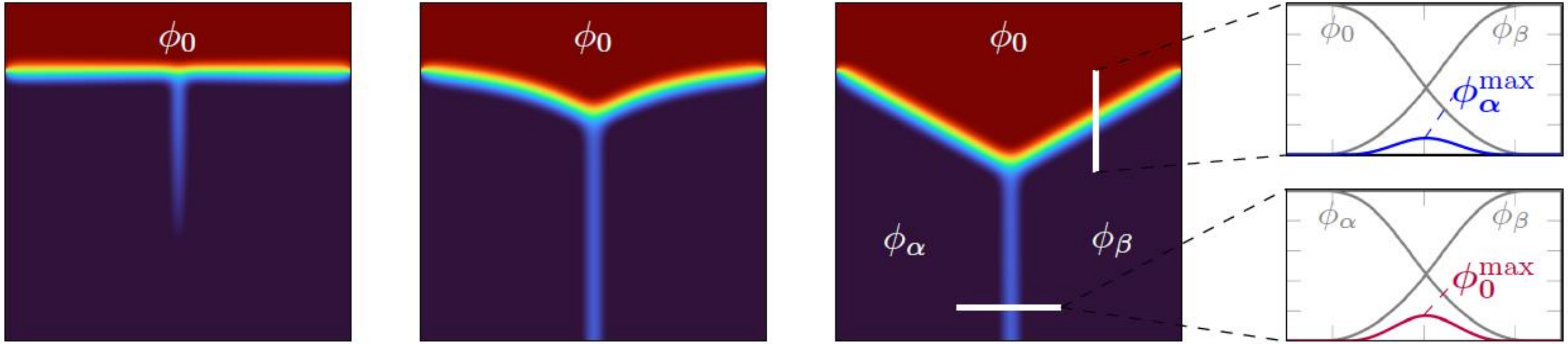
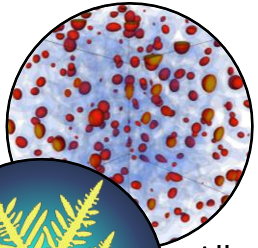
Triple junction benchmark – current state

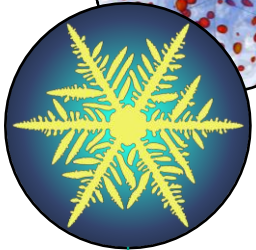
Simon Daubner, Paul Hoffrogge, Martin Minar, Britta Nestler



Motivation

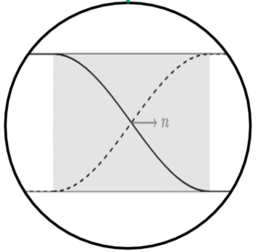


Cahn-Hilliard equation
(gradient + regular solution term)

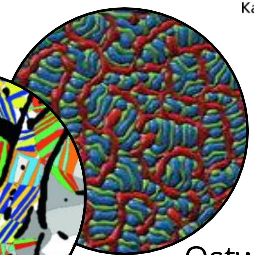


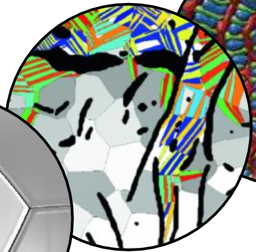
Allen-Cahn equation
(gradient + double-well/obstacle term)
+ anisotropy of interfacial energy
+ temperature field

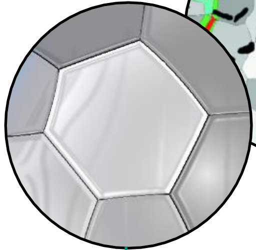
Validation



Study 1D interface in terms of
- Simulation studies
- Analytical solution
- Sharp / Thin interface asymptotics

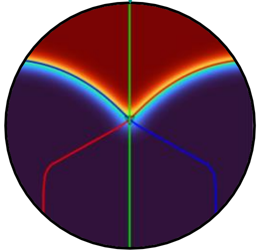






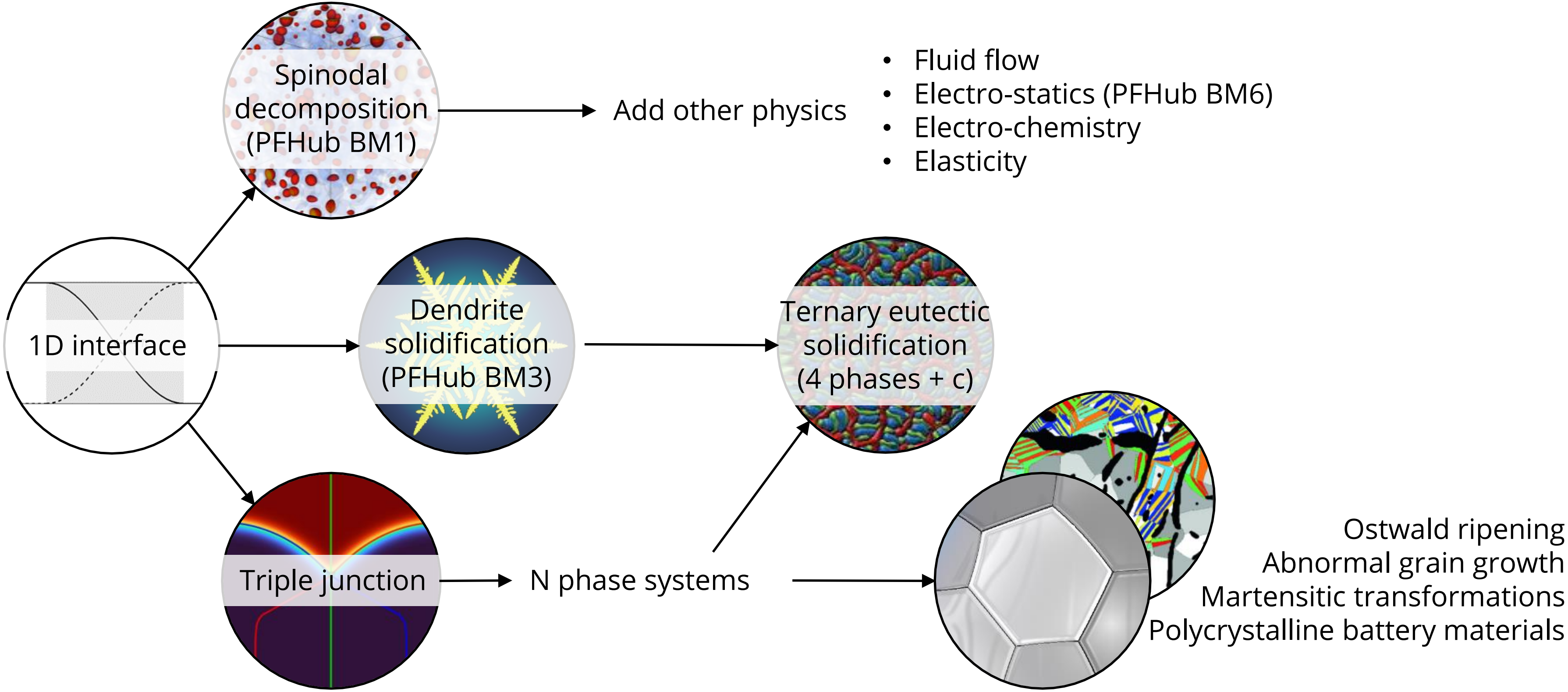
Ostwald ripening
Abnormal grain growth
Martensitic transformations
Polycrystalline battery materials

Validation

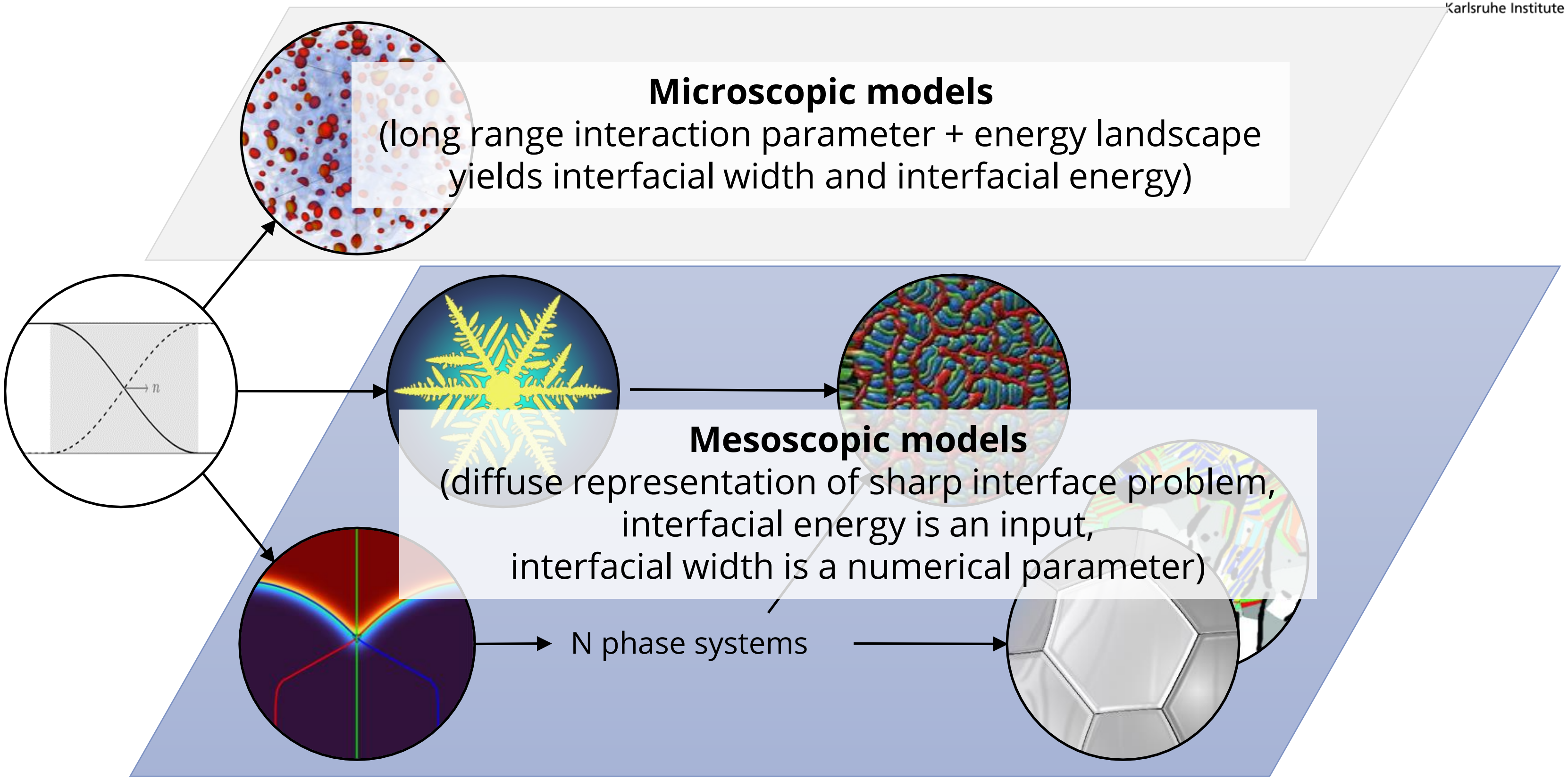


Study triple junction in terms of
- Simulation studies

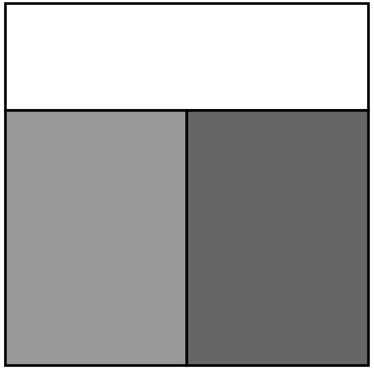
Motivation


Spinodal decomposition (PFHub BM1)
Add other physics
• Fluid flow
• Electro-statics (PFHub BM6)
• Electro-chemistry
• Elasticity
1D interface
Dendrite solidification (PFHub BM3)
Ternary eutectic solidification (4 phases + c)
Triple junction
N phase systems
Ostwald ripening
Abnormal grain growth
Martensitic transformations
Polycrystalline battery materials

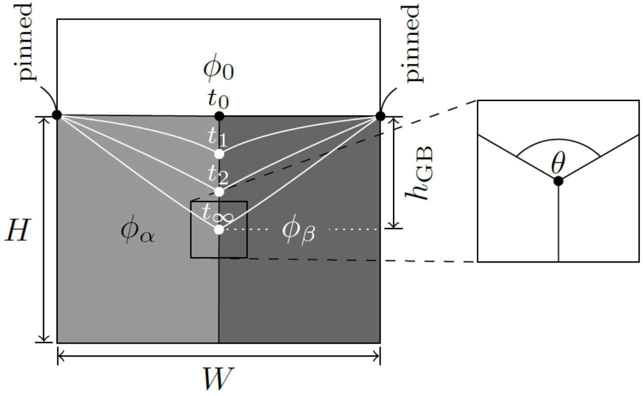
Motivation


Microscopic models
(long range interaction parameter + energy landscape
yields interfacial width and interfacial energy)
Mesoscopic models
(diffuse representation of sharp interface problem,
interfacial energy is an input,
interfacial width is a numerical parameter)
N phase systems

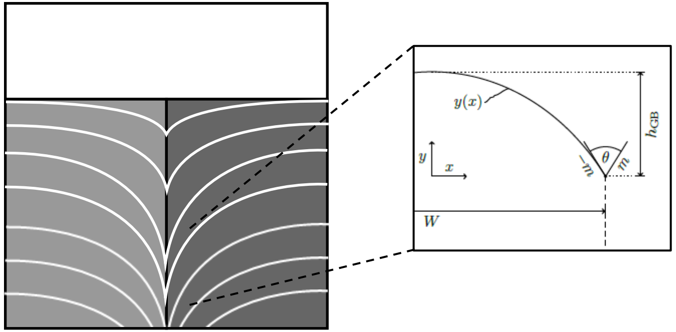
Triple junction benchmark

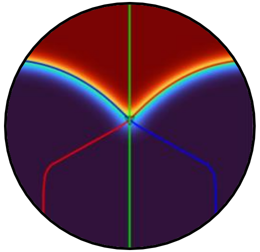


Static triple junction



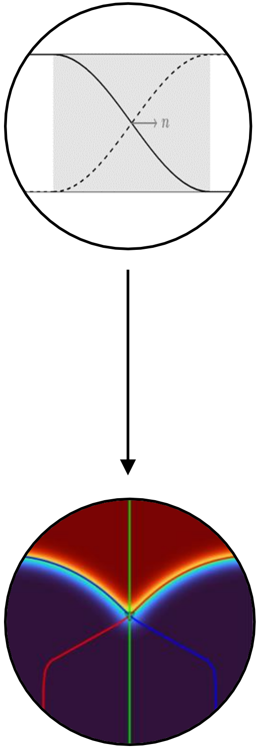
Steady state triple junction





Why a triple junction?

Multi-phase model formulation



$$\mathcal{F}_{\text{int}} = \int_V f_{\text{grad}} + f_{\text{well}} \, \mathrm{d}V$$
$$= \int_V \kappa |\nabla\phi|^2 + \Omega\phi^2(1-\phi)^2 \mathrm{d}V$$

All questions of generalizing a one order parameter formulation to N phases is already encapsulated in the three phase problem!

$$f^1_{\text{grad}} = \frac{\tilde{\kappa}}{2} \sum_\alpha |\boldsymbol{\nabla}\phi_\alpha|^2$$

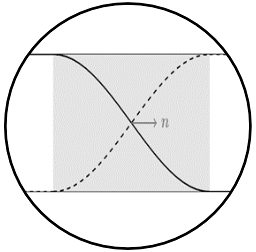
$$f^2_{\text{grad}} = -\sum_\alpha \sum_{\beta>\alpha} \kappa_{\alpha\beta} \boldsymbol{\nabla}\phi_\alpha \cdot \boldsymbol{\nabla}\phi_\beta$$

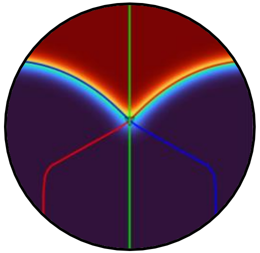
$$f^3_{\text{grad}} = \sum_\alpha \sum_{\beta>\alpha} \kappa_{\alpha\beta} |\phi_\alpha \boldsymbol{\nabla}\phi_\beta - \phi_\beta \boldsymbol{\nabla}\phi_\alpha|^2$$

Two-phase interface, N=2

$$\phi_\beta = 1 - \phi_\alpha$$
$$\boldsymbol{\nabla}\phi_\beta = -\boldsymbol{\nabla}\phi_\alpha$$
$$\boxed{\kappa |\boldsymbol{\nabla}\phi_\alpha|^2}$$

Multi-phase model formulation





$$\mathcal{F}_{\text{int}} = \int_V f_{\text{grad}} + f_{\text{well}} \,\mathrm{d}V$$

$$= \int_V \kappa |\nabla \phi|^2 + \Omega \phi^2 (1-\phi)^2 \mathrm{d}V$$

$$f_{\text{well}}^{\text{Moelans}} = \tilde{\Omega} \left(\sum_\alpha \sum_{\beta>\alpha} \chi_{\alpha\beta} \phi_\alpha^2 \phi_\beta^2 + \sum_\alpha \left(\frac{\phi_\alpha^4}{4} - \frac{\phi_\alpha^2}{2} \right) + \frac{1}{4} \right)$$

$$f_{\text{well}}^{\text{Toth}} = \tilde{\Omega} \left(\frac{1}{2} \sum_\alpha \sum_{\beta>\alpha} \phi_\alpha^2 \phi_\beta^2 + \sum_\alpha \left(\frac{\phi_\alpha^4}{4} - \frac{\phi_\alpha^3}{3} \right) + \frac{1}{12} \right)$$

$$f_{\text{well}}^{\text{Garcke}} = \sum_\alpha \sum_{\beta>\alpha} \Omega_{\alpha\beta} \phi_\alpha^2 \phi_\beta^2 + \sum_\alpha \sum_{\beta>\alpha} \sum_{\gamma>\beta} \Omega_{\alpha\beta\gamma} \phi_\alpha^2 \phi_\beta^2 \phi_\gamma^2$$

$$\Bigg\} \; \Omega \phi^2 (1-\phi)^2$$

Literature review - 1

Garcke, Nestler, Stoth (1999) SIAM J. APPL. MATH. Vol. 60, No. 1, pp. 295–315

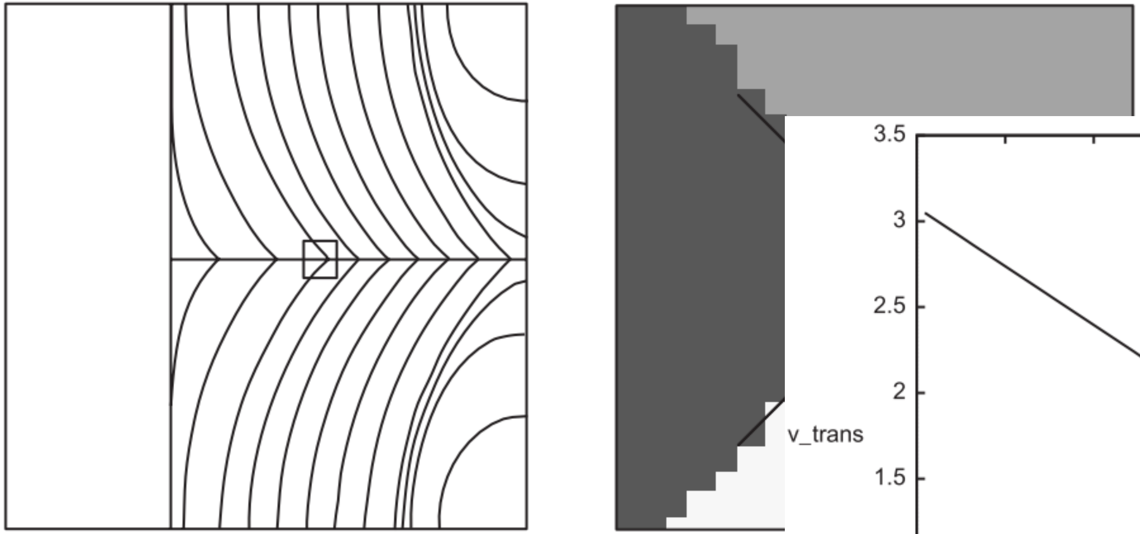
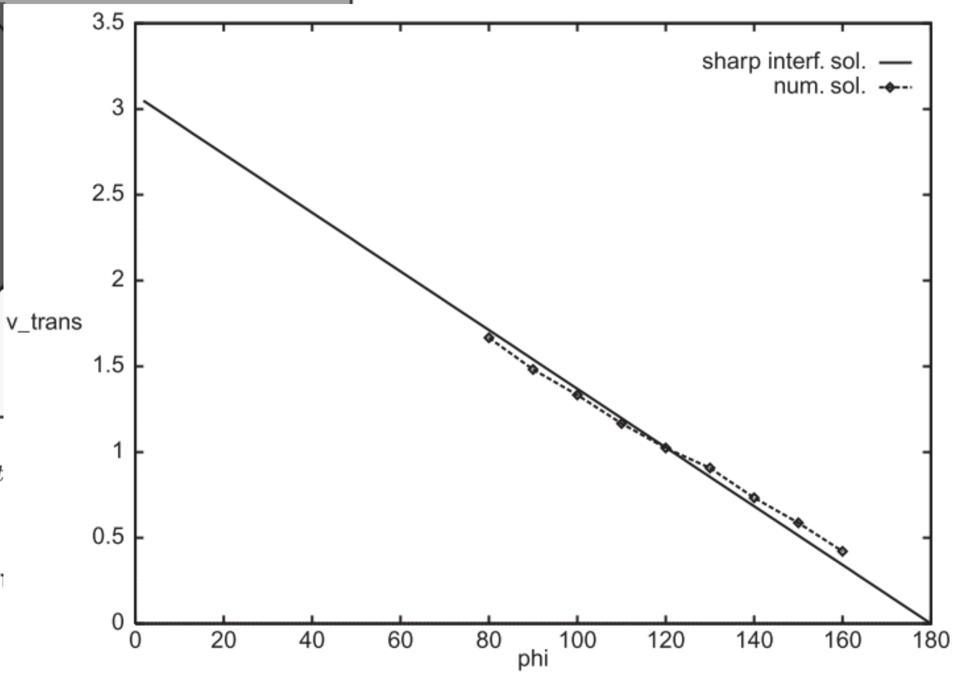
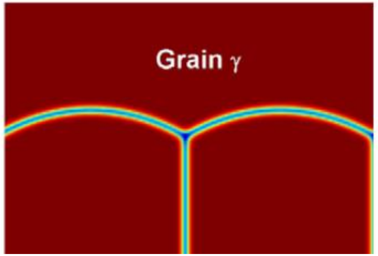


FIG. 7. *Simulated motion of the interfaces and the triple junct configuration for different times.*

$$f_{iso}(\mathbf{u}, \nabla \mathbf{u}) := \sum_{i<j} \frac{\tilde{\sigma}_{ij}}{\tilde{\mu}_{ij}} |u_i \nabla u_j - u_j \nabla u_i|^2. \qquad \Psi_{st}($$



Literature review - 2



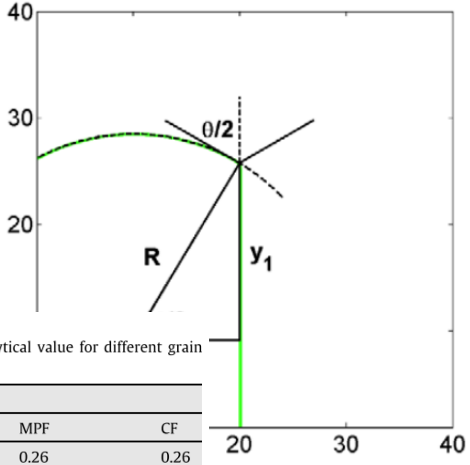
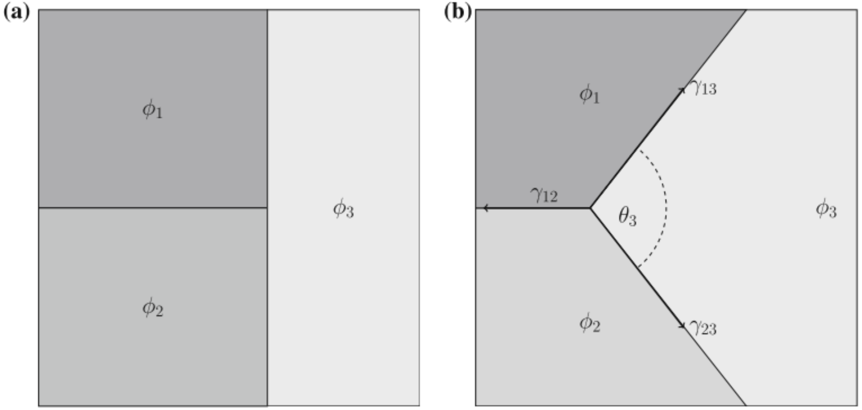


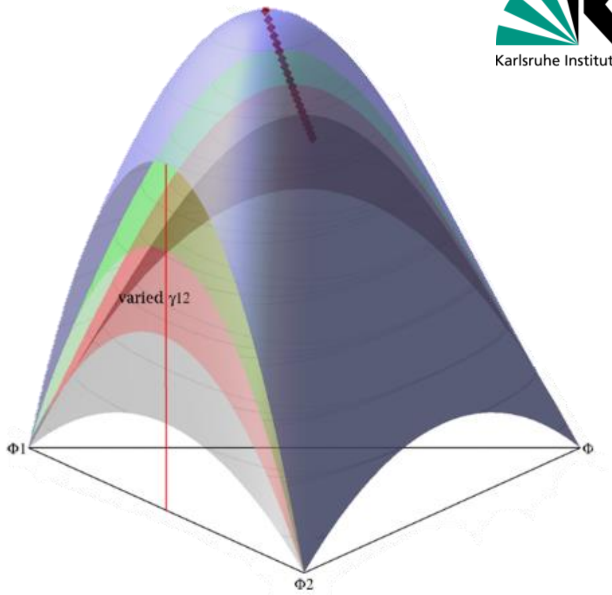
Table 3
Equilibrium angle at the triple junction and temporal evolution of the area of grain α for the MPF and CF model are compared with the analytical value for different grain boundary energy ratios $\sigma_{\alpha\beta}/\sigma_{\alpha\gamma}$, different grid spacings Δx and different interface widths ε. $\gamma_{\alpha\beta\delta}$ in the MPF potential is 3.0 for all cases.

σ	Δx, ε	θ			dA_α/dt		
		Anal.	MPF	CF	Anal.	MPF	CF
$\sigma_{\alpha\beta} = \sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.1$ $\varepsilon = 0.5$	120°	119°	119°	0.25	0.26 (2.8%)	0.26 (4.0%)
$\sigma_{\alpha\beta} = \sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.2$ $\varepsilon = 1.0$	120°	119°	118°	0.25	0.26 (2.8%)	0.26 (4.3%)
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.2$	$\Delta x = 0.1$ $\varepsilon = 0.5$	103°	100°	105°	0.25	0.26 (6.0%)	0.25 (1,1%)
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.2$	$\Delta x = 0.2$ $\varepsilon = 1.0$	103°	100°	104°	0.25	0.26 (6.0%)	0.25 (0.2%)
$\sigma_{\alpha\beta} = 0.2$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.2$ $\varepsilon = 0.5$	133°	135	133°	0.20	0.19 (5.9%)	0.20 (0,1%)
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.175$	$\Delta x = 0.2$ $\varepsilon = 1.0$	89°	84°	97°	0.25	0.27 (8.9%)	0.24 (4,7%)
$\sigma_{\alpha\beta} = 0.175$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.2$ $\varepsilon = 1.0$	139°	139°	139°	0.175	0.174 (0.6%)	0.173 (0.8%)
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.36$	$\Delta x = 0.2$ $\varepsilon = 1.0$	139°	139°	139°	0.25	0.25 (0.6%)	0.24 (0.8%)

"Comparative study of two phase-field models for grain growth" Moelans, Wendler, Nestler (2009) doi: 10.1016/j.commatsci.2009.03.037

Literature review - 3





$$\omega(\boldsymbol{\phi}) = \begin{cases} \overbrace{\frac{16}{\pi^2} \sum_{\substack{\alpha,\beta=1 \\ (\alpha<\beta)}}^{N,N} \gamma_{\alpha\beta}\phi_\alpha\phi_\beta}^{\text{second}-\text{order term}} + \overbrace{\sum_{\substack{\alpha,\beta,\delta=1 \\ (\alpha<\beta<\delta)}}^{N,N,N} \gamma_{\alpha\beta\delta}\phi_\alpha\phi_\beta\phi_\delta}^{\text{thirdorder term}}, & \boldsymbol{\phi} \in \Delta^{N-1}, \\ \infty, & \boldsymbol{\phi} \notin \Delta^{N-1}. \end{cases}$$

“Calibration of a multi-phase field model with quantitative angle measurement” Hötzer et. al., (2016) doi: 10.1007/s10853-015-9542-7

Literature review - 4

“Discussion of the Accuracy of the Multi-Phase-Field Approach to Simulate Grain Growth with Anisotropic Grain Boundary Properties” Eiken (2020) doi: 10.2355/isijinternational.ISIJINT-2019-722

$$v_n(x) = M_B \sigma_B \kappa(x) = M_B \sigma_B \frac{-y''(x)}{1+(y'(x))^2)^{1.5}}$$

$$v_x = M_B \sigma_B \frac{(\pi - 2\theta)}{H} = M_B \sigma_B \frac{2}{H} \arcsin\left(\frac{\sigma A}{2\sigma_B}\right)$$

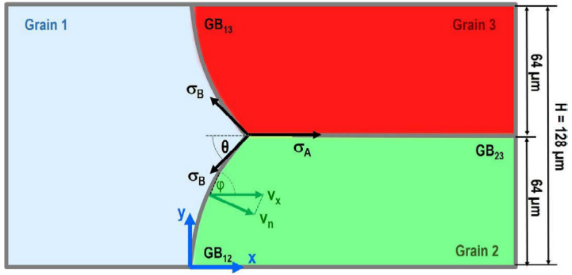
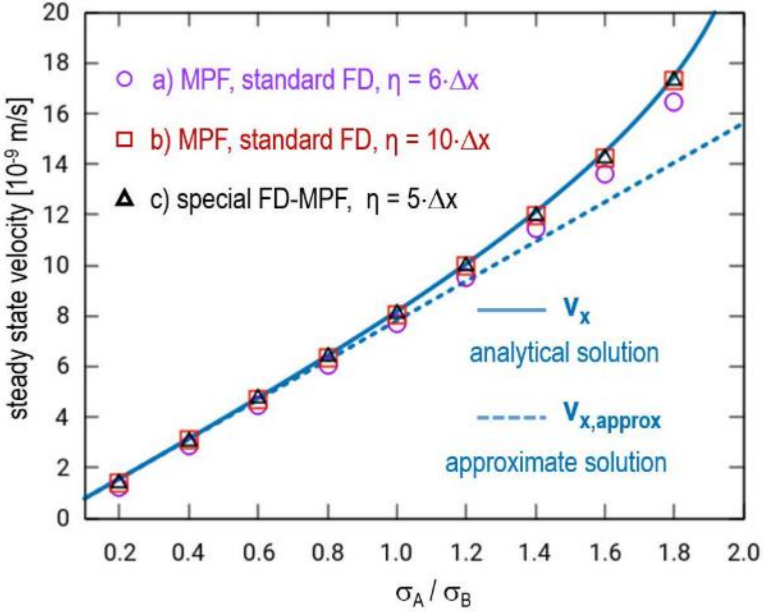


Fig. 1. Tri-crystal arrangement moving with steady-state velocity in horizontal direction. The existence of an unambiguous analytical solution enables a quantitative accuracy evaluation for anisotropic grain growth predictions. (Online version in color.)



Literature review - summary

Karlsruhe Institute of Technology

- Large zoo of model notations and formulations
- Analytical solution for triple junction theoretically well-known but still confusion within scientific community
- Varying simulation setups and varying metrics

σ	Δx, ε	θ		
		Anal.	MPF	CF
$\sigma_{\alpha\beta} = \sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.1$ $\varepsilon = 0.5$	120°	119°	119°
$\sigma_{\alpha\beta} = \sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.2$ $\varepsilon = 1.0$	120°	119°	118°
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.2$	$\Delta x = 0.1$ $\varepsilon = 0.5$	103°	100°	105°
$\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.2$	$\Delta x = 0.2$ $\varepsilon = 1.0$	103°	100°	104°
$\sigma_{\alpha\beta} = 0.2$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$	$\Delta x = 0.2$ $\varepsilon = 0.5$	133°	135	133°

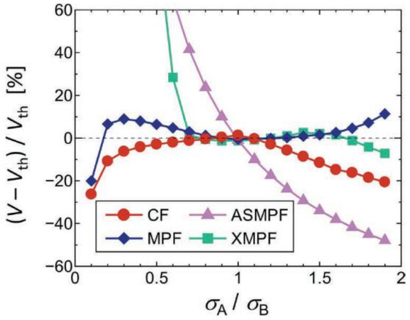
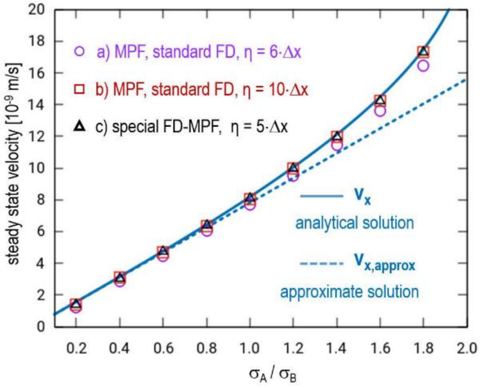
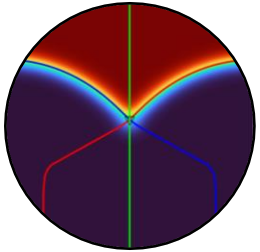


Fig. 3. Variations in relative error $(V - V_{th})/V_{th}$ depending on boundary energy ratio σ_A/σ_B, as calculated from different phase-field models. (Online version in color.)

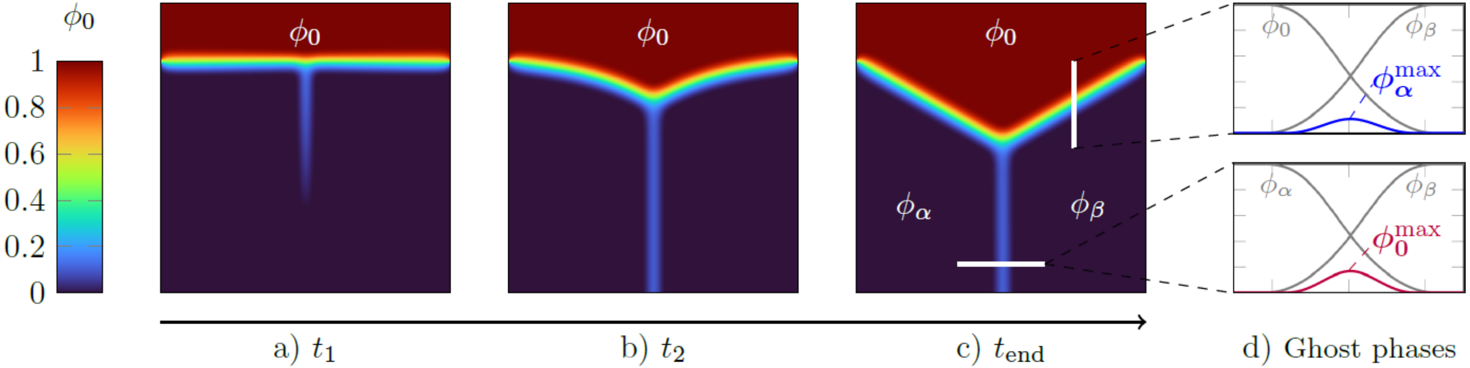




What can we learn?

S. Daubner, P. W. Hoffrogge, M. Minar, and B. Nestler. Triple junction benchmark for multiphase-field and multi-order parameter models. Computational Materials Science, 219:111995, 2023

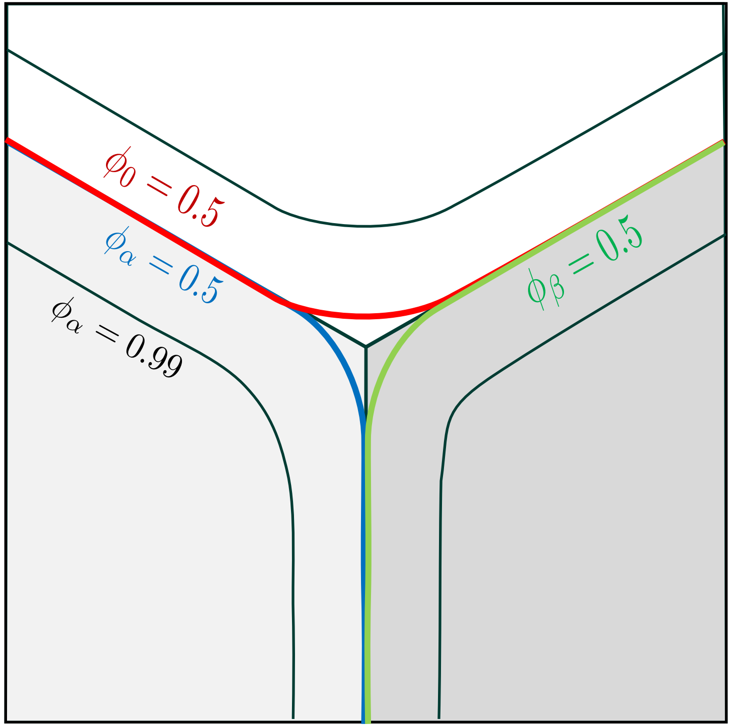
Static triple junction

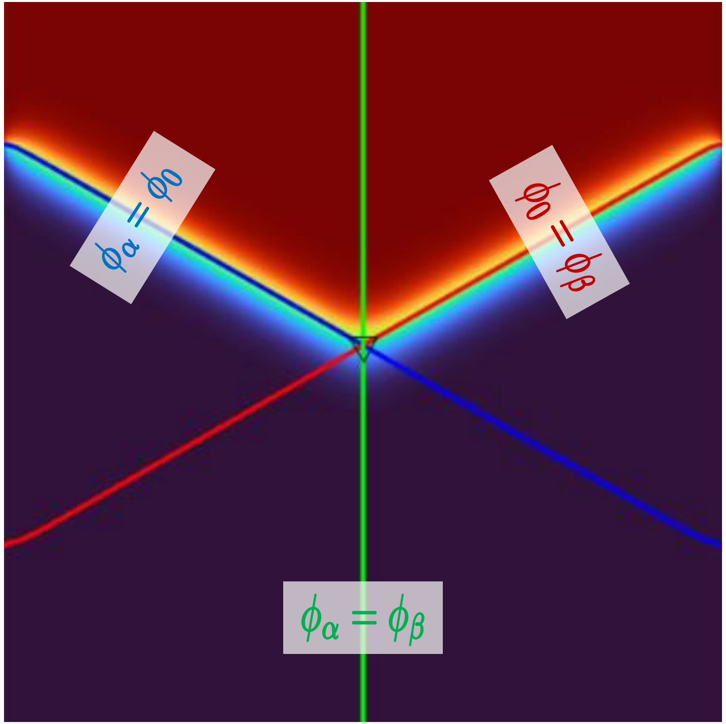


Metrics

- Total interfacial energy $\mathcal{F}_{int}(\phi, \nabla\phi) = \int_V f_{grad}(\phi, \nabla\phi) + f_{pot}(\phi)\mathrm{d}V$ $\quad \epsilon = |\mathcal{F}^n - \mathcal{F}^{n-1}|/\mathcal{F}^n$
- Dihedral angle θ is computed from position of the triple point. The numerical triple point is defined by the intersection of isolines $\varphi_\alpha = \varphi_0$ and $\varphi_\beta = \varphi_0$
- Spurious occurrence of φ_α, φ_β and φ_0 in the respective other two-phase interface

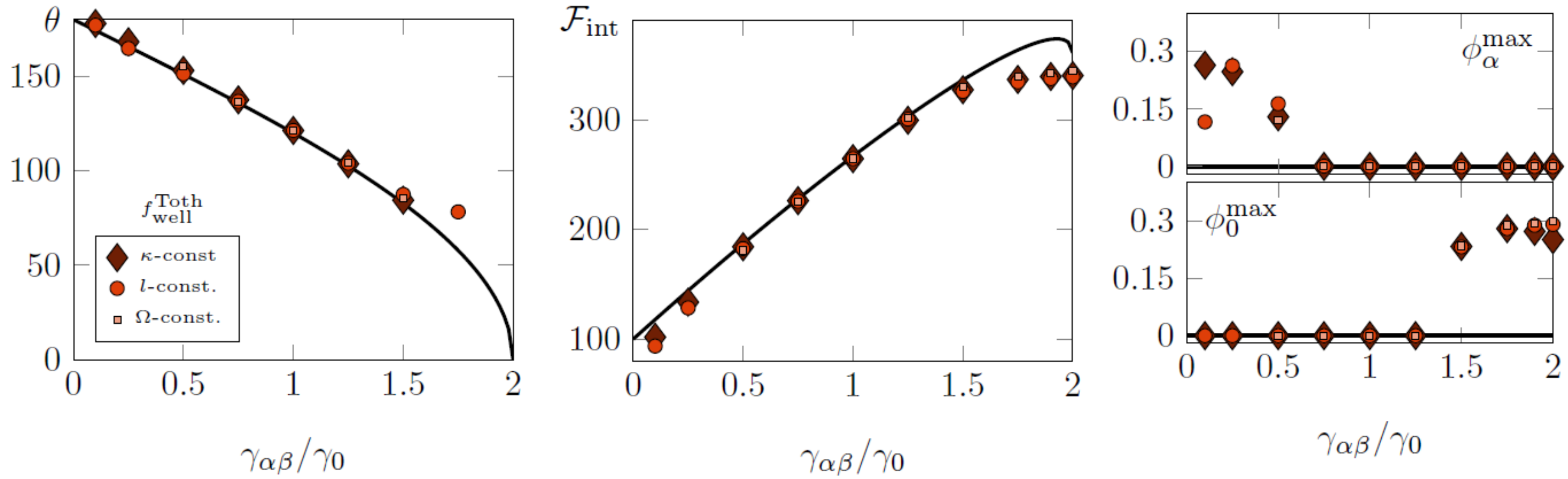
Static triple junction





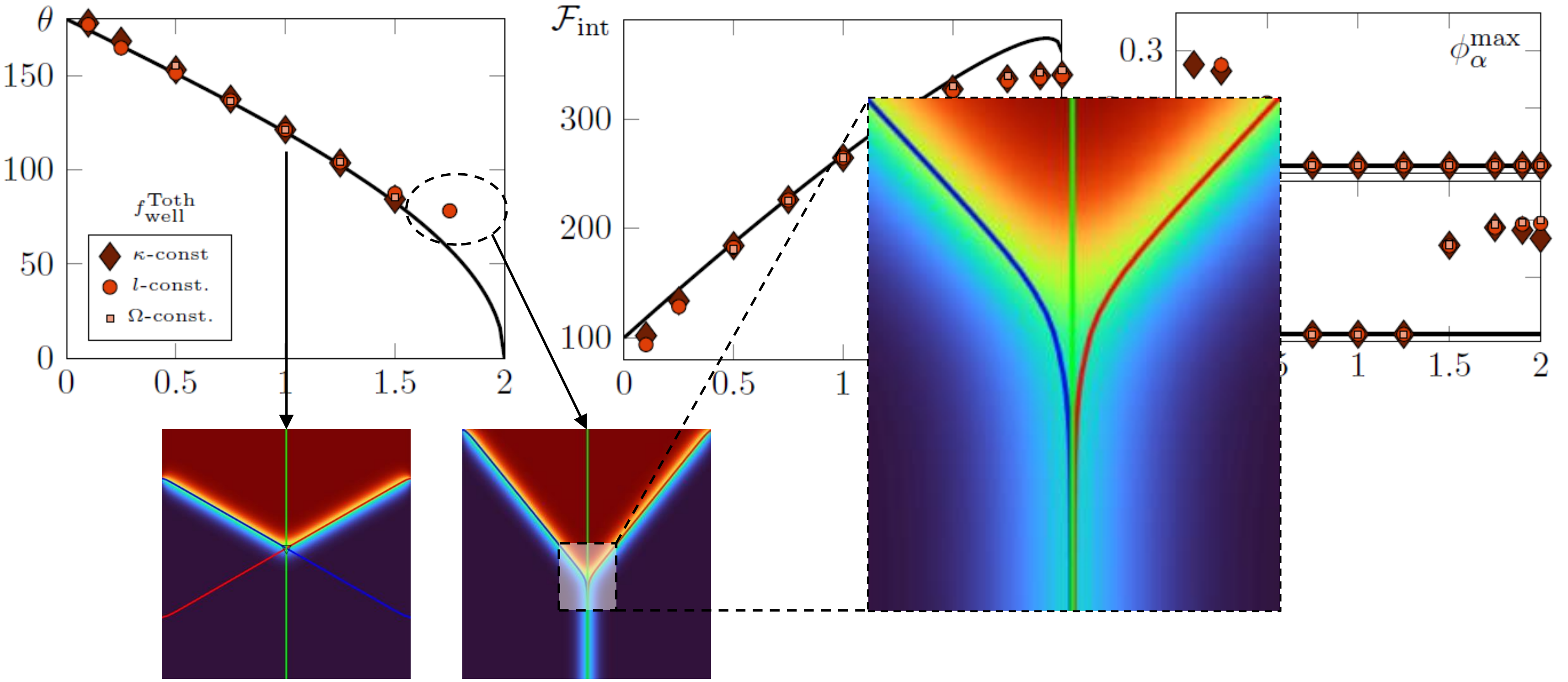
Static triple junction

Multi-order parameter models



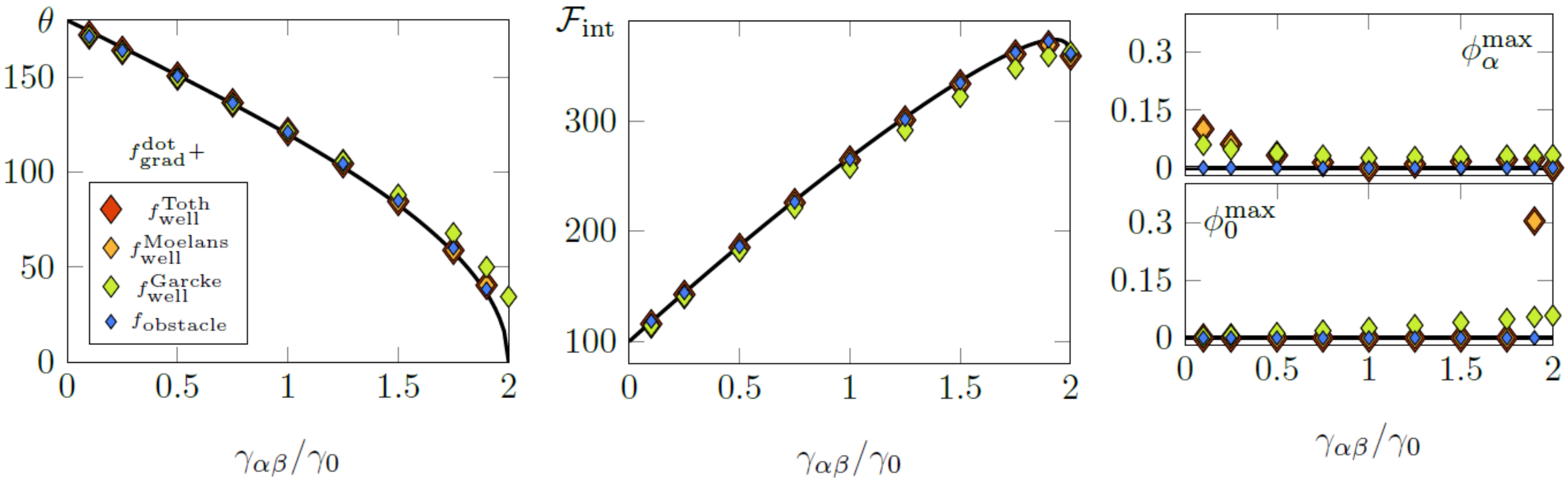
Static triple junction

Multi-order parameter models



Static triple junction

Multiphase-field models



Steady-state triple junction

Metrics

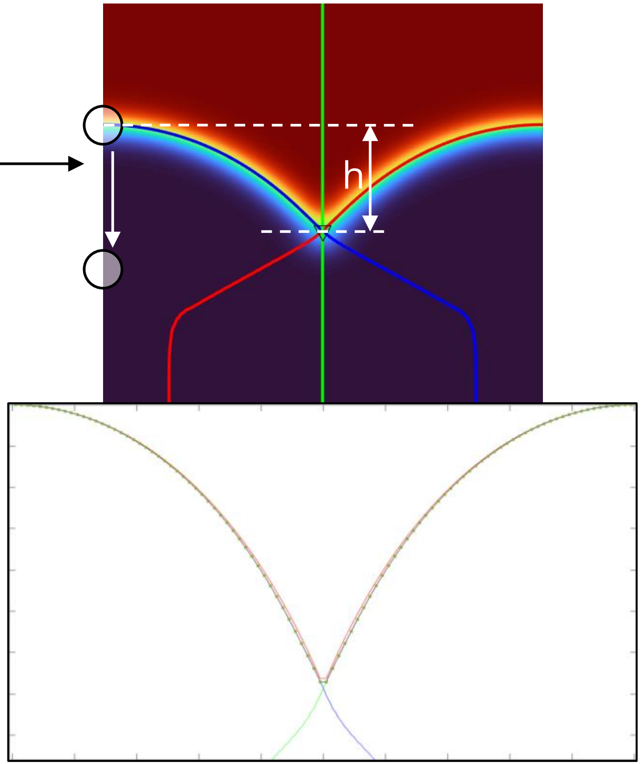
- Steady-state velocity is measured at left boundary

  $V = |(y^{x=0}_{\phi_0=\phi_\alpha})^n - (y^{x=0}_{\phi_0=\phi_\alpha})^{n-1}|/\Delta t$

- Dihedral angle θ is computed from position of the profile height. The numerical triple point is defined by the intersection of isolines $\varphi_\alpha = \varphi_0$ and $\varphi_\beta = \varphi_0$

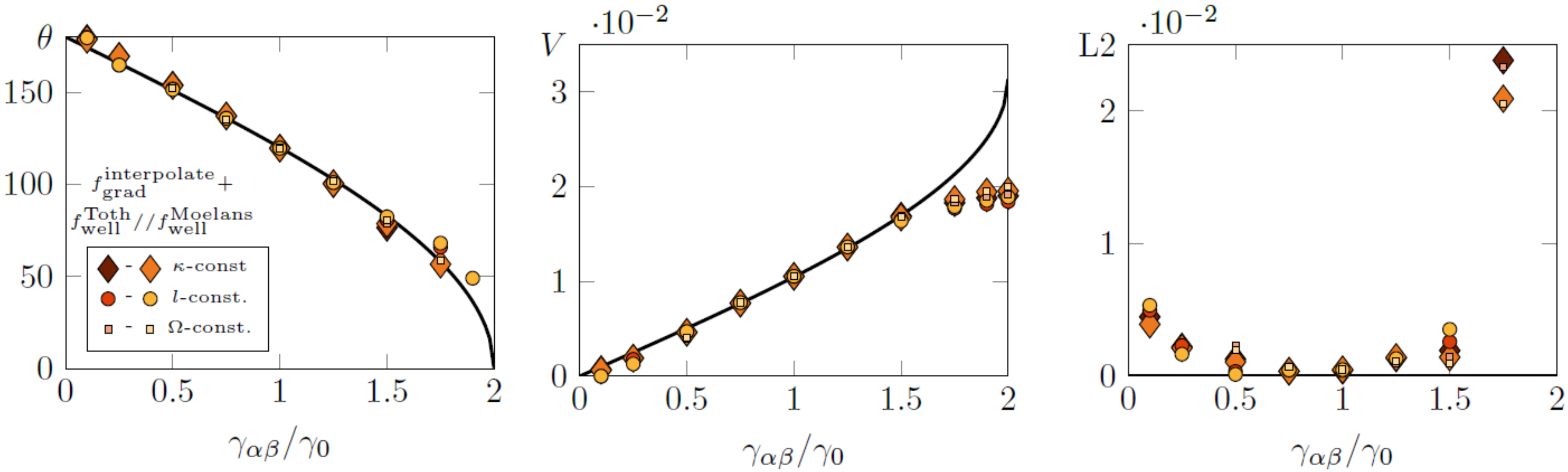
- (Mis-)match of numerical and analytical results for grain boundary geometry is measured by L2-norm

  $||y_{\text{numeric}} - y_{\text{analytic}}||_2 = \frac{1}{W}\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i^{\text{numeric}} - y_i^{\text{analytic}})^2}$



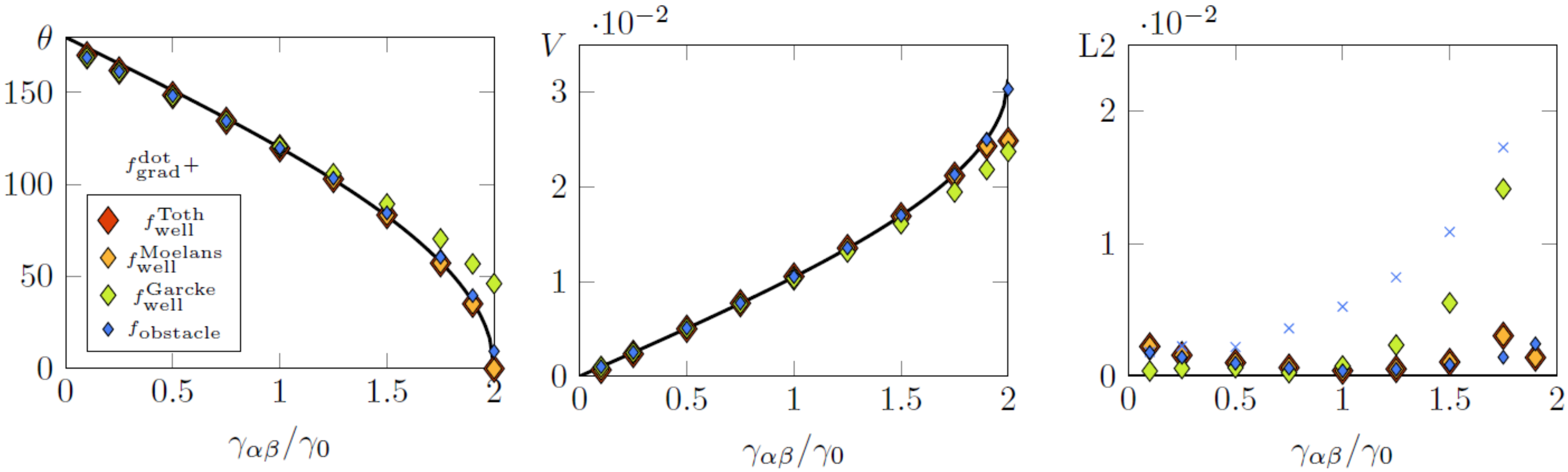
Steady-state triple junction

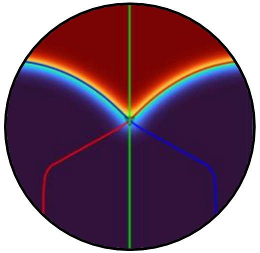
Multi-order parameter models



Steady-state triple junction

Multiphase-field models





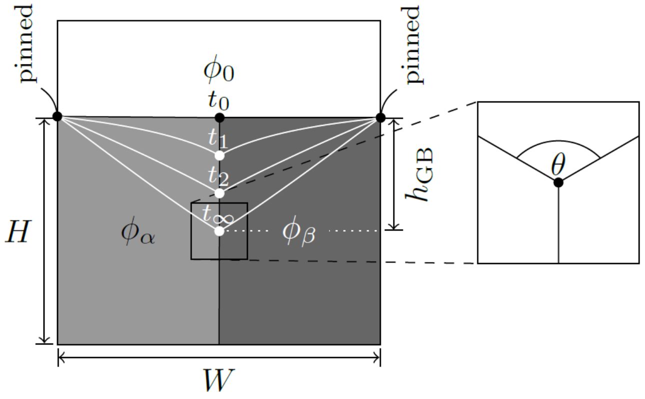
What else could we learn?

Triple junction benchmark

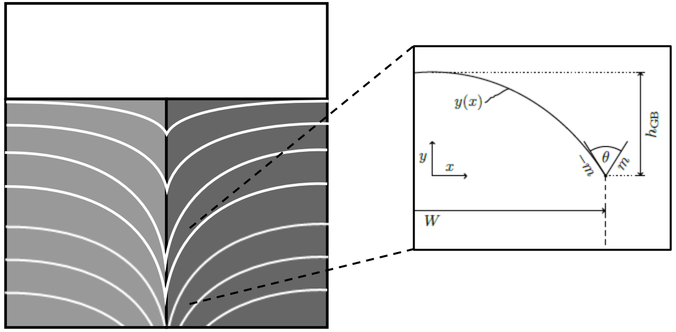
Possible studies

- Comparison of various model formulations
- Comparison of discretization, quantification of discretization error
- Evaluate computational cost/ efficiency (between various codes/ implementations)

Static triple junction



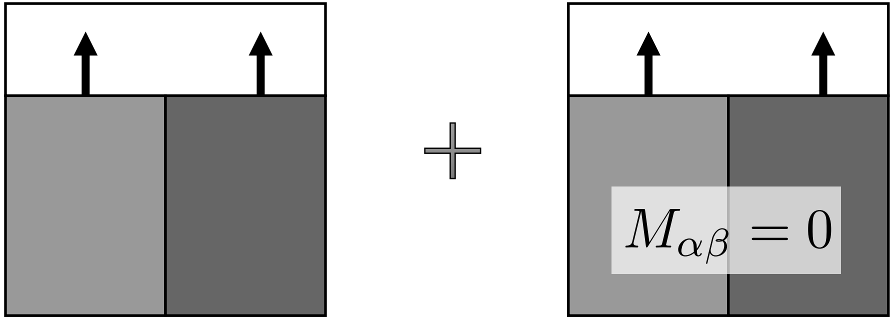
Steady state triple junction



Triple junction benchmark

Modifications to the benchmark

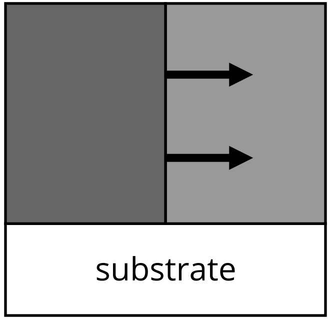
- Add driving force → solidification triple junction



- Modify pairwise phase mobilities

$$M_{\alpha\beta} = M$$

$$M_{\alpha 0} = M_{\beta 0} = 0$$



N. Enugala, Dissertation, 2021
“Some refinements in the phase-field and sharp interface treatments of eutectic growth”

Thank you for your attention!

Any Questions?

I thank all my colleagues who are involved in this work through vivid discussions. Special thanks to Paul Hoffrogge, Britta Nestler, Daniel Schneider and Ephraim Schoof.

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Comparison of Moelans and Toth potentials