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A semi-implicit conservative sharp-interface method for liquid-solid phase transition



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ABSTRACT

The solidification of an undercooled liquid is physically unstable. The dominating instability modes are affected by both the evolving temperature field in the solid and liquid phases, and characteristics of the phase interface such as the curvature and the propagation velocity. To capture the instability mode, therefore both the temperature field and the interface have to be represented accurately in a numerical model of the phase-change process. In this work, we develop conservative interface exchange terms for a sharp-interface formulation of liquid-solid phase transition. Conservation at the interface is maintained by explicit formulation of interface fluxes into both solid and liquid phases. We propose a semi-implicit level-set formulation to evolve the phase interface. A new formulation for the interface surface in a cut cell is derived, which includes the Stefan condition. We achieve low numerical dissipation by an explicit third-order Runge-Kutta scheme for time discretization, and a novel WENO-like (Weighted Essentially Non-Oscillatory) interface-gradient reconstruction. This distinguishes our level-set based sharp-interface model from previous level-set based approaches, which rely on finite-difference based interface treatment, and thus do not ensure discrete conservation at the interface. The flux terms in our approach take into account surface-tension and kinetic effects on the interface temperature (Gibbs-Thomson relation). The Stefan condition provides a relation between interface fluxes of mass and energy, and the interfacepropagation velocity. Computational efficiency is maintained by a multiresolution approach for local mesh adaptation, and an adaptive local time-stepping scheme.

We present one- and two-dimensional simulation results for the growth of a planar solidification front and a single parabolic dendrite affected by surface tension. The results agree well with experimental and analytical reference data, showing that the model is capable to capture both stable (planar) and unstable (dendritic-like) growth processes in the heat-diffusion dominated regime. The convergence order for successively finer meshes in the one-dimensional case is one for the interface location and the temperature field, outperforming previously reported level-set based approaches. We present numerical data of a growing crystal with four-fold symmetry. Our results indicate that the artificial dissipation of the underlying numerical scheme affects its capability to reproduce consistently physical tip-splitting instabilities. The proposed low-dissipation scheme is able to resolve such instabilities. Finally, we demonstrate the capability of the method to simulate multiple growing crystals with anisotropic surface-tension and kinetic effects.

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1. Introduction

Under suitable conditions, liquids can be cooled down to a temperature well below their solidification temperature. A disturbance of the undercooled liquid initiates sudden solidification processes, which manifest themselves as dendrites. Dendrites have a highly branched, tree-like structure. Anisotropic growth is caused by in-

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homogeneities of the phase-change process in preferred crystal growth directions. Small perturbations of the initial state of the undercooled liquid or during the growth process may cause significant changes in the resulting crystalline structure [21]. Although the dendritic growth process itself is inherently unstable, a steadystate solution exists for the tip radius and the growth velocity, which depend on both the material properties and the degree of undercooling. The steady-state growth mechanism can be characterized by diffusion or interface kinetics [46]. For the diffusiondominated regime, Langer and Müller-Krumbhaar [28-30,34] derived an analytical stability theory, which extends the seminal work of Ivantsov [20]. Their theory shows good agreement with experimental results [9,46–48] in the diffusion-dominated regime, but differs in the kinetics-dominated regime. Once tip radius and tip growth velocities exceed their stability region, tip-splitting or side-branching instabilities may occur that eventually lead again to a stable configuration.

The dendritic solidification process poses a Stefan problem at the phase interface, i.e. an initial-boundary value problem with moving boundary. Phase-interface dynamics are governed by the local temperature field and a Dirichlet boundary condition for the interface temperature considering local interface characteristics, such as the curvature or the propagation velocity. Therefore, an accurate representation of the topologically complex, timedependent solidification front in multiple dimensions is necessary [11]. Various multiphase models have been applied to solve the Stefan problem numerically, both for mesh-free [50-52] and meshbased discretization methods. For the mesh-based discretization, approaches can be related to either front-tracking [13,23,41] or front-capturing methods. Among the front-capturing methods, phase-field [2,3,10,14,25,27,35,49,57] and level-set [5-7,11,26,45,54-56] approaches are the most popular choices for representing the solidification front [21]. In the phase-field approach, an additional order parameter, the phase field variable, is introduced. This variable indicates the physical state at the location of interest. The phase interface is located in the transition region of this parameter, and the interface width is a model parameter. Hence, the interface is artificially thickened so it can be resolved on the given mesh. Phase-field models are therefore often classified as diffuseinterface model. The accuracy of the simulation depends on the thickness of the phase interface. Quantitatively accurate predictions of the phase front therefore require sufficiently small numerical grids, which may incur prohibitively high computational cost [21].

This difficulty is alleviated by the level-set approach. It also employs an order parameter, the level set, which describes the signed distance from the interface. The zero-level-set contour denotes the interface location. The sharp-interface property of the level set enables an accurate localization of the phase interface, and simplifies the computation of local interface characteristics. An approach to couple the interface velocity with the interface curvature was introduced by Osher and Sethian [37]. This work was a first step towards simulating dendritic solidification with the level-set method [44]. Chen et al. [6] extended this approach and proposed a model to solve the Stefan problem, focusing on crystal growth. They applied a finite difference approach to discretize the diffusion equation in solid and liquid phases on a homogenoeous grid, and used implicit time integration schemes. Their approach shows good agreement with the analytical solution obtained from solvability theory [26]. Higher-order stencils improved accuracy and convergence rates [11]. Overall computational efficiency was improved by a local mesh adaptation approach, which accounts for the different length scales near the phase interface [5]. Their approach was applied to compute the solidification of binary alloys by Theillard et al. [56]. An extended level-set model was introduced by Criscione et al. [7], who employed a finite-volume scheme using ghost cells to solve the temperature field. Good results were obtained for the simulation of both a stable, planar solidification front and the unstable growth of a single parabolic dendrite. Ramanuj et al. [39] presented simulations of unstable solidifying systems based on a second-order level-set approach [38]. They showed the advantages of high-order spatial schemes and explicit time integration schemes for dendrite-growth simulations. Yet, most previous works rely on implicit time integration schemes, introducing comparably large numerical dissipation and therefore require higher spatial resolutions to resolve topologically complex crystalline structures. In addition, non-conservative numerical interface models may compromise physically correct interface evolution.

In this work, we develop a conservative interface-interaction method for a sharp-interface formulation of liquid-solid phase transition of pure liquids. Conservation at the interface is maintained by explicit formulation of interface fluxes into both solid and liquid phases. We propose a semi-implicit level-set formulation to evolve the phase interface. A new formulation for the interface surface in a cut cell is derived, which includes the Stefan condition. We achieve low numerical dissipation by an explicit thirdorder Runge-Kutta scheme for time discretization [12,16], and a novel WENO-like (Weighted Essentially Non-Oscillatory) interfacegradient reconstruction [22]. This distinguishes our level-set based sharp-interface model from previously published level-set based approaches, which rely on finite-difference based interface treatment and may violate discrete conservation at the interface. The flux terms in our approach take into account surface-tension and kinetic effects on the interface temperature (Gibbs-Thomson relation), including anisotropic behavior. The Stefan condition provides a relation between interface fluxes of mass and energy, and the interface-propagation velocity. The sharp-interface property is ensured by extrapolating fluid states across the interface for the single-phase reconstruction of the cell-face fluxes near the interface [8]. Computational efficiency is improved by dynamic mesh adaptation with respect to the evolving interface and temperature field using the multiresolution approach of Harten [17]. We employ an adaptive local time-stepping scheme for efficient and robust time integration [24].

The structure of the paper is the following: in section 2, we describe the sharp-interface method for modeling solid-liquid phasetransition problems. The new conservative interface-interaction approach for liquid-solid phase transition is given in section 3, together with the employed level-set method. Section 4 provides one- and two-dimensional numerical example simulations for stable and unstable phase-change processes. We conclude the work in section 5.

2. Sharp-interface method for liquid-solid phase transition

The governing equations for the phase-change problem can be written as

$$\frac{\partial \mathbf{U}}{\partial t} = \nabla \cdot \mathbf{F}_k, \tag{1}$$

where $\mathbf{U} = (\rho, \rho c T)^T$ is the state vector of mass and energy, and $\mathbf{F}_k = (0, k \nabla T)^T$ represents heat conduction. Here, ρ is the density, c the specific heat capacity, T the temperature, and k the thermal conductivity. We solve eq. (1) separately for the solid and liquid subdomain, and assume the specific heat capacity c and the thermal conductivity k to be constant in each subdomain. The convection in the liquid phase is suppressed in order to focus on the phase-change model.

Eq. (1) needs to be completed by a set of interface conditions to fully describe the Stefan problem. We assume that the temperature field is continuous across the interface. The temperature at



Fig. 1. Schematic finite volume discretization of the domain Ω on a Cartesian quadratic grid.

the interface T_{Γ} is prescribed as Dirichlet boundary condition, and follows from the Gibbs-Thomson relation

$$T_{\Gamma} = T_m - \frac{\gamma I_m}{\rho L} \kappa - \epsilon_u ||\mathbf{u}_{\Gamma}||$$
⁽²⁾

including surface tension and kinetic effects. Here, T_m is the melting temperature of the material, γ the surface tension coefficient, L the latent heat, κ the interface curvature, ϵ_u the kinetic coefficient, and \mathbf{u}_{Γ} the interface velocity vector. Unless noted otherwise, we assume isotropic surface tension and kinetic coefficients. The Stefan condition represents the balance of local heat fluxes and the latent heat released by phase change and yields

$$\dot{m}[L + (T_{\Gamma} - T_m)(c_l - c_s)] = \rho \parallel \mathbf{u}_{\Gamma} \parallel [L + (T_{\Gamma} - T_m)(c_l - c_s)]$$

= $(k_s \nabla T_s - k_l \nabla T_l) \cdot \mathbf{n}_{\Gamma}.$ (3)

Here, \dot{m} is the mass rate of solidifying liquid, $\nabla_n T_{\Phi} = \nabla T_{\Phi} \cdot \mathbf{n}_{\Gamma}$ is the interface-normal temperature gradient of the solid ($\Phi = s$) and liquid ($\Phi = l$) phases, and \mathbf{n}_{Γ} is the interface-normal vector, which points from the solid to the liquid phase.

The governing equations (1) are discretized by a finite-volume approach in the domain Ω , which is divided into two subdomains Ω_l and Ω_s by a time-evolving interface Γ . Fig. 1 shows a sketch of the two subdomains with a sharp interface. We integrate eq. (1) in each computational cell S_{ij} of each subdomain Ω_{Φ} and apply Gauß' theorem to obtain

$$\int_{t^{(n)}}^{t^{(n+1)}} dt \int_{S_{ij} \cap \Omega_{\Phi}} dS_{ij} \frac{\partial \mathbf{U}}{\partial t} = \int_{t^{(n)}}^{t^{(n+1)}} dt \int_{\partial (S_{ij} \cap \Omega_{\Phi})} dS_{ij} \mathbf{F}_k \cdot \mathbf{n}$$
(4)

where $dS_{ij} = \Delta x_1 \Delta x_2$ denotes the cell volume in two dimensions, $S_{ij} \cap \Omega_{\Phi}$ each cell volume of phase Φ , $\partial(S_{ij} \cap \Omega_{\Phi})$ the cell face, and **n** the surface normal of this cell face. We replace $S_{ij} \cap \Omega_{\Phi}$ by $S_{ij}\alpha_{ij}$, where α_{ij} is the time-dependent volume fraction of phase Φ , with $0 \le \alpha_{ij} \le 1$. The cell face $\partial(S_{ij} \cap \Omega_{\Phi})$ can be approximated by the cell-face apertures A, $0 \le A \le 1$, and the segment of the interface Γ inside this cell, $\Delta \Gamma_{ij}$. Eq. (4) is then rewritten for a single forward-time integration step of phase Φ as

$$\alpha_{i,j}^{(n+1)} \mathbf{U}_{i,j}^{(n+1)} = \alpha_{i,j}^{(n)} \mathbf{U}_{i,j}^{(n)} + \frac{\Delta t}{\Delta x_1} (A_{i-1/2,j}^{(n)} \mathbf{F}_{\mathbf{k}_{i-1/2,j}}^{(n)} - A_{i+1/2,j}^{(n)} \mathbf{F}_{\mathbf{k}_{i+1/2,j}}^{(n)}) + \frac{\Delta t}{\Delta x_2} (A_{i,j-1/2}^{(n)} \mathbf{F}_{\mathbf{k}_{i,j-1/2}}^{(n)} - A_{i,j+1/2}^{(n)} \mathbf{F}_{\mathbf{k}_{i,j+1/2}}^{(n)}) + \frac{\Delta t}{\Delta x_1 \Delta x_2} \mathbf{X}_{\mathbf{S}_{i,j}}^{(n,n+1)} (\Delta \Gamma_{i,j})$$
(5)

where Δt denotes the timestep size, \mathbf{U}_{ij} the cell-averaged state vector of the considered phase in cell (i, j), and $\mathbf{F}_{\mathbf{k}_{i,j}}$ the fluxes in or out of this cell. The term $\mathbf{X}_{\mathbf{S},ij}$ describes the mass and energy exchange across the interface for the phase-change process. It vanishes if a cell is not a cut cell. We follow the approach of Hu et al. [19], and formulate the exchange terms as conservative interface fluxes. The fluxes also model the interface conditions (2) and (3). All terms on the right hand side are calculated at time $t^{(n)}$, except for the interface exchange term $\mathbf{X}_{\mathbf{S},ij}$, which is further detailed in the following section 3.

In this work, cell-face heat fluxes are reconstructed by a second-order central difference scheme. Low-dissipation time integration is achieved by a strongly stable third-order Runge-Kutta scheme

$$u^{(1)} = u^{(n)} + \Delta t L(u^{(n)})$$

$$u^{(2)} = \frac{3}{4}u^{(n)} + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)})$$

$$u^{(n+1)} = \frac{1}{3}u^{(n)} + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)})$$
(6)

[12,16]. The maximum admissible timestep size is determined from a CFL-type stability criterion considering the propagation speed of the phase interface and heat diffusion in both phases

$$\Delta t = \operatorname{CFL} \cdot \min\left(\frac{\Delta x}{|u_{\Gamma}|}, \frac{3}{14} \frac{(\Delta x)^2 \rho c}{k}\right). \tag{7}$$

In all examples we use CFL= 0.5. Advancing the flow field by this timestep size may lead to an unstable fluid state in cells with small volume fraction α . Therefore, we apply a mixing procedure in cells with α < 0.5 to maintain numerical stability [19].

Resolution of all scales of dendritic solidification on a homogeneous mesh is computationally expensive. Several orders of magnitude lie between the wavelength of the dominating instability modes of a growing dendrite and the size of the dendrite itself [56]. Therefore, spatial adaptation techniques are necessary to efficiently solve dendritic solidification problems numerically. We apply a block-structured wavelet-based multiresolution approach based on the work of Harten [17] to adapt the mesh to the progressing solidification front and the evolving temperature field [15,18,42]. The procedure is in detail described in Hoppe et al. [18]. In the multiresolution approach, the cell-averaged solution is represented by cell-averaged data on a coarse grid and a series of values on successively finer refinement levels. In this treebased structure, the two basic operations to communicate data between successive refinement levels are projection and prediction. The projection operation is applied to obtain data on a refinement level *l* from level l + 1. Cell-averaged data on level l + 1 can be interpolated from level *l* using the prediction operation. Projection and prediction operations are local and consistent, but not commutative, i.e:

- Applying first the prediction operation to obtain data on level *l* + 1 from level *l*, and afterwards again the projection operation results in exactly the same solution on level *l*.
- Applying first the projection operation to obtain data on level *l* from level *l* + 1, and interpolating afterwards the data on level *l* + 1 from level *l* using the prediction operation results in an error for data on level *l* + 1.

This motivates the definition of the so-called details d, which are the deviation of the predicted solution to the exact solution. The exact solution on the finest level can be replaced by a hierarchical data structure, which contains the exact solution on the coarsest level and the details of all successively finer levels. For implicit mesh adaptation, details are only considered when they are larger than a pre-defined level-dependent threshold

$$\varepsilon_l = \varepsilon_{\rm ref} \cdot e^{(-D \cdot (l - l_{\rm max}))}, \tag{8}$$

where l_{max} denotes the maximum level to which the mesh can be refined, *D* the number of dimensions, and ε_{ref} the admissible relative error on level *l*. If the details are sufficiently small, further grid refinement does not lead to significantly better results than interpolation from a coarser grid. In our simulations, we refine the mesh based on the local error of the energy field. In addition, the phase interface is enforced to be always on the finest level [15]. We apply dyadic refinement, where each cell can be refined into 2^{D} smaller cells. The reference error is set to $\varepsilon_{\rm ref} = 0.01$ for a refinement between the finest level and the next coarser one. Efficient time integration is obtained by applying a local time-stepping approach, where each refinement level is advanced with its level-dependent timestep size [36]. The method is described in detail in Kaiser et al. [24]. It allows for adapting the timestep size after each full Runge-Kutta cycle on the finest refinement level based on the CFL stability criterion (7).

3. Conservative interface-interaction model for liquid-solid phase transition

3.1. Conservative interface-exchange terms

The level-set function ϕ represents the phase interface as the zero-crossing of a multi-dimensional continuous function ϕ with>

$$\begin{split} & \mathbf{x} \in \Omega_s \to \phi(\mathbf{x}) < \mathbf{0}, \\ & \mathbf{x} \in \Omega_l \to \phi(\mathbf{x}) > \mathbf{0}, \text{ and} \\ & \mathbf{x} \in \Gamma \to \phi(\mathbf{x}) = \mathbf{0}. \end{split}$$

The absolute value of ϕ describes the normal distance of the cell center **x** to the interface Γ , which leads to the signed-distance property $|\nabla \phi| = 1$.

We develop conservative interface-exchange terms to model the phase-change process. We model mass and energy exchange across the interface, and for now suppress exchange of momentum. The interface fluxes for the solid phase are

$$\mathbf{X}_{\mathbf{S}_{s}} = \left(-\dot{m}\Delta\Gamma, -\dot{m}c_{s}T_{\Gamma}\Delta\Gamma + k_{s}(\nabla T_{s}\cdot\mathbf{n}_{\Gamma})\Delta\Gamma\right)^{T}, \qquad (9)$$

and for the liquid phase

$$\mathbf{X}_{\mathbf{S}_{l}} = (\dot{m}\Delta\Gamma, \, \dot{m}c_{l}T_{\Gamma}\Delta\Gamma + k_{l}(\nabla T_{l}\cdot\mathbf{n}_{\Gamma})\Delta\Gamma)^{l} \,. \tag{10}$$

The first term of the energy exchange describes the material transport through the interface, and the second term the heat flux into each material due to the Stefan condition (3). The interface temperature T_{Γ} is obtained from the Gibbs-Thomson relation eq. (2). If kinetic effects are taken into account, the interface temperature is computed using the interface velocity at time $t^{(n)}$ [11].

In previous work, the area of the interface segment in a cut-cell $\Delta\Gamma$ is computed from cut-cell apertures [19,31]. For $\dot{m} = \rho ||\mathbf{u}_{\Gamma}||$, the interface segment moves within the cut-cell by a distance $\Delta t ||\mathbf{u}_{\Gamma}||$. The linearized volume-fraction change is $\Delta t \Delta \Gamma ||\mathbf{u}_{\Gamma}||$. However, this formulation potentially violates conservation for multi-dimensional problems, see Fig. 2. The linearized volume-fraction change for the given case. Therefore, we propose a new way for determining $\Delta\Gamma$ based on a semi-implicit level-set approach (see section 3.2). First, we compute the time derivative of the liquid volume fraction $\dot{\alpha}$ from level-set fields $\phi^{(n)}$ and $\phi^{(n+1)}$

$$\dot{\alpha} = \frac{\partial \alpha}{\partial t} \approx \frac{\alpha(\phi^{(n+1)}) - \alpha(\phi^{(n)})}{\Delta t} \,. \tag{11}$$

It is thus possible to reformulate the mass exchange across the interface in terms of $\dot{\alpha}$ as $\dot{m}\Delta\Gamma = \rho\dot{\alpha}V_c$, where V_c denotes the cell volume. Second, we formulate the energy conservation in a single cut cell based on the Stefan condition, eq. (3),

$$\dot{Q}_{\dot{\alpha}} = \dot{Q}_{\lambda}$$

$$\dot{\alpha} \rho V_c [L + (T_{\Gamma} - T_m)(c_l - c_s)] = (k_s \nabla T_s - k_l \nabla T_l) \cdot \mathbf{n}_{\Gamma} \Delta \Gamma$$

where $\dot{Q}_{\dot{\alpha}}$ denotes the heat released in the phase-change process, and \dot{Q}_{λ} the released heat into both solid and liquid phases due to heat conduction. The interface area $\Delta\Gamma$ follows from

$$\Delta\Gamma = \frac{\dot{\alpha}\rho V_c \left[L + \left(T_{\Gamma_{i,j}} - T_m \right) (c_l - c_s) \right]}{(k_s \nabla T_s - k_l \nabla T_l) \cdot \mathbf{n}_{\Gamma}} = \frac{\dot{\alpha} V_c}{\| \mathbf{u}_{\Gamma} \|}$$
(12)



Fig. 2. Schematic of the volume-fraction change in a single cell during an Euler step. The included volume-fraction change is shown in blue. Fig. (a): change for the linearized approach. Fig. (b): the new semi-implict level-set approach, which correctly predicts the entire volume-fraction change.

Thus, the interface-exchange terms eqs. (9) and (10) can be written as

$$\mathbf{X}_{\mathbf{S}_{s}} = \left(-\rho_{s} \dot{\alpha} V_{c}, -\rho_{s} \dot{\alpha} V_{c} c_{s} T_{\Gamma} + k_{s} (\nabla T_{s} \cdot \mathbf{n}_{\Gamma}) \Delta \Gamma\right)^{T},$$
(13)

$$\mathbf{X}_{\mathbf{S}_{l}} = \left(\rho_{l}\dot{\alpha}V_{c}, \ \rho_{l}\dot{\alpha}V_{c}c_{l}T_{\Gamma} + k_{l}(\nabla T_{l}\cdot\mathbf{n}_{\Gamma})\Delta\Gamma\right)^{T}.$$
(14)

We compare our approach with the linearized formulation in section 4.3.

The overall accuracy and stability of the method are sensitive to the evaluation of the interface-normal temperature gradient [7]. A common method provided in previous work is to reconstruct the temperature at one or multiple points in a fixed normal distance to the interface. The interface-normal temperature gradient then is computed by a finite-difference scheme [7,32,40]. Through extensive numerical tests we found that a directional splitting approach with weighting of local interface-normal temperature gradients based on third-order WENO smoothness indicators [22] provides the best approximation of $\nabla_n T$ in terms of efficiency and accuracy, see Fig. 3. Filled dots mark cells which are considered for computing the interface-normal temperature gradient. First, we compute the interface temperature gradient in each cell for each direction with a finite difference stencil

$$\frac{\partial T}{\partial x_1}\Big|_{i+l,j} = \left| \left| \frac{T_{i+l,j} - T_{\Gamma}}{|\phi_{i,j}| + l \,\Delta x} \right| \left| \operatorname{sgn}(n_{\Gamma,x_1}), \frac{\partial T}{\partial x_2} \right|_{i,j+l} \right| \\ = \left| \left| \frac{T_{i,j+l} - T_{\Gamma}}{|\phi_{i,j}| + l \,\Delta x} \right| \left| \operatorname{sgn}(n_{\Gamma,x_2}) \right|$$
(15)

with $l \in \{1, 2, 3\}$, the sign function sgn() and n_{Γ,x_i} the component of the interface-vector in x_i -direction. We weight the cell-wise interface gradients based on the smoothness indicators of the third-order WENO scheme to obtain the overall interface-normal temperature gradient in the cut-cell (i,j) in each spatial direction $\partial T/\partial x_1$, $\partial T/\partial x_2$. These are then projected onto the normal direction

$$\nabla_n T = n_{\Gamma, x_1} \frac{\partial T}{\partial x_1} + n_{\Gamma, x_2} \frac{\partial T}{\partial x_2} \,. \tag{16}$$

Similar to Criscione et al. [7], the interface-normal temperature gradient finally is averaged within all direct neighbor cells. This procedure decreases spurious oscillations of the interface-normal temperature gradient.

3.2. Level-set evolution

The level-set field ϕ is evolved in time by an advection equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u}_{\Gamma} \cdot \nabla \phi = 0.$$
⁽¹⁷⁾

The level-set advection equation is solved for cut cells using the interface velocity \mathbf{u}_{Γ} , which is computed from the Stefan condition (eq. (3)) following

$$\|\mathbf{u}_{\Gamma}\| = \frac{k_s \nabla_n T_s - k_l \nabla_n T_l}{\rho [L + (T_{\Gamma} - T_m)(c_l - c_s)]}.$$
(18)

Non-cut cells are evolved using an interface velocity $\mathbf{\tilde{u}}_{\Gamma}$ extrapolated from adjacent cut cells, which is determined from the steady-state solution of the extrapolation equation

$$\frac{\partial \tilde{\mathbf{u}}_{\Gamma}}{\partial \tau} + \mathbf{n}_{\Gamma} \cdot \nabla \tilde{\mathbf{u}}_{\Gamma} = 0.$$
⁽¹⁹⁾

The level-set field is evolved with the phase states at time $t^{(n)}$ before advecting the fluid field. Thus, the solid and liquid phases can be updated afterwards from time $t^{(n)}$ to $t^{(n+1)}$ using the interface locations $\phi^{(n)}$ and $\phi^{(n+1)}$, e.g. when computing $\dot{\alpha}$ in eq. (11). We have found that this type of operator splitting improves mass conservation of the overall level-set scheme, see section 4.3 for a numerical example.

The numerical solution of the level-set advection does not maintain the signed-distance property $|\nabla \phi| = 1$. Therefore, the reinitialization equation

$$\frac{\partial \phi}{\partial \tau} + \operatorname{sign}(\phi_0)(|\nabla \phi| - 1) = 0$$
(20)

is iterated in pseudo time τ to steady state to restore the signeddistance property after each timestep [53]. Here, ϕ_0 is the levelset field prior the re-initialization step. Note that we also reinitialize cut cells to maintain the signed-distance property. The re-initialization of cells cut by the interface generally may affect the overall conservation of the level-set scheme by shifting the location of the zero-level-set [43]. This issue is, however, not relevant for the developed scheme, as the incorporation of the reinitialized level-set fields at $t^{(n)}$ and $t^{(n+1)}$ within the interface-exchange terms ensures local conservation, see section 3.1.

Similarly to the interface velocity extrapolation from the interface to the adjacent bulk cells, the fluid states are extrapolated across the interface to define a "ghost" fluid within the opposing phase [8]. These ghost-fluid states allow for the single-phase reconstruction of the cell-face fluxes near the interface. This maintains the sharp-interface property of the method.

	(i, j+3)			
	(i, j+2)			
	(i, j+1)			
	\mathbf{n}_{Γ} (i,j)	(i+1,j)	(i+2,j)	(i+3,j)
	Г			

Fig. 3. Schematic of the relevant cells for the computation of the interface-normal temperature gradient. Filled dots mark cell centers which are used to reconstruct the interface-normal temperature gradient.



Fig. 4. Schematic of the narrow-band approach: shown are the interface (blue), cut cells (dark gray), narrow-band cells (light gray), and bulk cells (white). The solid phase is on the left side of the interface ($\phi < 0$), the liquid phase on the right side ($\phi > 0$).

We introduce a narrow band around the interface to further improve the overall efficiency of our method. The narrow-band concept is shown in Fig. 4. Three cell types are distinguished:

- 1. Cut cells: cells that are cut by the interface.
- 2. Narrow-band cells: cells which are in the vicinity of the interface. The width of the narrow band depends on the applied spatial and temporal discretization schemes. As example, a narrow band with a width of four cells is shown in the figure.
- 3. Bulk cells: cells that are far away from in the interface.

All previously mentioned level-set operations (advection, reinitialization, interface velocity and ghost cell extrapolation) are only performed in cut cells and narrow-band cells. All bulk cells are set to a constant level-set value depending on whether they contain liquid (ϕ_+) or solid (ϕ_-) states. This approach limits costly level-set related operations to only a fraction of the domain, thus improving overall performance, without adversely affecting the accuracy of the method.

The Gibbs-Thomson relation given in eq. (2) includes the interface temperature as function of the interface curvature. The curvature is the divergence of the interface-normal vector $\kappa = \nabla \cdot \mathbf{n}_{\Gamma}$, which is numerically obtained from $\mathbf{n}_{\Gamma} = \nabla \phi / |\nabla \phi|$. The curvature is evaluated at the cell center by

$$\kappa = \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|}, \qquad (21)$$

using a third-order WENO scheme. Finally, the interface curvature is subjected to a subcell correction step depending on spatial di-

Table 1

Material parameters for the one-dimensional Stefan problem: water at 243.15K and ice at 263.15K.

	$\rho [\mathrm{kg}/\mathrm{m}^3]$	c [J/(kg K)]	<i>k</i> [W/(m K)]	L [kJ/kg]	T_m [K]
water	1000	4864.0	0.4829	333.6	273.15
ice	1000	2030.0	2.319		

mensionality D

$$\kappa_{\Gamma} = \frac{(D-1)\kappa}{D-1-\phi\kappa} \tag{22}$$

to take into account the distance between the cell center and the interface [33].

4. Numerical results

4.1. Growth of a planar solidification front (Stefan problem)

The classical Stefan problem describes the non-stationary growth of a planar solidification front, and is solved to investigate the accuracy of the model for non-stationary problems. We simulate the propagation of an ice front in undercooled water, as proposed by Rauschenberger et al. [40]. In a domain of length 2.5 mm, the phase interface is initially located at $x_{\Gamma,0} = 0$ and propagates into the semi-infinite liquid subdomain $x_{\Gamma}(t) > x_{\Gamma,0}$. Both phases are initially at constant temperatures of $T_s = 263.15$ K (solid) and $T_l = 243.15$ K (liquid). Material parameters are provided in Table 1. We prescribe a constant temperature $T_w = T_s = 263.15$ K at the wall, and use a zero-gradient boundary condition to represent a semi-infinite liquid subdomain. The domain size is chosen sufficiently large to prevent spurious effects from the far-field zero-gradient boundary condition on the ice-layer growth.

The numerical solution of the temperature field is compared to the analytical solution given by Carslaw & Jaeger [4]

$$0 < x < x_{\Gamma}(t), t > 0 : T(x,t) = T_{w} + (T_{m} - T_{w}) \frac{\operatorname{erf}\left(\frac{x - x_{\Gamma,0}}{2\sqrt{\alpha_{s}t}}\right)}{\operatorname{erf}(\beta)}$$
$$x > x_{\Gamma}(t), t > 0 : T(x,t) = T_{\infty} + (T_{m} - T_{\infty}) \frac{\operatorname{erfc}\left(\frac{x - x_{\Gamma,0}}{2\sqrt{\alpha_{t}t}}\right)}{\operatorname{erfc}(\tilde{\alpha}\beta)}$$
(23)

with

$$\beta \sqrt{\pi} = \frac{St_s}{\operatorname{erfc}(\beta)} e^{\left(-\beta^2\right)} + \frac{St_l}{\tilde{\alpha} \operatorname{erfc}(\tilde{\alpha} \beta)} e^{\left(-\tilde{\alpha}^2 \beta^2\right)}$$
(24)

and the ratio of the thermal conductivities $\tilde{\alpha} = \sqrt{\alpha_s/\alpha_l}$. The Stefan number *St* denotes the ratio of sensible heat to latent heat and is computed following

$$St_s = \frac{c_s(T_m - T_w)}{L}, \qquad St_l = \frac{c_l(T_m - T_\infty)}{L}.$$

Eq. (24) yields $\beta = 0.2685$ for the described case. The interface location at time *t* is given by

$$x_{\Gamma}(t) = x_{\Gamma,0} + 2\beta \sqrt{\alpha_s t} , \qquad (25)$$

and the interface velocity is

$$u_{\Gamma}(t) = \frac{dx_{\Gamma}(t)}{dt} = \beta \sqrt{\frac{\alpha_s}{t}}.$$
(26)

The simulations are initialized with the analytical solution for the temperature field from eq. (23) at t = 0.01, and a corresponding level-set field with the interface located at $x_{\Gamma}(t = 0.01)$ from eq. (25).

A temporal series of simulated temperature profiles is shown in Fig. 5, together with the corresponding analytical solutions. The effective resolution for this case is 512 cells in the entire domain. The



Fig. 5. Temperature profiles of the 1D Stefan problem at various instants for an effective resolution of 512 cells: analytical solution (-) and numerical results (symbols).



Fig. 6. Interface location for the one-dimensional Stefan problem for different resolutions: analytical solution (–) and numerical results (symbols).

agreement with the reference is good at all time instants. Steep temperature gradients in both phases diminish over time, as solid and liquid phases absorb the latent heat released by the solidifying undercooled liquid. Therefore, the propagation of the phase interface slows down.

The temporal evolution of the interface location is shown in Fig. 6 for successively finer meshes. The numerical results replicate the square-root behavior of the moving solidification front in time. The accuracy of the solution improves for successively finer meshes. Error plots are given in Fig. 7 for the interface location (left) and the temperature field (right) at t = 0.5, for effective mesh resolutions between 64 and 4096 cells. The temperature field error is given as L_{∞} norm, and as L_1 norm following

$$L_{1} = \frac{1}{V} \sum_{n} \frac{||T_{n,exact} - T_{n,sim}||}{T_{n,exact}} dV_{n}, \qquad (27)$$

with $T_{n,exact}$ being obtained from the analytical solution eq. (23). The global convergence order of the scheme is one for both the interface location and the temperature field, which is higher than for previously published level-set based approaches [40], underlining the advantages of applying high-order low-dissipation schemes.



(a) Error of the interface position

(b) Error of the temperature field

Fig. 7. Fig. (a): error of the interface location x_{Γ} at t = 0.5. Fig. (b): error of the temperature field (right) at t = 0.5. Given are reference convergence orders (dashed line) and simulation results (symbols).

4.2. Growth of a parabolic dendrite

The growth of a parabolic dendrite has been investigated analytically, experimentally, and numerically in the past. Based on the work of Ivantsov [20], Langer and Müller-Krumbhaar developed a stability theory for the growth of a single dendrite [28,29,34]. They derived a universal solution to compute the tip radius and velocity of a parabolic dendrite. First, the Péclet number of the growth process

$$Pe = \frac{r_t}{L} \tag{28}$$

is introduced, which describes the ratio of the tip radius r_t (i.e. the length scale of the growing dendrite) to the range of the diffusion field l given by

$$l = \frac{2\alpha}{u_{\Gamma}} \,. \tag{29}$$

Here, α denotes the thermal diffusivity of the melt and u_{Γ} is the interface velocity at the tip of the dendrite. For dendritic growth cases, Pe < 0.1 is usually valid. According to Langer et al. [29], the Stefan number and the Péclet number are related by

$$St \approx Pe \exp PeE_1(Pe)$$
 (30)

if the dendrite is of parabolic shape, rotationally symmetric, and isothermal. Here, E_1 describes the exponential integral.

A second non-dimensional parameter

$$\sigma = \frac{ld_c}{r_t^2} \tag{31}$$

can be formulated, which relates the capillary length scale

$$d_c = \frac{\gamma c T_m}{\rho L^2} \tag{32}$$

to the diffusion length l and the tip radius r_t . The parameter σ plays a crucial role in the stability analysis of dendritic growth. Depending on the number of dimensions D, Müller-Krumbhaar & Langer [34] derived that only solutions which satisfy

$$\sigma^* = \begin{cases} 0.020 \pm 0.007 & D = 2\\ 0.025 \pm 0.007 & D = 3 \end{cases}$$
(33)

are stable. Here, $\sigma = \sigma^*$ is the operating point of dendritic growth.

The tip radius and velocity for a given undercooling and material parameters are obtained as follows. First, eq. (30) is solved to

Table 2Material properties of ice and water at 273.15K [40].

	ho [kg m ⁻³]	<i>k</i> [W (m K) ⁻¹]	с [J (kg K) ⁻¹]	L [kJ kg ⁻¹]	γ [kg s ⁻²]
lce Water	1000.0 1000.0	2.216 0.5624	2103.0 4218.0	333.0	0.028

obtain the Péclet number. Then, the formula for the growth velocity

$$V = \sigma P e^2 = \frac{d_c u_\Gamma}{2\alpha} \tag{34}$$

is employed to compute the tip velocity and, eventually, the tip radius is found from eq. (28).

In the following, we compare the simulation results with both the analytical solution of the theory of Langer and Müller-Krumbhaar and experimental results [9,48] at various undercoolings ΔT . We prescribe a single dendrite of tip length l_D with the parametric function

$$x(s) = s \tag{35}$$

$$y(s) = -\frac{s^2}{r_t} + l_D,$$
(36)

 $s \in [0, \sqrt{r_t l_D/2}]$. We choose $l_D = 3r_t$, and an initial tip-radius which is half the tip radius expected from theory. We simulate only half a dendrite in a domain of size $[20r_t \times 40r_t]$, utilizing the symmetry of the problem, see Fig. 8 for the initial interface location together with a sketch of the multiresolution block structure. Each phase is initialized at constant temperature, the ice subdomain with $T_s = T_m$ and the undercooled water subdomain with $T_l = T_m - \Delta T$. Material parameters for water and ice at 273.15K are given in Table 2. The domain is chosen big enough to eliminate boundary effects. We resolve the domain with 256 × 512 cells. All far-field boundary conditions are assumed to be adiabatic.

Fig. 9 shows the transient tip velocity for an undercooling of $\Delta T = 10$ K for various refinement levels (Fig. 9 (a)), and the temperature field in the growing crystal (Fig. 9 (b)). The discontinuous temperature field at initialization leads to an overestimation of the tip velocity at early times, and the dendrite grows rapidly. The energy released by the solidifying melt results in a flattening



Fig. 8. Schematic of the simulation domain for the two-dimensional dendritic growth case, including the multiresolution block structure. The solidification front is shown in red. Note that the dendrite is not drawn to scale.

of the temperature gradient in both phases, and the tip velocity decreases. Note that the cell spacing only affects the early stages of the growth for t < 200 ns. Once a smooth temperature field has developed in the near field of the dendrite, the temporal evolution overlaps for different mesh sizes. Curvature effects on the interface temperature result in a heterogeneous temperature distribution in the parabolic dendrite (see Fig. 9 (b)). The minimum temperature occurs at the dendrite tip, which is where the interface velocity reaches its maximum.



(a) Temporal evolution of the tip velocity

Relative error of the presented results to the analytical soluti	on.
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ΔΤ [Κ]	1	2	5	8	10	15	20
error (u_{Γ}) [%]	11.6	12.8	16.0	10.2	9.0	9.7	10.3

Based on these results, we performed multiple simulations with various undercoolings to compare our model with analytical, experimental, and numerical reference data. Note that the interface radius r_t decreases with increasing undercooling ΔT . Therefore, we adapt the cell size to maintain a constant resolution per tip radius for all investigated cases. The strong initial temperature gradient results in a high interface velocity, so that the crystal grows rapidly. To assure that the crystal does not grow beyond its stability limit due to the initial transient, we initialize the dendrite with a tip radius smaller than what is predicted from the analtical solution $r_{t,0} < r_{t,LM-K}$. Once a smooth temperature field has developed, the tip curvature decreases. We evaluate the interface velocity once the tip radius is equal to the radius of the theory of Langer and Müller-Krumbhaar $r_{t,LM-K}$ [40]. Our results are presented in Fig. 10, together with the analytical solution [29] and previously published experimental [9,48] and numerical [7,40] data. The deviation to the analytical solution for each undercooling is presented in Table 3. The results of our model lie within the experimental scatter, and numerical errors are similar to previously published level-set based models [7,40]. For $\Delta T > 10$ K, experimental results deviate from analytically and numerically determined tip velocities. This deviation can be attributed to kinetic effects [48], which play an increasingly important role for such large undercoolings. and are neither included in the simulation models nor in the analytical model.

4.3. Growth of a crystal with four-fold symmetry

Juric and Tryggvason [23] proposed a test problem for the unstable growth of a crystal with four-fold symmetry. The initial phase interface is given by the parametric function

$$x(s) = x_c + (R_0 + R_s \cos(8\pi s)) \cos(2\pi s)$$
(37)

$$y(s) = y_c + (R_0 + R_s \cos(8\pi s)) \sin(2\pi s)$$
(38)



(b) Temperature field at the dendrite tip



Fig. 10. Tip velocity as function of the undercooling ΔT from the presented numerical simulations, numerical reference data [7,40], experimental reference data [9,48], and analytical results [29]. Present numerical results are marked with filled symbols, open symbols denote reference data from literature, and the solid and dashed lines give the analytical results together with the variance $\Delta \sigma$.

with $s \in [0, 1]$, $R_0 = 0.1$, $R_s = 0.02$, and $x_c = y_c = 2$ in a domain of size $[0, 4] \times [0, 4]$ with periodic boundary conditions. We use constant material parameters for the densities $\rho_l = \rho_s = \rho = 1$, the specific heat capacities $c_l = c_s = c = 1$, the thermal conductivities $k_l = k_s = k = 1$, and the latent heat L = 1. The melting temperature is set to $T_m = 1$, and the initial temperature field in the solid ($T_s = T_m$) and liquid ($T_l = 0.5$) phase is constant. The surfacetension coefficient and the kinetic coefficient are set to $\gamma = 0.002$ and $\epsilon_u = 0.002$, respectively [23].

The Stefan number of this problem is

$$St = \frac{c(T_m - T_l)}{L} = 0.5 = X_s(t \to \infty)$$

and indicates that at equilibrium, half of the domain is solidified, while the other half remains in a liquid state at melting temperature. The temporal evolution of the solid volume fraction X_s and of the mass *m* normalized with the initial mass m_0 are given in Fig. 11 for effective grid resolutions of 256, 320, 384, 448, and 512 cells per spatial direction. For the coarsest resolution, we find an overprediction of the steady-state solid volume fraction, but with increasing resolution this overshoot vanishes. The temporal behavior converges for increasing mesh refinement, too. At steady state, the solid and the liquid mass each account for approximately one half of the total mass, as expected for this setup. The total mass (Fig. 11 (b)) remains constant during the simulated time, confirming the conservation property of our method. For comparison, Fig. 12 shows the relative local deviation of the simulated density field ρ_{sim} to the exact solution $\rho = 1$ for an effective resolution of 256 cells per spatial direction at t = 0.4 with the linearized approach, Fig. 12 (a), and the semi-implicit scheme proposed here, Fig. 12 (b). The linearized scheme exhibits large density errors in cut cells where the main direction of the crystal growth deviates from the main grid axes, see e.g. the area between two neighbouring fingers, Fig. 12 (a). For the present scheme, the density errors vanish, Fig. 12 (b)).

Fig. 13 shows the isolines of the evolving solid-liquid interface for the previously mentioned grid resolutions. The time interval between isolines is $\Delta t = 0.05$. The initial four protrusions develop each into a single dendrite. The tip-splitting instability occurs at each of these protrusions. In previous studies, the onset of this instability was reported at $t \approx 0.3$ (e.g. [32,55]). Our low-dissipation simulations indicate that the numerical dissipation of the underlying numerical discretization scheme is critical for observing the first occurrence of tip-splitting, which in our case is at t = 0.15. This underlines the advantageous effect of low-dissipative spatial and temporal discretization schemes on the occurrence of interfacial instabilities, as already mentioned by Gibou et al. [11]. Such high-order methods benefit from their low intrinsic numerical diffusion which does not prevail over the physical instability mechanism. With increasing refinement, the secondary dendrites flatten, and the onset of additional tip-splitting instabilities is observed, see the results in Fig. 13 for resolutions above 384 cells. To the authors' knowledge, this kind of instability has not been reported for numerical simulations of this test case in previous literature.

The temperature field at t = 0.6 and t = 1 is given in Fig. 14. The anisotropic growth behavior is a consequence of the nonuniform temperature distribution in the solid and liquid phases, see t = 0.6. Between two neighboring fingers, the liquid temperature is close to the melting temperature, leading to a low growth velocity. Near the tips of the crystal, the liquid is still undercooled. In combination with the lower interface temperature at the tips, which follows from the Gibbs-Thomson relation for curved interfaces (eq. (2)), this results in a local increase of the growth velocity. At t = 1, the temperature is approximately homogeneous in solid and liquid phases. This results in small interface temperature gradients, thus the crystal ceases to grow.

4.4. Growth of multiple crystals with four-fold symmetry

Finally, we simulate the growth of a complex multi-crystal growth configuration in an undercooled liquid to mimic a realistic solidification microstructure. On a domain of size $[0, 8] \times [0, 4]$, we initialize four spherical seeds with initial radius r = 0.2. The arbitrarily chosen seed centers are located at (1, 2), (2.5, 3.5), (4, 1), and (6, 2). The initial temperature is $T_l = 0.2$ for the undercooled liquid, and $T_s = T_m = 1$ in the solid seeds. We use constant material parameters for the densities $\rho_l = \rho_s = \rho = 1$, the specific heat capacities $c_l = c_s = c = 1$, the thermal conductivities $k_l = k_s = k = 1$, the latent heat L = 1, and the kinetic coefficient $\epsilon_u = 0.002$. For the anisotropic surface tension, we use

$$\gamma(\Theta) = \gamma_0 \left\{ 1 + A_s \left[\frac{8}{3} \sin^4 \left(\frac{1}{2} m_s(\Theta - \Theta_0) \right) - 1 \right] \right\}$$
(39)

[1]. Here, γ_0 describes the undisturbed surface tension coefficient, A_s the magnitude of anisotropy, Θ the angle between the interface normal and the *x*-axis, Θ_0 the angle between the symmetry axis of the crystal and the *x*-axis, and m_s the symmetry mode of the crystal. We choose $\gamma_0 = 0.002$, $A_s = 0.4$, $\Theta_0 = 0$, and $m_s = 4$ for a crystal with four-fold symmetry. The maximum mesh resolution of the adaptive grid is 1024 × 512 cells, and periodic boundary conditions are applied in *x*- and *y*-direction.

Interface contour lines are given in Fig. 15, with an equal time spacing of $\Delta t = 0.005$ between isolines. The initial growth stages are similar to the growth of a single nucleus in an undercooled melt, since the growing crystals do not influence each other yet. The four-fold anisotropy of the surface tension causes the crystal to grow along four main directions, similarly to the case presented in section 4.3. Interfacial instabilities at the tip of each of the protrusions result in the characteristic tip-splitting patterns. At later stages, the growing crystals interact with each other and block each others growth, which results in the locally degenerated



Fig. 11. Fig. (a): evolution of the solid volume fraction for successively finer meshes. Fig. (b): evolution of the total mass, the liquid mass, and the solid mass for various resolutions. The total mass for for the different resolutions is shown in black, the mass in the liquid phase in green, and the mass in the solid phase in blue.



Fig. 12. Relative error of the density field at t = 0.4. Fig (a): linearized approach. Fig. (b): semi-implicit approach.

fingers. This behavior is connected to inhomogeneities in the temperature field, which is shown in Fig. 16 at t = 0.03 and t = 0.07. At t = 0.03, temperature-field inhomogeneities are restricted to the near field of each single crystal, while their surrounding consists of homogeneous undercooled liquid. Therefore, the shape of all four crystals is comparable to that of a single-crystal growth case, and symmetric to the main growth directions. The ongoing heat release during phase transition results in a temperature increase in the ambient undercooled liquid. At t = 0.07, the liquid between crystals 1 and 2 has reached the melting temperature locally, and the

growth ceases. The low numerical dissipation of the model ensures that the liquid areas between the solid crystals are preserved, and are not merged with each other. Between crystals 1 and 3, the fluid is still undercooled, thus the crystals grow in this direction.

5. Conclusion and outlook

We have presented a conservative interface-interaction method for a sharp-interface formulation of liquid-solid phase transition. Conservation at the interface is maintained by explicit formula-



Fig. 14. The temperature field for an effective resolution of 512 cells in each spatial direction. The solidification front is shown in black. Fig. (a): t = 0.6. Fig. (b): t = 1.0



Fig. 13. The solid-liquid interface for various grid resolutions. The time interval between isolines is $\Delta t = 0.05$.



Fig. 15. The solid-liquid interface for the growth of multiple cystals subjected to four-fold anisotropic surface tension. The time interval between two successive isolines is $\Delta t = 0.005$.

tion of interface fluxes into both solid and liquid phases. A semiimplicit level-set formulation is applied to evolve the phase interface. A new formulation for the interface surface in a cut cell has been derived, which includes the Stefan condition. The reconstruction of interface gradients based on third-order WENO smoothness indicators [22] and an explicit third-order Runge-Kutta scheme for time discretization [12,16] ensures low numerical dissipation. The interface-interaction model takes into account surface-tension and kinetic effects on the interface temperature (Gibbs-Thomson relation), including anisotropic behavior. The Stefan condition provides a relation between interface fluxes of mass and energy, and the interface-propagation velocity. The sharp-interface property is ensured by extrapolating fluid states across the interface for the single-phase reconstruction of the cell-face fluxes near the inter-



Fig. 16. The temperature field of the multi-crystal growth case. The solidification front is shown in black. Fig. (a): t = 0.03. Fig (b): t = 0.07.

face [8]. Computational efficiency is improved by dynamic mesh adaptation with respect to the evolving interface and temperature field using the multiresolution approach of Harten [17], and an adaptive local time-stepping scheme for efficient and robust time integration [24].

We have validated the presented method with analytical solutions for the one-dimensional Stefan problem and the growth of a two-dimensional parabolic dendrite. This shows that the model is capable to capture both unstable (dendritic-like) and stable (planar) growth processes accurately. Numerical results of a growing single crystal with four-fold symmetry and multiple crystals with four-fold symmetry demonstrate the capabilities of the method to model crystal-growth problems with complex interfaces, and that it recovers the tip-splitting instability correctly. Our results indicate that the numerical dissipation of the underlying numerical scheme is critical for the prediction of tip-splitting instabilities. Our simulation predicts an earlier onset of this instability than reported in previous literature which is consistent with lower numerical dissipation. The numerical examples presented here are limited to one and two dimensions, extension to three dimensions is subject of ongoing work.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

J.W.J. Kaiser: Conceptualization, Methodology, Software, Formal analysis, Visualization, Writing – original draft. **S. Adami:** Writing – review & editing, Supervision, Formal analysis, Resources, Project administration. **I.S. Akhatov:** Writing – review & editing, Supervision, Funding acquisition. **N.A. Adams:** Conceptualization, Writing – review & editing, Supervision, Funding acquisition, Project administration.

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References

- R. Almgren, Variational Algorithms and Pattern Formation in Dendritic Solidification, J. Comput. Phys. 106 (2) (1993) 337–354, doi:10.1016/S0021-9991(83) 71112-5.
- [2] D.M. Anderson, G.B. McFadden, A.A. Wheeler, A phase-field model of solidification with convection, Physica D 135 (2000) 175–194, doi:10.1016/ S0167-2789(99)00109-8.
- [3] C. Beckermann, H.J. Diepers, I. Steinbach, A. Karma, X. Tong, Modeling Melt Convection in Phase-Field Simulations of Solidification, J. Comput. Phys. 154 (1999) 468–496, doi:10.1006/jcph.1999.6323.
- [4], Conduction of heat in solids, H.S. Carslaw, J.C. Jaeger (Eds.), Oxford University Press, 1959.
- [5] H. Chen, C. Min, F. Gibou, A numerical scheme for the Stefan problem on adaptive Cartesian grids with supralinear convergence rate, J. Comput. Phys. 228 (16) (2009) 5803–5818, doi:10.1016/j.jcp.2009.04.044.
- [6] S. Chen, B. Merriman, P. Smereka, S. Osher, A simple level set method for Stefan problems, J. Comput. Phys. 135 (1997) 8–29.
- [7] A. Criscione, D. Kintea, Ž. Tuković, S. Jakirlić, I.V. Roisman, C. Tropea, Crystallization of supercooled water: A level-set-based modeling of the dendrite tip velocity, Int. J. Heat Mass Transf. 66 (2013) 830–837.
- [8] R.P. Fedkiw, T.D. Aslam, B. Merriman, S. Osher, A Non-oscillatory Eulerian Approach to Interfaces in Multimaterial Flows (The Ghost Fluid Method), J. Comput. Phys. 152 (2) (1999) 457–492.
- [9] Y. Furukawa, W. Shimada, Three-dimensional pattern formation during growth of ice dendrites - its relation to universal law of dendritic growth, J. Cryst. Growth 128 (1993) 234–239, doi:10.1016/0022-0248(93)90325-Q.

- [10] M. Gaoyang, X. Lingda, W. Chunming, J. Ping, Z. Guoli, Two-dimensional phasefield simulations of competitive dendritic growth during laser welding, Mater. Design 181 (2019) 107980.
- [11] F. Gibou, R. Fedkiw, R. Caflisch, S. Osher, A level set approach for the numerical simulation of dendritic growth, J. Sci. Comput. 19 (1) (2003) 183–199.
- [12] S. Gottlieb, C.-W. Shu, Total variation diminishing Runge-Kutta schemes, Math. Comput. 67 (221) (1998) 73–85.
- [13] R.D. Groot, Second order front tracking algorithm for Stefan problem on a regular grid, J. Comput. Phys. 372 (2018) 956–971.
- [14] Z. Guo, P. Lin, A thermodynamically consistent phase-field model for twophase flows with thermocapillary effects, J. Fluid Mech. 766 (2015) 226–271, doi:10.1017/jfm.2014.696.
- [15] L.H. Han, X.Y. Hu, N.A. Adams, Adaptive multi-resolution method for compressible multi-phase flows with sharp interface model and pyramid data structure, J. Comput. Phys. 262 (2014) 131–152, doi:10.1016/j.jcp.2013.12.061.
- [16] A. Harten, High resolution schemes for hyperbolic conservation laws, J. Comput. Phys. 135 (1983) 260–278, doi:10.1016/0021-9991(83)90136-5.
- [17] A. Harten, Adaptive Multiresolution Schemes for Shock Computations, J. Comput. Phys. 115 (1994) 319–338.
- [18] N. Hoppe, I. Pasichnyk, M. Allalen, S. Adami, N.A. Adams, Node-Level Optimization of a 3D Block-Based Multiresolution Compressible Flow Solver with Emphasis on Performance Portability, in: International Conference on High Performance Computing & Simulation (HPCS), 2019.
- [19] X.Y. Hu, B.C. Khoo, N.A. Adams, F.L. Huang, A conservative interface method for compressible flows, J. Comput. Phys. 219 (2) (2006) 553–578, doi:10.1016/j.jcp. 2006.04.001.
- [20] G. Ivantsov, Doklady Akademii Nauk SSSR (1947) 558-567.
- [21] M.A. Jaafar, D.R. Rousse, S. Gibout, J.P. Bédécarrats, A review of dendritic growth during solidification: Mathematical modeling and numerical simulations, Renew, Sust. Energ. Rev. 74 (March 2016) (2017) 1064–1069, doi:10.1016/ j.rser.2017.02.050.
- [22] G.-S. Jiang, C.-W. Shu, Efficient implementation of weighted ENO schemes, J. Comput. Phys. 126 (1996) 202–228.
- [23] D. Juric, G. Tryggvason, A Front-Tracking Method for Dendritic Solidification, J. Comput. Phys. 123 (1996) 127–148.
- [24] J.W.J. Kaiser, N. Hoppe, S. Adami, N.A. Adams, An adaptive local time-stepping scheme for multiresolution simulations of hyperbolic conservation laws, J. Comput. Phys. X 4 (2019) 100038.
- [25] A. Karma, W.-J. Rappel, Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetrics, Phys. Rev. E 53 (1996).
- [26] Y.-T. Kim, N. Goldenfeld, J. Dantzig, Computation of Dendritic Microstructures using a Level Set Method, Phys. Rev. E 62 (2) (2000) 2471–2474.
- [27] R. Kobayashi, Modeling and numerical simulations of dendritic crystal growth, Physica D 63 (1993) 410–423, doi:10.1016/0167-2789(93)90120-P.
- [28] J.S. Langer, H. Müller-Krumbhaar, Theory of dendritic growth-I. Elements of a stability analysis, Acta Metall. 26 (11) (1978a) 1681–1687, doi:10.1016/ 0001-6160(78)90078-0.
- [29] J.S. Langer, H. Müller-Krumbhaar, Theory of dendritic growth-II. Instabilities in the limit of vanishing surface tension, Acta Metall. 26 (11) (1978b) 1689–1695, doi:10.1016/0001-6160(78)90079-2.
- [30] J.S. Langer, J. Müller-Krumbhaar, Stability effects in dendritic crystal growth, J. Cryst. Growth 42 (C) (1977) 11–14, doi:10.1016/0022-0248(77)90171-3.
- [31] E. Lauer, X.Y. Hu, S. Hickel, N.A. Adams, Numerical investigation of collapsing cavity arrays, Phys. Fluids 24 (5) (2012) 052104, doi:10.1063/1.4719142.
- [32] K. Ling, W.Q. Tao, A sharp-interface model coupling VOSET and IBM for simulations on melting and solidification, Comput. Fluids 178 (2019) 113–131.
- [33] J. Luo, X. Hu, N.A. Adams, A conservative sharp interface method for incompressible multiphase flows, J. Comput. Phys. 284 (2015) 547–565, doi:10.1016/ j.jcp.2014.12.044.
- [34] H. Müller-Krumbhaar, J.S. Langer, Theory of dendritic growth-III. Effects of surface tension, Acta Metall. 26 (11) (1978) 1697–1708, doi:10.1016/0001-6160(78) 90080-9.
- [35] B. Nestler, A.A. Wheeler, L. Ratke, C. Stöcker, Phase-field model for solidification of a monotectic alloy with convection, Physica D 141 (2000) 133–154, doi:10.1016/S0167-2789(00)00035-X.
- [36] S. Osher, R. Sanders, Numerical Approximations to Nonlinear Conservation Laws With Locally Varying Time and Space Grids, Math. Comput. 41 (164) (1983) 321–336.
- [37] S. Osher, J.A. Sethian, Fronts Propagating With Curvature Dependent Speed: Algorithms Based on Hamilton-Jacobi Formulations, J. Comput. Phys. 79 (1988) (1988) 12–49.
- [38] V. Ramanuj, R. Sankaran, High Order Anchoring and Reinitialization of Level Set Function for Simulating Interface Motion, J. Sci. Comput. 81 (3) (2019) 1963–1986, doi:10.1007/s10915-019-01076-0.
- [39] V. Ramanuj, R. Sankaran, B. Radhakrishnan, A sharp interface model for deterministic simulation of dendrite growth, Comput. Mater. Sci. 169 (May) (2019) 109097, doi:10.1016/j.commatsci.2019.109097.
- [40] P. Rauschenberger, A. Criscione, K. Eisenschmidt, D. Kintea, S. Jakirlić, Ž. Tuković, I.V. Roisman, B. Weigand, C. Tropea, Comparative assessment of Volume-of-Fluid and Level-Set methods by relevance to dendritic ice growth in supercooled water, Comput. Fluids 79 (2013) 44–52, doi:10.1016/j.compfluid. 2013.03.010.
- [41] A.R. Roosen, J.E. Taylor, Modeling Crystal Growth in a Diffusion Field Using Fully Faceted Interfaces, J. Comput. Phys. 114 (1994) 113–128, doi:10.1006/jcph. 1994.1153.

- [42] D. Rossinelli, B. Hejazialhosseini, D.G. Spampinato, P. Koumoutsakos, Multicore/multi-gpu accelerated simulations of multiphase compressible flows using wavelet adapted grids, J. Sci. Comput. 33 (2) (2011) 512–540.
- [43] G. Russo, P. Smereka, A Remark on Computing Distance Functions, J. Comput. Phys. 163 (2000) 51–67.
- [44] J.A. Sethian, J. Straint, Crystal growth and dendritic solidification, J. Comput. Phys. 98 (2) (1992) 231-253, doi:10.1016/0021-9991(92)90140-T.
- [45] J. Shaikh, A. Sharma, R. Bhardwaj, On sharp-interface level-set method for heat and/or mass transfer induced Stefan problem, Int. J. Heat Mass Transf. 96 (2016) 458–473, doi:10.1016/j.ijheatmasstransfer.2015.12.074.
- [46] A.A. Shibkov, Y.I. Golovin, M.A. Zheltov, A.A. Korolev, A.A. Leonov, Morphology diagram of nonequilibrium patterns of ice crystals growing in supercooled water, Physica A 319 (2003) 65–79, doi:10.1016/S0378-4371(02)01517-0.
- [47] A.A. Shibkov, Y.I. Golovin, M.A. Zheltov, A.A. Korolev, A.A. Vlasov, Kinetics and morphology of nonequilibrium growth of ice in supercooled water, Crystallogr. Rep. 46 (3) (2001) 496–502, doi:10.1134/1.1376484.
- [48] A.A. Shibkov, M.A. Zheltov, A.A. Korolev, A.A. Kazakov, A.A. Leonov, Crossover from diffusion-limited to kinetics-limited growth of ice crystals, J. Cryst. Growth 285 (2005) 215–227.
- [49] R. van der Sman, Phase field simulations of ice crystal growth in sugar solutions, Int. J. Heat Mass Transf. 95 (2016) 153–161.
- [50] D. Sun, S. Pan, Q. Han, B. Sun, Numerical simulation of dendritic growth in directional solidification of binary alloys using a lattice Boltzmann scheme, Int. J. Heat Mass Transf. 103 (2016) 821–831.

- [51] D. Sun, Y. Wang, H. Yu, Q. Han, A lattice Boltzmann study on dendritic growth of a binary alloy in the presence of melt convection, Int. J. Heat Mass Transf. 123 (2018) 213–226.
- [52] D. Sun, M. Zhu, J. Wang, B. Sun, Lattice Boltzmann modeling of bubble formation and dendritic growth in solidification of binary alloys, Int. J. Heat Mass Transf. 94 (2016) 474–487.
- [53] M. Sussman, P. Smereka, S. Osher, A Level Set Approach for Computing Solutions to Incompressible Two-Phase Flow, J. Comput. Phys. 114 (1994) 146–159.
- [54] L. Tan, N. Zabaras, Modeling the growth and interaction of multiple dendrites in solidification using a level set method, J. Comput. Phys. 226 (2007) 131–155, doi:10.1016/j.jcp.2007.03.023.
- [55] L. Tan, Z. Zabaras, A level set simulation of dendritic solidification with combined features of front-tracking and fixed-domain methods, J. Comput. Phys. 211 (2006) 36–63, doi:10.1016/j.jcp.2005.05.013.
 [56] M. Theillard, F. Gibou, T. Pollock, A Sharp Computational Method for the Simu-
- [56] M. Theillard, F. Gibou, T. Pollock, A Sharp Computational Method for the Simulation of the Solidification of Binary Alloys, J. Sci. Comput. 63 (2015) 330–354, doi:10.1007/s10915-014-9895-0.
- [57] H. Xing, K. Ankit, X. Dong, H. Chen, K. Jin, Growth direction selection of tilted dendritic arrays in directional solidification over a wide range of pulling velocity: A phase-field study, Int. J. Heat Mass Transf. 117 (2018) 1107–1114, doi:10.1016/j.ijheatmasstransfer.2017.10.086.