Phase field modelling of dendritic solidification by using an adaptive meshless solution procedure

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Abstract. A novel numerical procedure is developed for modelling two-dimensional dendritic solidification in dilute binary alloys. The evolution of the phases and the solute concentration is described by the partial differential equations, obtained from the phase field model. The meshless radial basis function-generated finite difference (RBF-FD) method is used for the spatial discretisation of the partial differential equations. The forward Euler scheme is used for the time-stepping. In order to reduce the computational cost, an adaptive procedure is developed, based on the quad-tree strategy, ensuring the highest density of the computational nodes at the solid-liquid interface. In the procedure, the computational domain is divided into overlapping sub-domains which can be dynamically refined or coarsened. The regular or scattered node distribution with constant node density is used for discretisation of each sub-domain. The adaptive procedure is ensured by the constant product between the area of a sub-domain and the computational node density. The accuracy and speedup in comparison to the solution on a uniform node distribution are assessed by solving the benchmark problem for dendritic solidification in dilute binary alloys. The main originality of the model represents the first use of RBF-FD method for the spatial discretisation of the PF equations in combination with adaptive solution procedure. The RBF-FD method can be used on unstructured node distributions, which is especially advantageous in the solution of PF model for dendritic growth, since the solution is very sensitive to the regularity of the node distribution. The developed spatial-temporal-adaptive numerical model represents an accurate and computationally efficient tool for the prediction of the dendrite morphology and micro-segregation during the solidification in binary alloys.

1. Introduction

Dendritic morphology is one of the most commonly observed microstructures in the industrial casting of metallic alloys. The microstructure evolution significantly determines the material properties of the final product [1, 2]. The theoretical and computational studies of dendritic growth can therefore be used to better understand and optimise the casting procedure.

The phase field (PF) approach [3, 4] represents a one-domain formulation for the simulation of dendritic solidification. Different phases are formulated by different values of PF, a continuous variable, which is constant in the bulk of the phases and smoothly varies over the interfaces between them. In the first step of the derivation of a PF model [5], a free-energy functional is constructed, describing the thermodynamics of a phase change and the capillary effects. Next, the kinetic equations for PF and other thermodynamic variables are derived by minimising the free-energy functional. Finally, appropriate free PF model parameters [6] have to be set in order to correctly capture the underlying physics of the phase
change. Additionally, in some cases, the kinetic equations have to be modified [7] in order to ensure quantitatively correct simulation results. In this paper, a PF model of dendritic solidification in dilute binary alloys [8] is considered. The model consists of two partial differential equations (PDEs), one for the PF and one for the dimensionless supersaturation.

In the numerical solution of the PF model, the spacing between the neighbouring computational nodes has to scale with the PF interface thickness. Although the interface thickness can be increased by using the thin-interface limit of the PF model [6], the ratio between the size of the computational domain and the interface thickness usually remains to be in the range of a few orders of magnitude, making the PF simulations computationally extremely costly. In the last few decades, a spectra of different numerical techniques [9, 10] have been applied for the solution of the PF models. One of the most popular techniques for PF model is the adaptive mesh refinement [11, 12], where the node density is dynamically increased near the solid-liquid interface and dynamically decreased in the bulk of the solid and liquid phase. This reduces the computational efforts while sustaining the accuracy of the numerical solution.

The PF model is in the present paper solved by a novel adaptive meshless solution procedure, based on the numerical technique for modelling of solidification by using a novel next-generation adaptive mesh refinement [12]. The computational domain is divided into the computational sub-domains with different computational node densities by using a quad-tree data structure [13]. Computational sub-domains are dynamically refined/de-refined in order to ensure the highest node density in the areas with the largest gradients of PF and dimensionless supersaturation. The meshless RBF-FD method [14] is used for spatial discretisation of the PF equations. The solution of PF equations is propagated in each sub-domain independently, while the boundary conditions are set by the weighted least squares method (WLS) [15] interpolation from the overlapping neighbouring sub-domains. The forward Euler scheme is used for temporal discretisation of PDEs on each of the sub-domains, where a suitable stable time step depends on the node density in a sub-domain. The synchronisation between the neighbouring sub-domains with different node densities only occurs when they are integrated to the same simulation time.

In the paper, firstly, the PF model for solidification of dilute binary alloys is presented. Next, the adaptive solution procedure and the RBF-FD method are described. The benchmark problem for solidification in binary alloys is used for the assessment of the accuracy and the efficiency of newly developed numerical algorithm.

2. Governing equations

We study solidification of a dilute binary alloy [8] by solving a coupled system of two partial differential equations, one for the PF \( \phi \) and one for the dimensionless supersaturation \( U \). The values \( \phi = 1 \) and \( \phi = -1 \) represent the solid and the liquid phase, respectively. The dimensionless supersaturation is defined as \( U = (\exp(u) - 1)/(1 - k_0) \), where \( u \) measures the dimensionless departure of the chemical potential from the equilibrium value and \( k_0 \) stands for the partition coefficient, respectively. The departure is defined as

\[
\frac{2c \phi}{1 + k_p - (1 - k_p) \phi},
\]

where \( c \) and \( c_0 \) stand for the concentration and the equilibrium concentration in the liquid phase, respectively.

It is convenient for numerical analysis to write PF model in dimensionless form by introducing the dimensionless spatial coordinates, the dimensionless time, and the dimensionless diffusivity of the solute in the liquid phase

\[
(x, y) = (x / W_0, y / W_0), \quad \bar{t} = t / \tau_0, \quad \overline{D} = D \tau_0 / W_0^2,
\]

where \( D \) is the diffusivity of the solute in the liquid phase and \( W_0 \) and \( \tau_0 \) stand for the characteristic interface thickness and the characteristic time of attachment of the atoms, respectively. The dimensionless governing equations in case of a negligible interface kinetics [8] are given as
\[
\left(1 + (1 - k_p) \tilde{R}_c, T\right) a^2(n) \partial \phi = \nabla \cdot \left( a^2(n) \nabla \phi \right) + \sum_{x,y} \nabla \cdot \left[ \left( \nabla \phi \right)^2 a(n) \frac{\partial a(n)}{\partial \phi} \right] - \phi - \phi^3 - \lambda(1 - \phi^2) \left(U - R_c, T\right) - \left(1 + k_p - \frac{1 - k_p}{2}\right) \partial _t U = 0
\]

where \( \lambda \) is the coupling constant and \( n=(n_x,n_y) \) stands for the normalized gradient of PF. The dimensionless cooling rate is defined as

\[
\tilde{R}_c = R_c \tau_0 / \Delta T_0, \quad \Delta T_0 = |m_l|(1-k_p)\epsilon_{40},
\]

where \( R_c \) and \( m_l \) stand for the cooling rate and the liquidus slope, respectively. In the case of the solid phase with a cubic crystal structure, the following anisotropy function \( a(n) \) is in use

\[
a(n) = 1 - 3 \epsilon_4 + 4 \epsilon_4 (n_x^4 + n_y^4),
\]

where \( \epsilon_4 \) is the strength of anisotropy.

The thin-interface limit of the PF model [6-8], yields the following relations between the physical and the PF parameters

\[
W_0 = \lambda d_o / a_1, \quad \tau_0 = a_2 \lambda W_0^2 / D,
\]

where \( a_1 = 0.8839 \) and \( a_2 = 0.6267 \). The constant \( d_o = \Gamma/\Delta T_0 \) is the chemical capillary length, where \( \Gamma \) is the Gibbs-Thomson coefficient. The thin-interface limit yields only one free parameter in the PF model. It has to be set consistently with the validity condition \(|\psi|\ll 1\), where \( \psi \) is the dimensionless interface velocity. As stated in [8], the convergence of the model actually starts to break at \(|\psi|\approx 0.2\), yielding more freedom in the selection of the free parameter.

3. Solution procedure

3.1. Adaptive discretisation of computational domain

In the solution procedure, the computational domain \( \Omega \) is decomposed into \( N_p \) overlapping computational sub-domains \( \Omega^i, i=1,2,3,...N_p \). The boundaries of \( \Omega^i \) and \( \partial \Omega^i \) are denoted as \( \Omega^i \) and \( \partial \Omega^i \), respectively. \( \partial \Omega^i \) can lie partially in \( \partial \Omega \) and partially in the neighbouring \( \Omega^j, j \neq i \). In the latter case, the boundary condition on \( \partial \Omega^i \) is set according to the solution in \( \Omega^j \), \( j \neq i \).

In our case, we consider a rectangular \( \Omega \) which is recursively divided into smaller rectangular sub-domains \( \Omega^i \) by using the balanced quad-tree data structure [13] as seen in figure 1(a). A quad-tree is balanced if the level difference between any two neighbouring leafs is less than or equal to one. \( \Omega^i \) is constructed by extending \( \Omega_{i-1} \) in order to obtain the overlapping sub-domains. For each \( \Omega^i \), uniform, regular or scattered node distribution is generated as seen in figure 2(b). The details of algorithm for construction of scattered node distribution are given in [16]. The boundary condition in computational nodes from \( \Omega^j \), lying on \( \partial \Omega^j \cap \partial \Omega \) is defined by the physical problem, while the Dirichlet boundary condition is assumed in computational nodes on \( \partial \Omega^j \cap \Omega^i \), \( j \neq i \). The values of Dirichlet boundary condition in such nodes are interpolated from \( \Omega^i \).

In order to accurately capture the details of the solution during simulation, i.e. if the refinement condition is fulfilled, the domain \( \Omega^i \) is divided into four new sub-domains with twice reduced spacing \( h_0^i \). Additional \( \Omega^i \) have to be refined too in order to maintain the balanced quad-tree. Similarly, four \( \Omega^i \) can be merged into one \( \Omega^{i'} \) with twice increased spacing \( h_0^i \), if de-refinement condition is fulfilled. De-refinement can only occur, if the quad-tree is still balanced after the potential merger of four \( \Omega^i \).
The computational node density in $\Omega^*$ is determined as $\rho^* = 1/ h^*$, where the spacing is given as $h^* = 2^{N-M} h_{\text{min}}$, where $h_{\text{min}}$ is the minimum spacing, and $N$ and $M$ stand for the level of $\Omega^0$ and the maximum level of the quad-tree, respectively. The length and height of $\Omega^0$ are given as $L^0 = n_l h^*$ and $H^0 = n_h h^*$, respectively, where $n_l$ and $n_h$ are the number of regularly distributed nodes per length and height, respectively. The length and height of $\Omega^*$ depends on the position of $\Omega^0$ in $\Omega$; in the case from figure 1(a), they are given as $L^* = (n_l + n_{\text{buff}}) h^*$ and $H^* = (n_h + 2 n_{\text{buff}}) h^*$, where the parameter $n_{\text{buff}}$ controls the area of overlapping.

**Figure 1.** (a) Rectangular computational domain $\Omega$, divided by the quad-tree algorithm into subdomains $\Omega^0$, which are extended in order to obtain the overlapping sub-domains $\Omega^*$. A quad-tree subdomain is extended by constructing boundary of computational domain $\partial \Omega^*$ which lies inside the neighbouring sub-domains. (b) Regular or scattered node distribution is used for discretisation of $\Omega^*$. (c) Illustration of a computational domain $\Omega^*$ and boundary $\Gamma^*$. The solid circles and empty triangles represent the interior and the boundary computational nodes, respectively. The dashed line represents the boundary of a local sub-domain, containing only interior nodes. The boundary of a local sub-domain containing the interior and the boundary nodes is represented by the dotted line.

3.2. Discretisation of PDEs on overlapping sub-domains

The spatial differential operators in each $\Omega^*$ are evaluated by the use of RBF-FD method. In the section, notation $\Omega^*$ is used instead of $\Omega^*_{\text{int}}$, since the procedure is the same for every $\Omega^*$ in $\Omega$. The method is based on the interpolation of the field value over a local sub-domain $\Omega^*$, centred at a node $r^*$ from $\Omega^*$, by the use of $N_{\text{loc}}$ radial basis functions (RBFs) and $N_{\text{aug}}$ augmentation monomials. $\Omega^*$ consists of $r^*$ and its $N_{\text{loc}} - 1$ nearest neighbours as seen in figure 1(c). The details of the method are given in our very recent work [14]. The RBF-FD has a finite-difference-like structure, i.e., a general spatial differential operator $\Theta$ at $r^*$ is approximated as

$$\Theta \eta(r^*) \approx \sum_{k}^{N_{\text{loc}}} w_k^* \eta_k^*,$$

where $\eta$ is an arbitrary scalar field, $w_k^*$ is a finite-difference-like coefficient, and $\eta_k^*$ field value at k-th node in $\Omega^*$. Similar approximation can be written for discretisation of $\Theta$ acting on a vector or tensor field. WLS method [15] is used for interpolation of field values to the boundary nodes in the neighbouring sub-domains. WLS has also a finite-difference-like structure, however, the weighted least squares minimisation is used instead of collocation in the calculation of the finite-difference-like coefficients.

The forward Euler scheme is used for the temporal discretisation of the partial differential equations. The interpolation of boundary values between neighbouring sub-domains only occurs, when they are at the same simulation time, since the explicit time step in $\Omega_{\text{int}}^*$ is calculated as

$$\Delta t^* = \frac{h^*}{12 \max(D,1/\min(a(n)))}.$$
4. Numerical results

4.1. Benchmark definition and model parameters

The solution procedure is verified by solving the benchmark problem for solidification in dilute binary alloys proposed by Karma [8]. In the benchmark, growth of a single dendrite into a supersaturated melt is considered while the cooling rate is set to zero. The growth velocity and the concentration profile in the solid phase are used to verify the numerical model.

A square $\Omega$ with the side length $L/d_0=740$ is used in the simulation, while a small circular nucleus with radius $R_0/d_0=22$ is put in the south-west corner of $\Omega$. Initial supersaturation in the whole $\Omega$ is set to $U=-0.55$. Zero flux Neumann boundary conditions are used for $\phi$ and $U$ on $\Gamma$. The growth velocity and the concentration profile in the solid phase are used to verify the numerical model.

A regular node distribution is used for discretisation of $\Omega$ in the present work. Irregular distribution can be easily employed too, because of the meshless concept. Second-order accurate RBF-FD method [14] is used by setting augmentation with monomials up to the second order while $N_{loc}=13$ fifth-order poly-harmonic splines are used as RBFs. The interpolation of boundary values in the neighbouring sub-domains is performed by WLS [15] with $N_{loc}=6$.

4.2. Results

The rescaled concentration profile $c/c_l$ at time $tD/d_0^2=26000$ is shown in figure 2(a). Non-overlapping computational sub-domains $\Omega_0^*$, determined by the quad-tree algorithm are also shown. The actual computation is done on extended overlapping sub-domains $\Omega_0^*$. The adaptive algorithm dynamically ensures that the solid-liquid interface lies in sub-domains with $h^*_i=h_{\text{min}}/W_0=0.4$ while larger values of $h^*_i$ are used in the bulk of the solid and the liquid phase. The concentration profile in the middle of the trunk is shown on the right in figure 2(b). A plot of the dendrite’s tip velocity as a function of time is shown in figure 3(c). Both, $c/c_l$ and $V_d/D$, are very close to the benchmark values [7].

![Figure 2](image_url)

**Figure 2.** (a) Concentration profile and quad-tree subdomains at the end of the simulation. Each extended sub-domain in the interior of $\Omega$ contains $(n_L+2n_{\text{buff}})\times(n_H+2n_{\text{buff}})=324$ computational nodes. (b) Concentration profile in the middle of the dendrite’s trunk.
Figure 3. (a) Dendrite’s tip velocity as a function of time. (b) Speedup of adaptive solution procedure as a function of time. The speedup is defined as a ratio between ERTs on adaptive and uniform node distribution.

The same simulation is run also on uniform node distribution with parameters $h_{\text{min}}/W_0=0.4$, $n_L=n_H=512$, and $M=0$ in order to assess the speedup of adaptive solution procedure. In the adaptive procedure, we reduce the number of the computational nodes and the number of time iterations, however, we introduce some additional computational work due to the interpolation of boundary values and the adaptation of the sub-domains. The speedup of the adaptive numerical model in comparison with the solution on the fixed node distribution is shown in figure 3(b). The speedup is divided into three parts: we compare the iteration elapsed real time (ERT) on uniform node distribution to ERT needed only for iteration, sum of ERTs for iteration and interpolation of boundary values, and sum of ERTs for iteration, interpolation, and adaptation. As expected, the speedup is a decreasing function of the solid-liquid interface area. Each extra term in the sum of ERTs reduces speedup. The highest speedup is observed at the beginning of the simulation. The highest growth velocity is observed initially, hence, a lot of time is spent for adaptation of computational sub-domains. The adaptation time is reduced as the velocity decreases.

5. Conclusions
An adaptive meshless solution procedure for the PF simulation of dendritic growth is developed. In the procedure, a rectangular computational domain is dynamically refined or de-refined into sub-domains with different node density by the use of quad-tree data structure. The procedure ensures that the solid-liquid interface is in the sub-domains with the highest node density. RBF-FD method and WLS are used for discretisation of PDEs and interpolation of boundary values to the neighbouring sub-domains, respectively. Simple forward Euler scheme is applied for time stepping.

The newly developed model is verified by solving the PF benchmark problem for solidification in dilute binary alloys. We have compared the segregation profile in the solid phase and the dendrite’s growth velocity. Both quantities are in good agreement with results from the benchmark problem [7]. We have also assessed the speedup of the adaptive algorithm by comparing ERTs on adaptive and uniform node distributions. The speedup drops with time as more and more sub-domains are created as the size of the solid-liquid interface increases. Naturally, the communication between neighbouring sub-domains and refinement/de-refinement procedure reduce the speedup of the method.

In the current version of the method, the finite-difference-like coefficients in the RBF-FD and WLS method are calculated whenever a new sub-domain is created. The finite-difference-like coefficients will only be calculated at the beginning of the simulation and then copied and appropriately rescaled as new sub-domain is created in the future foreseen version of the numerical implementation. This improvement will decrease the adaptation ERT, however, speedup will remain reduced due to communication. In the future, the PF model for solidification in dilute multi-component alloys [17] will
be numerically solved by the developed numerical method and integrated into the simulation system for direct-chill casting of aluminium alloys [18] and continuous casting of steel [19].

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References
[1] Dantzig J A and Rappaz M 2009 Solidification (Lausanne, Switzerland: EFPL Press)
[2] Glicksman M E 2011 Principles of Solidification (New York, USA: Springer New York)
[3] Chen L-Q 2002 Phase-field models for microstructure evolution Annu. Rev. Mater. Res. 32 113–40
[4] Boettinger W J, Warren J A, Beckermann C and Karma A 2002 Phase-field simulation of solidification Annu. Rev. Mater. Res. 32 163–94
[5] Provatas N and Elder K 2010 Phase-Field Methods in Materials Science and Engineering (Weinheim, Germany: Wiley-VCH)
[6] Karma A and Rappel W-J 1998 Quantitative phase-field modeling of dendritic growth in two and three dimensions Phys. Rev. E 57 4323
[7] Karma A 2001 Phase-Field Formulation for Quantitative Modeling of Alloy Solidification Phys. Rev. Lett. 87 115701
[8] Echebarria B, Folch R, Karma A and Plapp M 2004 Quantitative phase-field model of alloy solidification Phys. Rev. E 70 061604
[9] Karma A and Tourret D 2016 Atomistic to continuum modeling of solidification microstructures Curr. Opin. Solid State Mater. Sci. 20 25–36
[10] Dong X, Xing H, Weng K and Zhao H 2017 Current development in quantitative phase-field modeling of solidification J. Iron. Steel. Res. Int. 24 865–78
[11] Provatas N, Goldenfeld N and Dantzig J 1998 Efficient computation of dendritic microstructures using adaptive mesh refinement Phys. Rev. Lett. 80 3308–11
[12] Greenwood M, Shampur K N, Ofori-Opoku N, Pinomaa T, Wang L, Gurevich S and Provatas N 2018 Quantitative 3D phase field modelling of solidification using next-generation adaptive mesh refinement Comput. Mater. Sci 142 153–71
[13] Dobravec T, Mavrič B and Šarler B 2017 A cellular automaton – finite volume method for the simulation of dendritic and eutectic growth in binary alloys using an adaptive mesh refinement J. Comput. Phys 349 351–75
[14] Dobravec T, Mavrič B and Šarler B 2020 Reduction of discretisation-induced anisotropy in the phase-field modelling of dendritic growth by meshless approach Comput. Mater. Sci 172 109166
[15] Hatić V, Mavrič B and Šarler B 2018 Simulation of a macrosegregation benchmark with a meshless diffuse approximate method Int. J. Numer. Method. H. 28 361–80
[16] Hatić V, Mavrič B, Košnik N and Šarler B 2018 Simulation of direct chill casting under the influence of a low-frequency electromagnetic field Appl. Math. Model. 54 170–88
[17] Ohno M 2012 Quantitative phase-field modeling of nonisothermal solidification in dilute multicomponent alloys with arbitrary diffusivities Phys. Rev. E 86 051603
[18] Šarler B, Dobravec T, Glavan G, Hatić V, Mavrič B, Vertnik R, Cvahte P, Gregor F, Jelen M and Petrovič M 2019 Multi-Physics and Multi-Scale Meshless Simulation System for Direct-Chill Casting of Aluminium Alloys J. Mech. Eng. 65 658–70
[19] Vertnik R, Mramor K and Šarler B 2019 Solution of three-dimensional temperature and turbulent velocity field in continuously cast steel billets with electromagnetic stirring by a meshless method Eng. Anal. Bound. Elem. 104 347–63