Diffuse interface models provide an elegant description of microstructure evolution involving phase or domain boundary motion. As compared to sharp interface descriptions, the difficult problem of explicit interface tracking is avoided, which allows for any topological evolution of the phase or domain structures, such as interface instabilities, shape bifurcations, coagulation events, particle nucleation or dissolution. Phase-field methods are extensively used in the simulation of complex evolution problems, such as solidification [2], solid-state transformations [3], crack propagation [4–7], dislocation dynamics [8–10], ferro-electric domain evolution [11], grain growth [12, 13], as well as many other [14].

Quite often, the width of the diffuse interface appears to be the smallest length-scale in the system. Obviously, in all these cases one is interested in choosing the smallest possible width, while still keeping the benefits from the diffuse interface description. So far, artificial gird friction or grid pinning in the phase-field equation, which naturally results from the numerical discretization, has been the major limiting factor in this regard.

Recently Finel et al. found a striking new way to eliminate these effects in the 1D phase-field equation. The key is to restore the translational invariance (TI), that has been broken by the numerical discretization. Then a one-grid point interface resolution is possible without grid pinning [1]. The method is related to previous suggestions to improve the numerical performance of phase-field solvers via a nonlinear scaling of the phase-field equation [15, 16]. Similar formulations involving the sectional defined sinus like phase-field profile have been independently proposed by J. Eiken [17].

We consider the stationary motion of a planar interface between two phases at different bulk free energy levels. The bulk free energy difference drives the growth of the low energy phase on the expense of the high energy phase. The coupling of the phase-field to the bulk energy density difference is prototypical for many advanced phase-field models, where the driving forces are calculated from local concentrations or strains [18–27].

Keeping the simple cubic computational grid with grid spacing $h$ as fixed, we investigate the influence of varying interface orientations on the stationary motion, see Fig. 1. Deviations of the resulting interface velocity from theorectic expectations reveal the effect of artificial grid friction and pinning.

### Sharp Phase-Field Modeling

The derivation of the phase-field models is stated from a Helmholtz free energy functional

$$ F[\phi] = \int_V \left( \frac{\lambda \Gamma (\nabla \phi)^2}{2C_T} + \Gamma \frac{g(\phi, \lambda)}{\lambda C_T} + \mu \rho(\phi) \right) dV, \quad (1) $$

where $V$ is the volume of the system, and $\nabla$ denotes the gradient. The equilibrium potential $g(\phi, \lambda)$, depends on the phase-field $\phi$ and and on $\lambda = \lambda/h$. It has to vanish at the two local minima at $\phi = 0$ and $\phi = 1$, which correspond to the distinct phases of the system. $\lambda$ denotes the width of the diffuse interface, $\Gamma$ is the interface energy density, and $C_T$ is a dimensionless calibration factor. The calibration factor $C_T$ is calculated via $C_T = \int f(\phi_0, \nabla \phi_0)_{\mu = 0} d\Gamma$, where $n$ denotes the interface normal direction, and the phase-field $\phi_0$ is given by Eq. (3). For further information, we refer to the supplementary material. A positive bulk free energy density difference $\mu$ favors the growth of phase $\phi = 0$ on the expense of phase $\phi = 1$. The interpolation function $\rho(\phi)$ satisfies $\rho(0) = 0$ and $\rho(1) = 1$ and further provides vanishing slope at $\phi = 0$ and $\phi = 1$.

![Figure 1. The simulation configuration: Stationary motion of a planar interface.](image-url)
The time derivative of the phase-field, $\partial_t \phi$, is proportional to the variational derivative of the free energy functional (1), $-\delta_\phi F$. We write the equation of motion as $3\Gamma \cdot \partial_t \phi = -2M \delta_\phi F$ [28], and obtain

$$\partial_t \phi = \frac{2M}{3\Gamma} \left( \nabla^2 \phi - \frac{1}{\lambda^2} \partial_\phi g(\phi, \tilde{\lambda}) \right) - \frac{2M}{3\Gamma} \mu \partial_\phi p(\phi),$$  

(2)

where $\nabla^2$ denotes the Laplace operator, $M$ is a kinetic coefficient comparable to a diffusion coefficient with dimension $[M] = m^2 s^{-1}$, and $\partial_\phi$ abbreviates the partial derivative with respect to the phase-field $\phi$.

During stationary interphase motion a constant amount of energy per unit time interval dissipates via the preceding phase transformation. Thus, the phase transformation rate and interface velocity is exactly determined by the diving force $\mu$ via $v_{th} = -M\mu/\Gamma$. Choosing $g(\phi, \infty) = 8\phi^2 (1 - \phi^2)$ and $p(\phi) = p_1(\phi) = \phi^2 (3 - 2\phi)$, the following special analytic solution for Eq. (2) can be found

$$\phi_0(\mathbf{r}, t) = \left(1 - \tanh \left(2(\mathbf{r} \cdot \mathbf{n} - r_n) / \lambda \right)\right)/2.$$  

(3)

Here $\mathbf{n}$ is the unit normal interface vector, $\mathbf{r}$ is the position vector and $r_n = v_{th} t$ denotes the central interface position, moving with the velocity $v_{th}$.

For vanishing driving forces $\mu = 0$ and vanishing phase-field motion $\partial_t \phi = 0$, Eq. (2) reduces to the equilibrium condition, which reads in the discrete form as

$$\sum_{k=1}^3 \lambda^2 / h^2 \left( \phi_{i+k} - 2\phi_i + \phi_{i-k} \right) - \partial_\phi g(\phi, \tilde{\lambda}) = 0,$$  

(4)

where $i$ denotes the grid points of the simple cubic 3D numerical lattice and the lattice vector $\mathbf{u}_k$ connects two neighboring grid points along the direction $\mathbf{e}_k$ with a spacing $h = |\mathbf{u}_k|$. Similar to [1], the equilibrium potential is decomposed into $g(\phi, \lambda) = \sum_{k=1}^3 g_k(\phi, \lambda)$. The 3D equilibrium condition (4) is satisfied, if all three 1D cartesian contributions are independently satisfied at the same time. Interestingly, the $k$–th component of the condition (4) can be satisfied at any real time during the propagation of the interface by using the following addition property of the hyperbolic tangent profile (3) [1]:

$$\phi_{i \pm \mathbf{u}_k} = \frac{(1 \pm a_k) \phi_i}{1 \pm (2\phi_i - 1) a_k},$$  

(5)

where the grid coupling parameters $a_k$ are defined as

$$a_k = \tanh \left(2\mathbf{u}_k \cdot \mathbf{n} / \lambda \right) = \tanh \left(2hn_k / \lambda \right).$$  

(6)

$n_k$ denotes the projection of $\mathbf{n}$ onto the direction $\mathbf{e}_k$. Using Eq. (5) and (4) we obtain the $k$–th component of the derivative of the equilibrium potential

$$\partial_\phi g_k(\phi, \tilde{\lambda}) = a_k^2 \lambda^2 \frac{4\phi (1 - \phi) (1 - 2\phi)}{1 - a_k^2 (1 - 2\phi)^2}.$$  

(7)

The actual potential is given by the integral, $g(\phi, \tilde{\lambda}) = \int_0^\infty \sum_k \partial_\phi g_k(\phi', \tilde{\lambda}) d\phi'$ (also see [1]). In the continuum limit $h \to 0$, this potential converges the original quartic double well potential, since $\lim_{n_{th} \to 0} \lambda^2 d_k^2 = 4$.

For an accurate determination of the local grid coupling parameters $a_k$, we propose the following scheme based on the addition property Eq. (5), $a_k = (a_k^+ + a_k^-)/2$, where

$$a_k^\pm = \frac{\pm (\phi_{i \pm \mathbf{u}_k} - \phi_i)}{\phi_i - 2\phi_{i \pm \mathbf{u}_k} \phi_i + \phi_{i \pm \mathbf{u}_k}}.$$  

(8)

By inserting the derivative (7) into the equilibrium condition (4) the explicit dependence on the interface width $\lambda$ cancels out. Then, the phase-field width is solely controlled by the grid coupling parameters (8). In contrast to the original formulation by Finel et al. [1], here, these parameters depend on the interface normal vector, which is calculated locally by (8). Consequently, without additional length control of $\mathbf{n}$ the width of the diffuse interface wouldn’t be defined in the model. Therefore, we locally calculate the components $n_k = \lambda \arctan h a_k/2$, restore unit length via $\mathbf{n}^{\text{new}} = \mathbf{n} / |\mathbf{n}|$ and re-calculate corrected grid coupling parameters $a_k^{\text{new}}(\mathbf{n}^{\text{new}})$ using (6).

Testing the translational invariance, we calculate the system integral over the equilibrium condition (4) using the discrete 3D phase-field as given by the ideal profile function (3). When the ideal profile is moved across several grid points, the discrete force integral oscillates. In Fig. 2, we plot the force oscillation amplitude $A$ for different interface orientations. Large oscillation amplitudes indicate broken translational invariance (TI), as for the classical no TI formulation shown by the black curve. Fixed grid coupling parameters, as proposed by Finel et al. [1], restore translational invariance for fixed interface orientations (fixed TI). The new TI model (green curve) restores translational invariance locally in the interface normal direction, leading to evenly small force oscillation amplitudes $A$, regardless of the interface orientation.
rithmic complexity, than the original model proposed by A. Finel.

Possible range of driving forces Grid friction and pinning during stationary motion has been studied earlier [29, 30]. It leads to a reduction of the average interface width and velocity. Both, the velocity and the width oscillate as the center of the interface passes one grid point after the other. With decreasing phase-field width, we obtain increasingly larger drops of the average values as well as increasing oscillation amplitudes. This culminates in a vanishing velocity, where the phase-field is pinned the to computational grid.

In Fig. 3, we plot the relative deviation of the measured interface velocity $v$ from its theoretic expectation $v_{th}$ as function of the driving force $\hat{\mu} = \mu h / \Gamma$. The mean error is depicted by the thick solid/dashed lines. The continuous lines indicate a constant time resolution of $M \mu \Delta t / (\Gamma h) = 6 \cdot 10^{-8}$, where $\Delta t$ is the time step. For all these driving forces the interface center has passes at least four grid points. The dashed lines indicate shorter simulations, where the interface center has not been advanced by the distance of a full grid point. The difference between the oscillation amplitude and the mean value is plotted as transparently colored area. When the colored area is found above the mean value, we have the “healthy” situation that the measured interface velocity oscillates around the theoretic expectation. In contrast, colored areas below the mean value denote the “unhealthy” case, when the theoretic expectation is located somewhere outside the oscillation interval.

Without restoring of translational invariance (no TI), grid friction leads to substantial errors in the interface velocity. Even for interfaces as wide as $\lambda = 5$, grid pinning occurs for driving forces below $\mu h / 4 \Gamma < 10^{-7}$. In contrast, the 1D SPFM is not subjected to this limitation, even if the phase-field width is chosen as small as $\lambda = 0.6$. For the SPFM the error in the interface velocity only depends on the error in the time discretization!

Conceptually allowed values for driving forces have to be small enough to guarantee the meta-stability of the high energy phase. In other words, the two local minima of the potential energy at $\phi = 0$ and $\phi = 1$ have to be separated by a maximum. Considering the potentials, $g(\phi, \infty)$ and $p_3(\phi)$, this requires the absolute value of the driving force to be below $|\mu| < 4 / \lambda$, with $\hat{\mu} = \mu h / \Gamma$ denoting the dimensionless driving force. For a fixed interface energy the range of possible driving forces is smaller the wider the interface is! This circumstance can be quite restricting as the appearance of interface instabilities, such as the diffusional Mullins-Sekerka [31] or the elastic Asaro-Tiller-Grinfeld instability [32, 33], require the interface energy to be comparably small [34, 35]. Using the SPFM potentials $p_3(\phi)$ and $g(\phi, \lambda = 0.6)$ together with the energy calibration $C_T = 0.238$, we calculate the range of possible driving forces for an interface as sharp as $\lambda = 0.6$ to be $|\mu| \lesssim 230$! The upper bounds for the driving force for the different cases are indicated by respectively colored dash-dotted vertical lines in Fig. 3.

Using interpolation functions of higher polynomial order can also extend the theoretic range of possible driving forces. However, the effect of using interpolation functions other than the natural function, $\partial_\phi p_3 = 6 \phi(1 - \phi)$, for which a steady state solution of Eq. (2) exists, is that the nonequilibrium phase-field profile is altered, see Fig. 4. The steeper interpolation function, $\partial_\phi p_5 = 30 \phi^2 (1 - \phi)^2$ [19, 29], provide decreasing phase-field widths with increasing driving forces. Lower order interpolation functions, such as $\partial_\phi p_{\text{min}} = 8 \sqrt{\phi(1 - \phi)} / \pi$ [20], lead to an increase in phase-field width as the driving force increases. The 1D SPFM in conjunction with $p_5$ provides significant oscillations in the measured interface width for $\hat{\mu} \geq 1$, as indicated by the dark-orange colored area in Fig. 4. A further extension of the range of possible driving forces within the 1D SPFM by using $p_5(\phi)$ requires to account for the altered nonequilibrium profile.

Frictionless interfaces motion in 3D In 3D the direction of interface motion appears as an important additional degree of freedom. We consider interface orientations $\mathbf{n}$ resulting from rotations around the two different axes $[001]$ and $[011]$, as sketched in Fig. 5. The simulation of interface propagation in directions other than
the \((100)\) -directions of the computational grid requires special wetting-angle boundary conditions for the phase-field \([36-38]\). These have to account for the contact angle \(\alpha\) between the boundary direction \(\mathbf{e}_b\) and the interface normal \(\mathbf{n}\). The boundary value at \(\mathbf{b}\) is calculated as

\[
\phi_b = \frac{(1 - a_n) \phi_{b+u_b}}{1 - a_n (2 \phi_{b-u_b} - 1)},
\]

with \(a_n = \tanh(2h \sin \alpha / \lambda)\). The idea is to calculate the boundary value at \(\mathbf{b}\) from the neighboring phase-field value at \(\mathbf{b} + \mathbf{u}_b\) using the addition theorem for the hyperbolic tangent profile \((5)\), and imposing a profile-shift by the length \(s_n = h_k \sin \alpha\) along the interface normal direction.

In Fig. 5, we compare the orientation dependent error in the interface velocity for two different models. The classical model with no restored translational invariance (no TI) and \(\tilde{\lambda} = 5\) is shown in blue color. The green curve in Fig. 5 shows the behavior of the new model, where translational invariance has been restored in the direction of interface motion. It provides very accurate interface velocities for all orientations, even if the phase-field width is as small as \(\lambda = 0.6\). As for the 1D SPFM, the resulting velocity error only depends on the error in the time discretization. Thus, the new model indeed provides frictionless motion of planar interfaces with arbitrary orientations! This study is partly comparable to the sphericity study of a growing sphere as presented in Fig. 2 in \([1]\) showing the respective behavior of the original 3D SPFM.

**Diffusion limited solidification** The feasibility to deal with time dependent and inhomogeneous driving forces \(\mu\) is demonstrated by considering the thermal diffusion limited solidification of a pure substances within a thermally isolated system. We introduce the dimensionless temperature field \(U(x,t) = C (T(x,t) - T_M) / L\), where \(T_M\), \(C\) and \(L\) denote melting temperature, latent heat and heat capacity, respectively. \(\mu\) is proportional to the temperature field by \(\mu = U T_0 / \Delta T\), where \(\Delta T = \Gamma T_M C / L^2\) denotes the capillary length, which scales with the interface energy density \(\Gamma\). The temperature obeys a diffusion equation, \(\partial_t U = D \nabla^2 U + \partial_t \mu \partial_t \phi\), with the thermal diffusion coefficient \(D\) \([39-41]\). The new model is capable to simulate diffusion limited solidification with interfaces as sharp as \(\lambda = 0.6\)! For an initial undercooling temperature of \(U(x,0) = -0.3\) the smallest possible capillary length is \(d_0 / h = 0.003\). This value is about a factor 30 smaller than the smallest value used in \([29]\). It is small enough to resolve a full dendrite with side-arms within a \(60 \times 30 \times 30\) -system (see Fig. 6). Such a small capillary length to grid spacing ratio relates to a maximal dimensionless driving force of \(\mu_{\text{max}} = U(x,0) / d_0 = 100\). Therefore, the SPFM related extension of the range of possible driving forces is accessible in practical 3D simulations of thermal diffusion limited solidification!

The interface energy anisotropy, necessary for the dendritic selection \([42]\) visible in Fig. 6, results from the underlying cubic grid. Equilibrium particle shape calculations with conserved phase volumes \([29, 43-45]\) show that for \(\lambda = 0.6\) the new TI model provides a lattice anisotropy corresponding to \(\epsilon_4 = (R_{\text{max}} - R_{\text{min}}) / 2R_{\text{max}}\), or \(\epsilon_4 = 0.064\), or \(\epsilon_4 = 0.881\), where, \(R_{\text{min}}\) and \(R_{\text{max}}\) denote the smallest and largest distance between the nonlinear \(\phi = 1/2\) -contour and the particle's center, respectively.

**Conclusion** The effect of artificial grid friction on the stationary motion of planar interfaces is investigated in a classical phase-field model as well as variants of the Sharp Phase-Field Model (SPFM) \([1]\)

- With a one-grid point interface resolution the SPFM provides a largely extended range of possible driving forces.
- The extended parameter range is accessible in 3D simulations of thermal diffusion limited solidification.
- The newly proposed model with translational in-
variance in the direction of interface motion provides frictionless motion of marginally resolved diffuse interfaces for arbitrary interface orientations.

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* michael.fleck@uni-bayreuth.de

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Whenever, the energy is evaluated across the diffuse interface region, the model should provide the exact amount of energy excess, which corresponds to the imposed value interface energy density $\Gamma$. Therefore, the calibration factor $C\Gamma$ for the interface energy can be calculated via the following line integral

$$C\Gamma = \int f(\phi_0, \partial_i \phi_0)_{\mu=0} d\mathbf{n} / \Gamma,$$

where $\mathbf{n}$ denotes the direction normal to the interface, and $\phi_0$ denotes a phase-field profile function, which contains one respectively oriented interface, where the phase-field variable undergoes the full transition from $\phi = 0$ to $\phi = 1$. In Fig. 7, we plot the interface energy calibration factor $C\Gamma$ as function of the dimensionless interface grid resolution number $\lambda/h$. For the marginally resolved diffuse interfaces, we obtain values for the calibration line integral mentioned above that substantially differ from the continuum value.

1. **Grid friction**

Fig. 8 illustrates the influence from artificial grid friction on the stationary motion of planar interfaces in one dimension. An animated version of Fig. 8 is also provided in the supplementary material. We compare the resulting interface motion for different choices of the ratio between the phase-field width and the numerical grid spacing $\lambda/h$. On top a snapshot of the phase-field values at different grid points (full symbols) around the interface are plotted. This is accomplished by a least square fit of the profile function (Eq. (3) in the manuscript) to the phase-field values, as indicated by the solid lines. Below, first the energy density and then the fitting value for the phase-field width are plotted both as function of the advancing center of the interface $x_0 = v_{th}t$.

Due to artificial grid friction, the average values of the measured interface width and energy are both smaller than the analytic expectations. The squeezed interface propagates with a clearly smaller average velocity than expected. Further, we obtain oscillations in the interface energy and the fitted width as the center of the interface passes one grid point after the other. With decreasing phase-field width, we obtain increasingly larger drops of the average values as well as increasing oscillation amplitudes. For the conventional model this culminates in fully destroyed interface kinetics, which is commonly referred to as grid pinning. In contrast, the translationally invariant one dimensional Sharp Phase-Field Model (1D SPFM) by A. Finel et al. [1], as shown by the green curves in Fig. 8, is not subjected to this effects even though the phase-field width has been chosen as small as $\lambda/h = 0.5$.

![Figure 7. Plot of the interface energy calibration factor $C\Gamma$ as a function of the interface grid resolution number $\lambda/h$.](image)

![Figure 8. The influence of artificial grid friction on the motion of a planar interface. Comparison of a conventional phase-field formulation for different phase-field widths $\lambda/h$ with the one dimensional Sharp Phase-Field Model (1D SPFM), as proposed by [1], for a marginally diffuse interface (green curves).](image)
2. Measure of the interface position

It should be mentioned that for marginally diffuse interfaces the conventional measure of the interface position by a linear interpolation of the $\phi = 1/2$ contour-position is not the best choice to approximate the real center of the phase-field profile. Especially, when the phase-field width is small compared to the grid spacing, a linear interpolation can provide a quite different result as compared to the interface position resulting from a least square fit using the analytic profile function. On the other hand performing a least square-fit only to get a measure for the local interface position is most often not appropriate.

Therefore, we propose a nonlinear interpolation of the interface position based on the analytic phase-field profile. The interpolated position, where the phase-field profile takes the arbitrary contour-level $l$ ($0 < l < 1$) can be calculated as

$$x_k^{\text{int}}(i) = ih + \frac{\lambda}{2n_k} \left| \text{arctanh} \left( \frac{l - \phi_i}{2l(\phi_i - \phi_i - l)} \right) \right|,$$  \hspace{1cm} (10)

where $n_k$ denotes the projection of the unit normal interface orientation vector onto the $k$–th cartesian direction, which also corresponds to one of the principle directions of the simple cubic numerical lattice in this case. In order to further regularize the resulting interface position as function of time, we impose an averaging between the two slightly different interface positions $x_k^{\text{int}}(i)$ and $x_k^{\text{int}}(i + u_k)$ of the two neighboring grid points, connected by the principle lattice vector $u_k$, next to the position of the contour-level $l$, i.e. we have the condition $(\phi_i - l) \cdot (\phi_i + u_k) - l \leq 0$.

We attach three movies to this supplemental material:

1. Supplementary_material_2_Pinning-animation.mpg: This movie is an animated version of Figure 1 in the manuscript. Thus it illustrates the influence of artificial grid-friction on the motion of a planar interface in one dimension. We compare the behavior of the conventional phase-field formulation for different phase-field widths $\lambda/h$ with the behavior of the Sharp Phase-Field Model (1D SPFM), as proposed by [1], for a marginally diffuse interface (green curves).

2. Supplementary_material_3_Steady_state-interface_motion.mpg: This movie is an animated visualization of the evolution of the phase-field during the simulation of stationary motion of a planar interface with propagates under an angle of 45° with respect to the computational grid.

3. Supplementary_material_4_ContactAngleBD.mpg: This movie illustrates the function of the newly proposed boundary conditions. They enforce a finite contact angle between the interface normal and the boundary plane. In this movie, we show a simulation of the shape-evolution of an initially cubic particle toward its spherical equilibrium shape under conserved phase volume. The particle is in contact with the bottom boundary, where a contact angle of 80° with respect to the boundary plane is enforced.