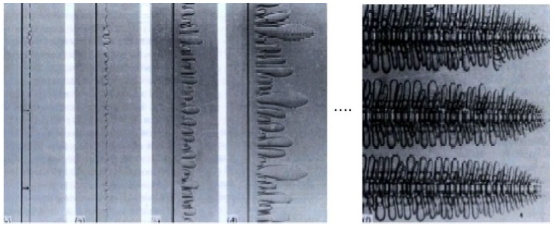
Microstructure evolution

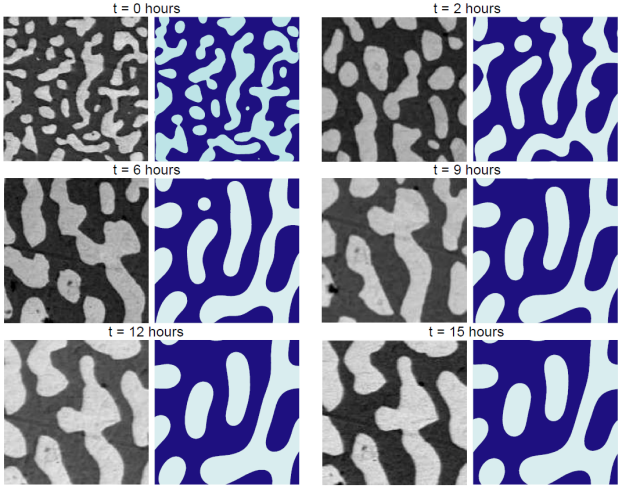
- Directional solidification, dendritic growth, ...



[Provatas & Elder, 2010]

Microstructure evolution

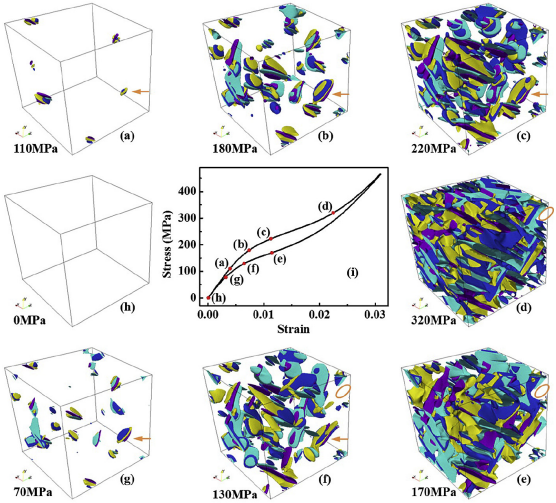
- Spinodal decomposition – microstructure coarsening by diffusion



Thermal ageing of tin–lead solder at 150° [Ubachs, Schreurs & Geers, *JMPS* 2004]

Microstructure evolution

- Martensitic transformation



[Zhu et al, 2017]

Phase-field method: diffuse-interface modelling approach

→ tracking of interfaces is avoided (interfaces are diffuse)

→ microstructure evolution is simulated on a fixed (but fine!) computational grid

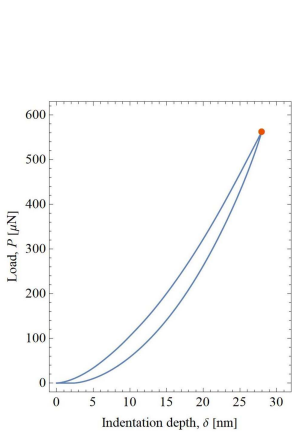
→ various physical phenomena can be included

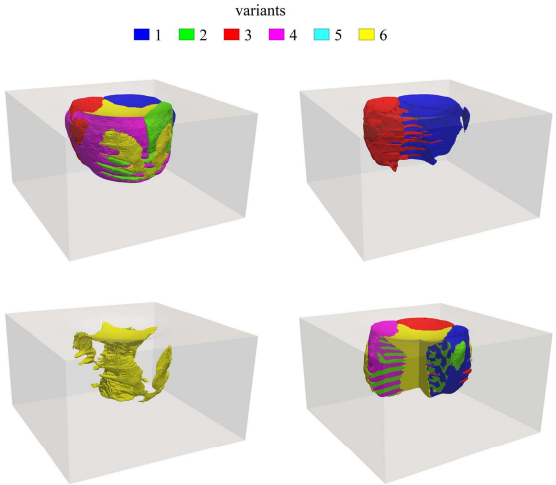
Some literature references on the phase-field method:

- general reviews [Chen, 2002; Moelans et al, 2008; Steinbach, 2009; Provatas & Elder, 2010; Wang & Li, 2010]
- phase-field method for martensitic transformation [Wang & Khachaturyan, 1997; Artemev et al, 2000; Wen et al, 2000; Levitas & Preston, 2002; Ahluwalia et al, 2008; Shu & Yen, 2008; Lei et al, 2010; Hildebrand & Miehe, 2012; Borukhovich et al, 2014; Schoof et al, 2019; Liu et al, 2024, ...]
- finite-element-based finite-strain phase-field models [Levitas et al, 2009; Clayton & Knap, 2011; Hildebrand & Miehe, 2012; Mosler et al, 2014; Tůma et al, 2016, 2018, 2021; Bartels & Mosler, 2017; Kiefer et al, 2017; Basak & Levitas, 2019; Rezaee-Hajidehi & Stupkiewicz, 2020, 2021]

Martensitic transformation in CuAlNi during nano-indentation

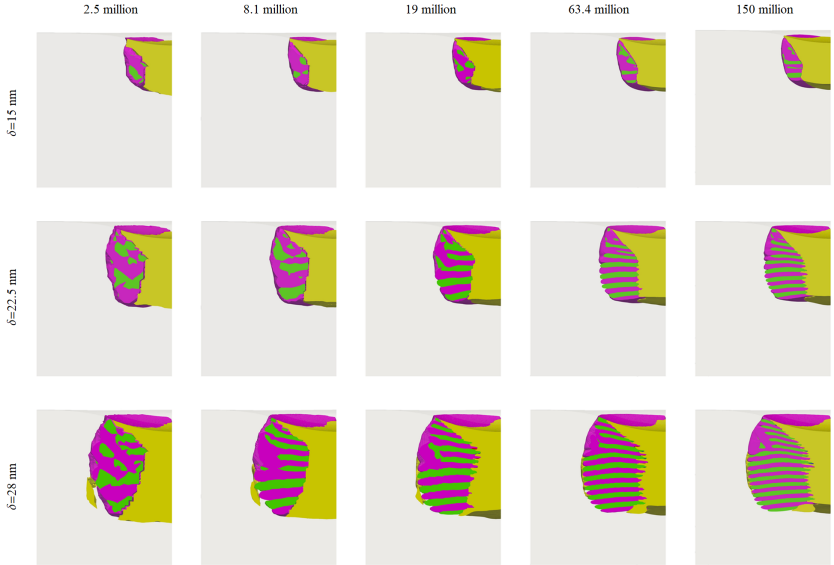
[Tůma, Rezaee-Hajidehi, Hron, Farrell & S, *CMAME* 2021]





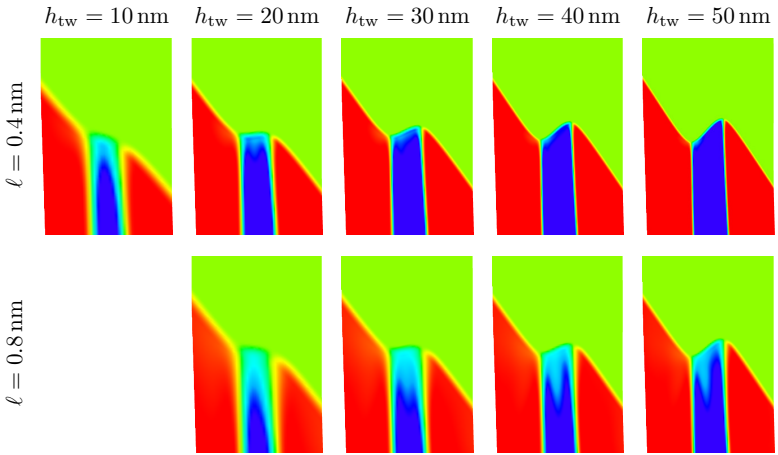
Fine mesh is needed $\rightarrow$ large-scale problems

$\ell = \text{const}$



[Tůma et al, 2021]

So why not to increase ℓ?



[Tůma & S, *IJSS* 2016]

Aim of our work

- Can we improve computational efficiency of the phase-field method?
  - sharper interfaces $\rightarrow$ larger element size $\rightarrow$ reduced computational cost
  - keeping simplicity (e.g., avoid XFEM)

$\rightarrow$ sharp phase-field method [Finel et al, 2018] – but relying on the finite difference method

Outline

1. Conventional phase field method
2. LET: lamination-based treatment of weak discontinuities
3. LET-PF: hybrid diffuse-semisharp approach for evolving interfaces

Outline

Prototype phase-field model

- Assumptions:
  - → two phases
  - → viscous evolution
- Constitutive framework for each phase: elasticity with eigenstrain ($i = 1, 2$)

$$F_i(\boldsymbol{\varepsilon}) = F_i^0 + \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^{\mathrm{t}}) \cdot \mathbb{L}_i(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^{\mathrm{t}}), \qquad \boldsymbol{\sigma} = \mathbb{L}_i(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^{\mathrm{t}})$$

- Phase transformation: continuous order parameter $\phi \approx$ volume fraction $(0 \le \phi \le 1)$
- Bulk free energy density

$$F_{\mathrm{B}}(\boldsymbol{\varepsilon}, \phi) = F^0 + \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{t}}) \cdot \mathbb{L}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{t}})$$

Interpolated properties:

$$\begin{aligned} \boldsymbol{\varepsilon}^{\mathrm{t}}(\phi) &= (1-\phi)\boldsymbol{\varepsilon}_1^{\mathrm{t}} + \phi\boldsymbol{\varepsilon}_2^{\mathrm{t}} \\ \mathbb{L}(\phi) &= (1-\phi)\mathbb{L}_1 + \phi\mathbb{L}_2 \\ F^0(\phi) &= (1-\phi)F_1^0 + \phi F_2^0 \end{aligned}$$

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Interpolated properties:

$$\begin{aligned} \boldsymbol{\varepsilon}^{\mathrm{t}}(\phi) &= (1 - h(\phi))\boldsymbol{\varepsilon}_1^{\mathrm{t}} + h(\phi)\boldsymbol{\varepsilon}_2^{\mathrm{t}} \qquad h(0) = 0,\ \ h(1) = 1,\ \ h'(0) = h'(1) = 0 \\ \mathbb{L}(\phi) &= (1 - h(\phi))\mathbb{L}_1 + h(\phi)\mathbb{L}_2 \\ F^0(\phi) &= (1 - h(\phi))F_1^0 + h(\phi)F_2^0 \end{aligned}$$

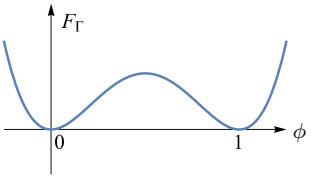
Prototype phase-field model (2)

- Bulk free energy density

$$F_{\mathrm{B}}(\boldsymbol{\varepsilon},\phi) = F^0(\phi) + \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{t}}(\phi)) \cdot \mathbb{L}(\phi)(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{t}}(\phi))$$

- Interfacial free energy density (so-called double-well potential)

$$F_\Gamma(\phi,\nabla\phi) = \gamma\left(\frac{6}{\ell}\,\phi^2(1-\phi)^2 + \frac{3\ell}{2}|\nabla\phi|^2\right)$$



- Total free energy density

$$F(\boldsymbol{\varepsilon},\phi,\nabla\phi) = F_{\mathrm{B}}(\boldsymbol{\varepsilon},\phi) + F_\Gamma(\phi,\nabla\phi)$$

- Dissipation potential (of viscous type)

$$D(\dot{\phi}) = \frac{1}{2m}\,\dot{\phi}^2$$

+ variational framework $\rightarrow$ complete model

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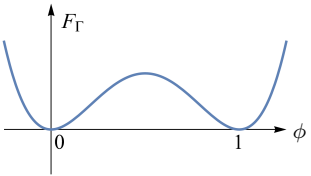

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Variational framework

- Potential energy functional

$$\mathcal{E}[\boldsymbol{u},\phi] = \mathcal{F}[\boldsymbol{u},\phi] + \Omega[\boldsymbol{u}], \qquad \mathcal{F}[\boldsymbol{u},\phi] = \int_B F(\nabla_{\mathrm{s}}\boldsymbol{u},\phi,\nabla\phi)\,\mathrm{d}V$$

  → $\Omega[\boldsymbol{u}]$ – potential of external loads, e.g., $\Omega[\boldsymbol{u}] = -\int_{\partial_t B} \boldsymbol{t}^* \cdot \boldsymbol{u}\,\mathrm{d}S$

- Global rate potential

$$\Pi[\dot{\boldsymbol{u}},\dot{\phi};\boldsymbol{u},\phi] = \dot{\mathcal{E}}[\dot{\boldsymbol{u}},\dot{\phi};\boldsymbol{u},\phi] + \mathcal{D}[\dot{\phi}], \qquad \mathcal{D}[\dot{\phi}] = \int_B D(\dot{\phi})\,\mathrm{d}V$$

- Minimization problem [Miehe, 2011; Hildebrand & Miehe, 2012; Tůma, Petryk & S, 2016, 2018]

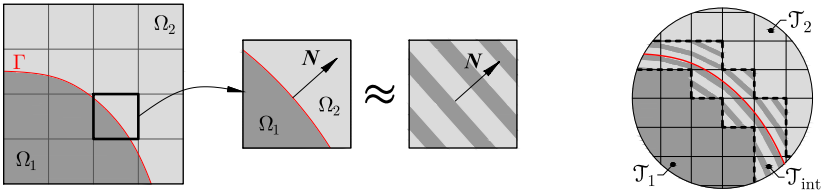
$$\{\dot{\boldsymbol{u}},\dot{\phi}\} = \arg\min_{\dot{\boldsymbol{u}},\dot{\phi}} \Pi[\dot{\boldsymbol{u}},\dot{\phi};\boldsymbol{u},\phi]$$

  - $\delta_{\dot{\boldsymbol{u}}}\Pi = 0$ → equilibrium equation (virtual work principle)
  - $\delta_{\dot{\phi}}\Pi = 0$ → evolution equation for ϕ

Outline

Laminated element technique (LET)

[Dobrzański, Wojtacki & S, *Comput. Struct.* 2024]



- Interfaces defined implicitly by a level set function ϕ
- Total free energy (FE discretization + LET)

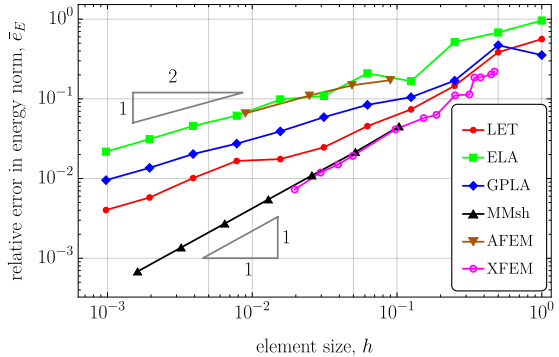
$$\mathcal{F} = \mathcal{F}_{\mathrm{B}} = \sum_{i=1}^{2} \left(\sum_{\omega \in \mathcal{T}_i} \int_{\omega} F_i \, \mathrm{d}V \right) + \sum_{\omega \in \mathcal{T}_{\mathrm{int}}} \int_{\omega} \overline{F} \, \mathrm{d}V$$

  - microstructure of the laminate (η, $\boldsymbol{N}$) depends on the position of the interface within the element
  - overall (homogenized) bulk energy of simple laminates within laminated elements, $\omega \in \mathcal{T}_{\mathrm{int}}$

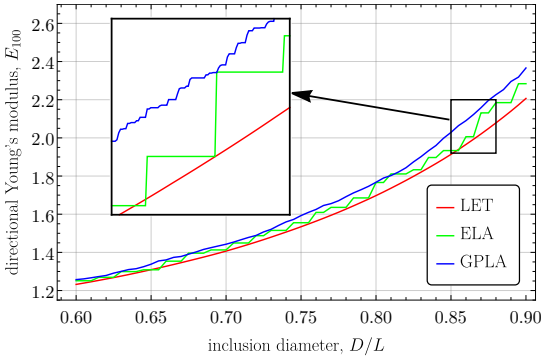
$$\overline{F} = \overline{F}(\boldsymbol{\varepsilon}, \eta, \boldsymbol{N}) = (1-\eta)F_1 + \eta F_2$$

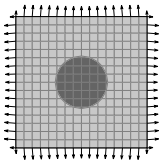
LET performance: elastic inclusion problem

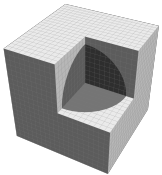
convergence with mesh refinement



response as a function of radius







Outline

LET-PF: combining the phase-field method with LET

- Total free energy

$$\mathcal{F} = \mathcal{F}_{\mathrm{B}} + \mathcal{F}_{\Gamma}$$

- Interfacial free energy $\rightarrow$ diffuse treatment of interfaces by the phase-field (PF) method

$$\mathcal{F}_{\Gamma} = \sum_{\omega \in \mathcal{T}} \int_{\omega} F_{\Gamma} \, \mathrm{d}V, \qquad F_{\Gamma} = \gamma \left(\frac{6}{\ell} \, \phi^2 (1-\phi)^2 + \frac{3\ell}{2} |\nabla \phi|^2 \right)$$

- Bulk free energy $\rightarrow$ semisharp treatment of interfaces by LET

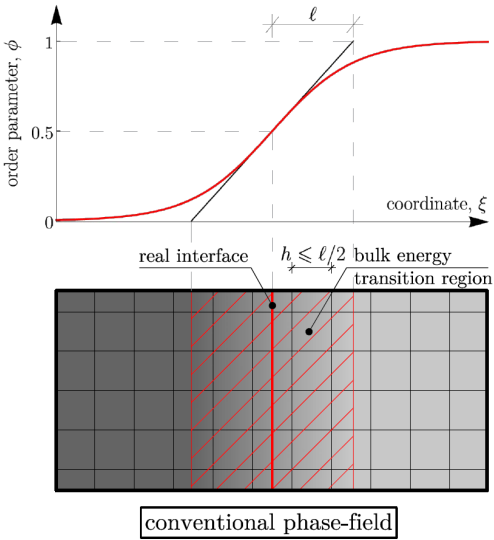
$$\mathcal{F}_{\mathrm{B}} = \sum_{i=1}^{2} \left(\sum_{\omega \in \mathcal{T}_i} \int_{\omega} F_i \, \mathrm{d}V \right) + \sum_{\omega \in \mathcal{T}_{\mathrm{int}}} \int_{\omega} \overline{F} \, \mathrm{d}V$$

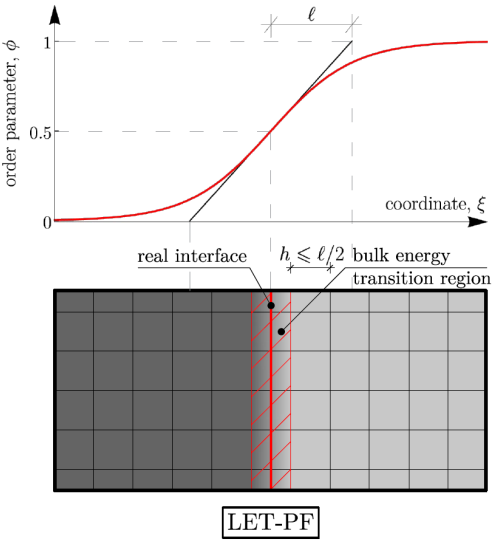
  - the order parameter ϕ plays the role of a level set function ($\phi = \frac{1}{2} \rightarrow$ interface)

- Variational framework

$$\Pi = \dot{\mathcal{F}} + \mathcal{D} \quad \rightarrow \quad \min$$

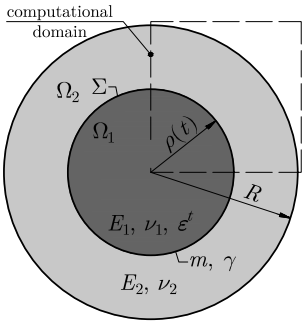
LET-PF: combining the phase-field method with LET

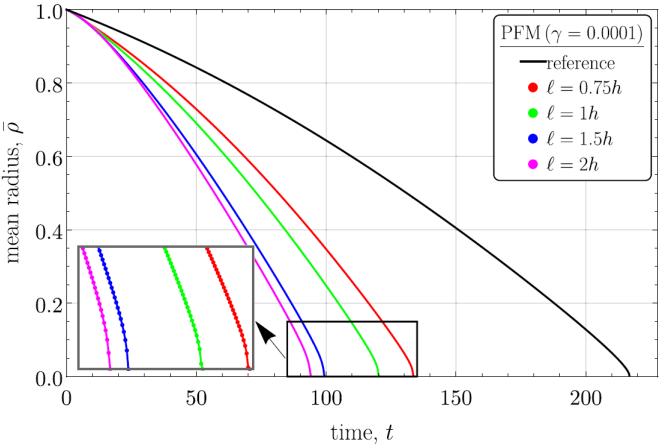




Evolving (vanishing) circular inclusion: conventional phase-field method

- evolution driven by elastic strain energy, large time increments, coarse mesh (2D)
- analytical solution of the reference 1D sharp-interface problem





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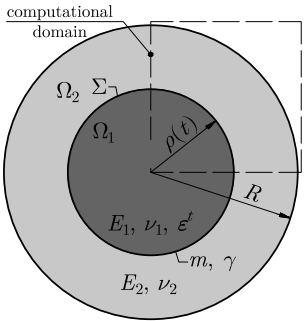
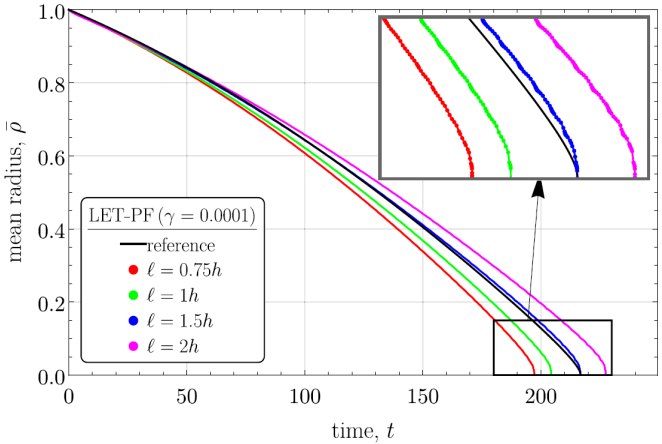
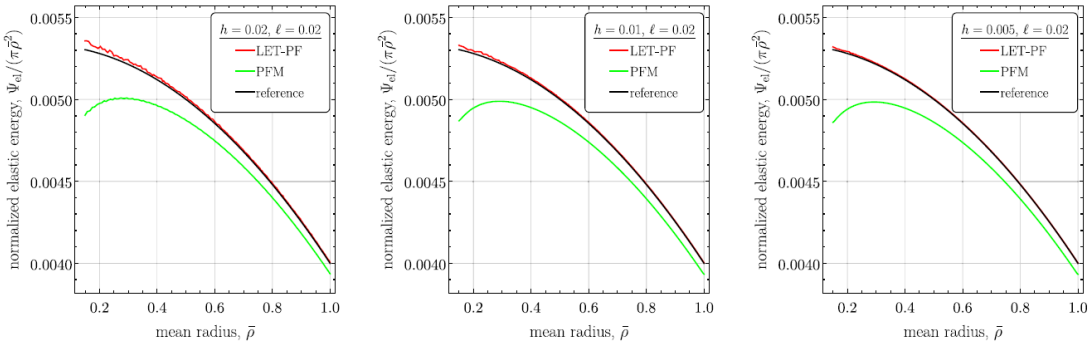




Evolving (vanishing) circular inclusion: effect of mesh refinement

- elastic strain energy as a function of inclusion radius, $\ell = \text{const}$



- error due to the finite thickness of the diffuse interface in the conventional phase-field method
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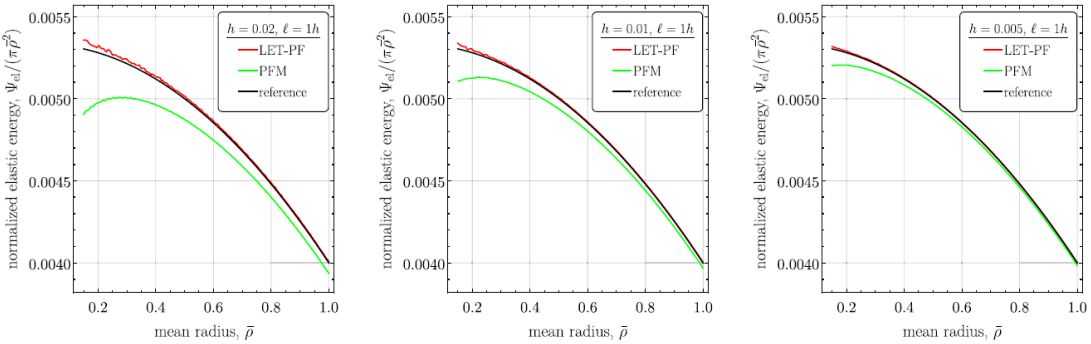
- elastic strain energy as a function of inclusion radius, $h/\ell = \text{const}$



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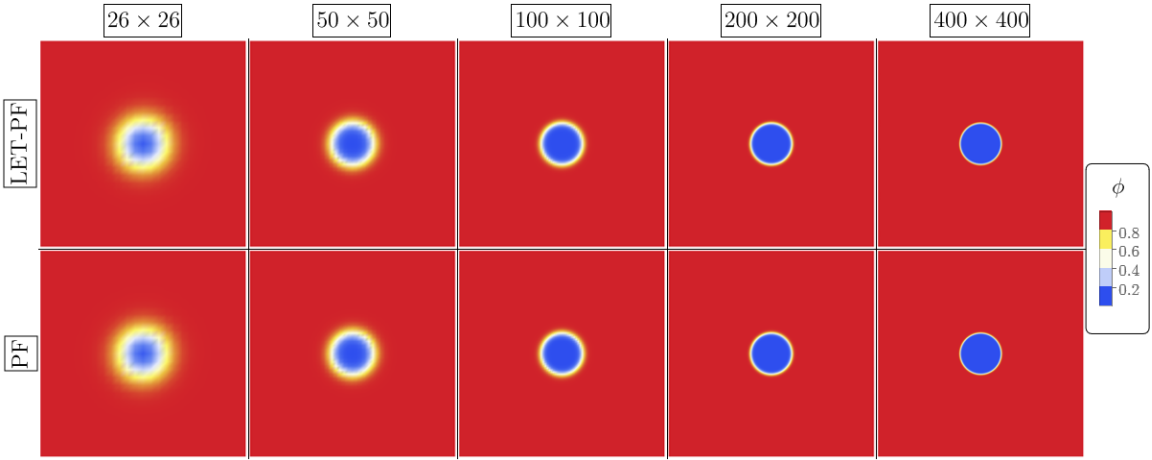
Evolving inclusion in a constrained domain: effect of mesh size

- LET-PF vs. conventional phase-field (PF), $h/\ell = \text{const}$ – initial state



Evolving inclusion in a constrained domain: effect of mesh size

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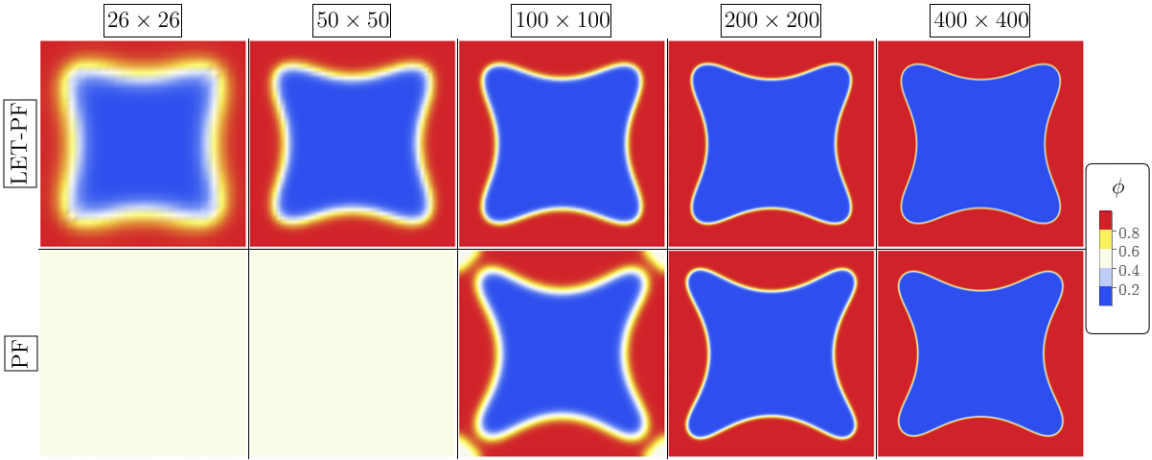

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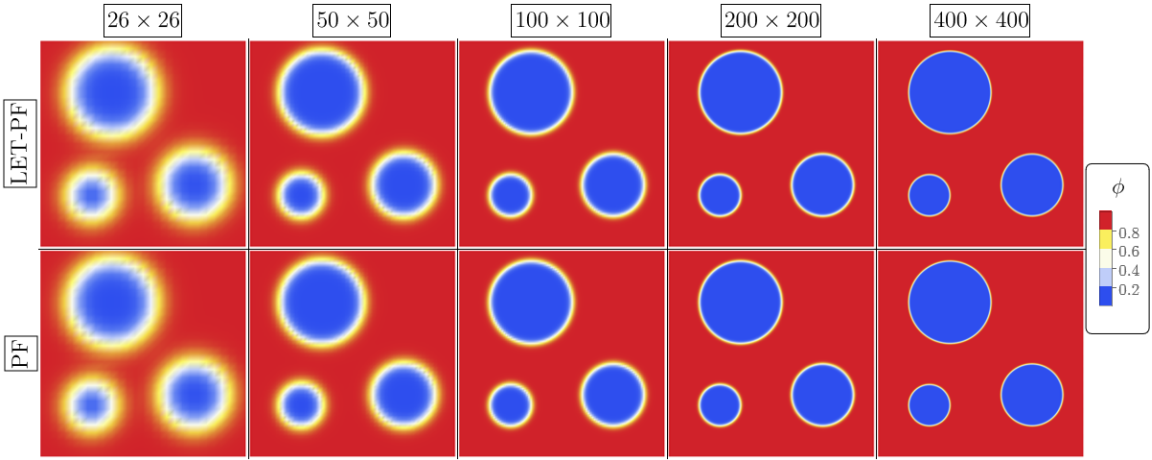

Summary

In short:

- *Proof of concept* of a new approach to phase-field modelling of microstructure evolution

In more detail:

- LET-PF, a hybrid diffuse–semisharp approach combining
  1. phase-field method – interfacial energy contribution
  2. laminated element technique (LET) – bulk energy contribution
- Features:
  - simple (element-based implementation)
  - for the problems studied, LET-PF exhibits higher accuracy than the conventional phase-field method

Even more details:

J. Dobrzański, K. Wojtacki & S. Stupkiewicz, Lamination-based efficient treatment of weak discontinuities for non-conforming finite element meshes, *Comput. Struct.* **291**, 107209, 2024.

J. Dobrzański & S. Stupkiewicz, Towards a sharper phase-field method: A hybrid diffuse-semisharp approach for microstructure evolution problems, *Comp. Meth. Appl. Mech. Eng.* **423**, 116841, 2024.

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