The phase-change heat conduction analysis during solidification processes by a hybrid generalized FDM

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Abstract. In this paper, the single-domain enthalpy model is adopted for heat transfer analysis of phase change during solidification processes. The resulting second-order parabolic partial differential equations (PDEs) with varying thermophysical coefficients is numerically solved by a hybrid generalized finite difference method (GFDM) under mixed boundary conditions. The spatial derivatives in the PDEs are approximated by the Taylor series expansions combining with the moving-least squares technique. The temporal derivative is evaluated with a six-point symmetric difference by the classical Crank-Nicholson technique. The Newton-Raphson iteration method is used to solve the resulting nonlinear algebraic equations. Finally, the transient temperature field and the moving phase-change interface are obtained by analysing the nodal temperature distribution. Several examples are presented for verify the stability and effectiveness of this meshless method.

1. Introduction
The solidification processes are widely existed in material manufacturing and processing, such as casting, welding, metal purification, laser cladding, and selective laser sintering, etc. In the process of material solidification and structure forming, the accompanying high temperature gradient and phase change will cause significant changes in the thermodynamic properties, which may lead to uneven thermal stress distributions in the formed structures. This is the primary reason of undesirable residual stress distribution in metal castings. Therefore, the effective analysis of phase change and heat transfer during solidification processes is of great importance to evaluate and improve the casting quality.

The solid-liquid interface existing in phase change problems is varying with time, which cannot be determined in advance. To solve such problems with moving interface become very complicated, which was termed as the Stefan problem [1]. The early studies on phase-change heat transfer problems were devoted to find the analytical solutions to some simplified models. Cho and Sunderland [2] derived an analytical solution of the phase transition problem in a semi-infinite plate. Goodman and Shea [3] obtained the approximate solution of solidification problem in a finite area. The analytic solutions for more complex cases are extremely difficult. Accordingly, numerical methods become the preferred approaches to deal with these problems.

Various numerical methods have been applied to the phase-change problems, involving the boundary element method (BEM), the finite element method (FEM), the finite volume method (FVM), and the finite difference method (FDM). Honnor and Davies [4] used both the generalized Newmark dual reciprocity BEM and the single-step DRBEM for solving nonlinear transient field problems with phase change. Danaila et al. [5] utilized the adaptive FEM to capture the solid-liquid interface in two-
dimensional (2D) phase-change problem, and used the concealed source term to simulate the phase transition. Archibald et al. [6] studied the heat transfer and fluid flow problems using FVM. Chernogorova and Vabishchevich [7] applied FDM for solving the solidification problem of multi-component alloys in cylindrical molds, in which the solid phase composition of the mushy zone was assumed to be a known function of temperature.

Because the element remeshing or variable time-step techniques are required for dealing with the moving phase-change interface, the computing efficiencies of these traditional numerical methods are drastically degraded. Accordingly, the meshless methods are more suitable for this problem. As a real meshless method, the generalized finite difference method (GFDM) directly discretizes the PDEs and do not need any numerical integration, which makes it feasible to dealing with the nonlinear phase-change problems. The idea of the GFDM stems from Jesen’s introduction of irregular grids into the classical FDM by using the six-point stars [8]. However, the early stage of this method was trapped by the frequent singularity or ill-conditioning of the star. Later in 1998, Orkisz [9] proposed an improved version of the GFDM algorithm by introducing an eight-point star and moving least squares (MLS) interpolation, which greatly improved the stability of the algorithm. The latest version of GFDM is more stable and has been successfully applied to various problems. For example, Gu et al. [10] solved the inverse Cauchy problem associated with 3D non-uniform Helmholtz equations. Lei et al. [11] successfully applied it to solve in-plane crack problems. Gu et al. [12] studied the inverse problem of 3D transient heat conduction.

In this paper, a hybrid GFDM is utilized to analyze the phase change problems by combining the GFDM for spatial domain with Crank-Nicolson scheme for time domain. A brief outline of this paper is organized as follows: the mathematical description for phase-change heat conduction is presented in section 2; Section 3 introduces the algorithm and numerical implementation of the GFDM; Next in Section 4, several examples are studied to show the effectiveness and accuracy of this method. Finally, some conclusions are presented.

2. Mathematical description of phase-change heat conduction
The heat conduction equation for phase change and heat transfer problems during metal solidification processes can be formulated by the following expression [13]

\[ C(T) \frac{\partial T(x,t)}{\partial t} = \lambda \nabla^2 T(x,t), \quad x \in \Omega, \]

in which \( C(T) \) is the substitute thermal capacity; \( \lambda \) is the thermal conductivity; \( T, x \) and \( t \) denote temperature, spatial co-ordinates and time, respectively.

The substitute thermal capacity of the metal material is defined as follows

\[ C(T) = \begin{cases} c_s & T < T_s \\ c_p + \frac{L}{T_L - T_s} & T_s \leq T < T_L \\ c_L & T \geq T_L \end{cases} \]

where \( c_s, c_p, c_L \) are the volumetric specific heats of liquid, mushy zone and solid state, respectively; \( L \) is the latent heat. It is assumed that the temperature of the mushy zone is in the range of \( T_s \) to \( T_L \).

The initial condition is assumed as

\[ T(x,t) = T_p, \quad x \in \Omega, \]

in which \( T_p \) is the pouring temperature.

The mixed boundary conditions (BCs) including Dirichlet and Neumann BCs are considered:

\[ T(x,t) = T_b, \quad x \in \Gamma_t, \]

\[ (q_w)_t = -\lambda \frac{\partial T}{\partial n} = q_w, \quad x \in \Gamma_q, \]

where \( T_b \) and \( q_w \) are the prescribed boundary temperature and flux, respectively.
The generalized finite difference method (GFDM)

The meshless GFDM is used to discrete the space domain and the Crank-Nicolson scheme \[14\] for temporal discretization. The temperature field and the moving interphase surface under different thermal conduction BCs are obtained by a Newton-Rapson iterative solution. For the sake of simplification, the PDE (1) is rewritten in the following simplified form

\[
\frac{\partial T}{\partial t} = L_2[T]
\]

with \( L_2[T] = \lambda / C(T) \nabla^2 \) being the nonlinear second-order partial differential operator.

3.1. Discrete space domain by GFDM

A partial derivative formula is obtained by combining Taylor series expansion and moving least squares (MLS) approximation. It is assumed that a cluster of \( N \) nodes are randomly scattered in the solution domain \( \Omega \), which can be represented by the set \( S = \{ x^1, x^2, ..., x^N \} \). All these nodes can be classified into three sets: \( S_1 \) for all interior nodes; \( S_2 \) for the boundary nodes satisfying the Dirichlet BCs (4); \( S_3 \) for the remaining boundary nodes satisfying the Neumann BCs (5).

The subset including \( m \) nearest nodes \( x^I \) \((I=1,2, ..., m)\) are partitioned for each node \( x^0 \). Thus, the influence domain of a central node is obtained. Following with the expression in Gavete et al. [15], the subset \( E_0 = \{ x^0, x^1, ..., x^m \} \) including the support nodes \( x^I \) with the central node \( x^0 \) is termed as ‘star’, see figure 1. It should be noted that each node is assigned an associated star in the solution domain.

Let us suppose \( T^I = T(x^I) \) being the function value of the node \( x^I \) in the subset \( E_0 \). By using the Taylor’s expansion, the value \( T^I \) can be approximated by the Taylor series in the neighborhood of \( x^0 \) as follows:

\[
T^I \approx T^0 + h_I T^0_I + k_i T^0_i + \frac{1}{2} h_i^2 T^0_{i1} + \frac{1}{2} k_i^2 T^0_{i2} + h_i k_i T^0_{i12} = T^0 + p^I D
\]

where \( h_i = x^I_i - x^0 \) and \( k_i = x^I_i - x^0_i \) are the coordinate steps from the central point \( x^0 \) to the support node \( x^I \). The following expressions

\[
D(T^0) = \begin{bmatrix} T^0_1 & T^0_2 & T^0_{11} & T^0_{12} \\ T^0_2 & T^0_{12} & T^0_{22} & T^0_{23} \end{bmatrix}
\]

\[
p^I(x^I, x^0) = \begin{bmatrix} h_i & k_i & h_i^2 / 2 & k_i^2 / 2 & h_i k_i \end{bmatrix}
\]

are introduced into the equation (7) with the partial derivative vector \( D(T^0) \) at the central point \( x^0 \) and the nominal basis \( p^I \). Then, a residual function \( B(T) \) is defined by the following expression

3. Figure 1. An irregular cloud of points and the selection of stars for 2D

...
\[ B(T) = \sum_{i=1}^{m} \left( T^0 - T^i + p_i^T D \right)^2 \omega_i \]  

which is expressed as the value that Taylor series has truncated after expanding the second-order. In which, \( \omega_i \) denotes the weighting function and the following compactly supported function is adopted in this paper:

\[
\omega_i = \omega(d_i) = \begin{cases} 
1 - 6 \left( \frac{d_i}{d_M} \right)^2 + 8 \left( \frac{d_i}{d_M} \right)^3 - 3 \left( \frac{d_i}{d_M} \right)^4, & \text{if } d_i \leq d_M \\
0, & \text{if } d_i > d_M 
\end{cases}
\]  

with \( d_i = |x_i - x^0| = \left( h_i^2 + k_i^2 \right)^{1/2} \) being the distance between \( x^0 \) and \( x_i \). \( d_M = \max \{d_1, d_2, \ldots, d_m\} \) is defined as the maximal distance between the farthest support node and the central node.

Then, the extremum of the residual function \( B(T) \) with respect to the partial derivatives \( D(T^0) \) is obtained by \( \partial B(T) / \partial D(T^0) = 0 \), which will lead to the following linear equation system

\[
AD = b
\]

in which \( A \) is a symmetric matrix and takes the following form

\[
A = PW^{T}\tau
\]

where \( P = \{p_1, p_2, \ldots, p_m\} \) and \( W = \{\omega_1^2, \omega_2^2, \ldots, \omega_m^2\} \) is a diagonal matrix.

By introducing the vector \( T = \{T^0, T^1, \ldots, T^m\}^{T} \) for \( m \) function values of all the support nodes \( x^i \) (\( i = 1, \ldots, m \)) and \( T_0 = \{T^0, T^0, \ldots, T^0\}^{T} \) for the center node \( x^0 \), the partial derivative vector \( D(T^0) \) can be expressed in the following matrix form

\[
D(T^0) = A^{-1}b = A^{-1}PW(T - T_0)
\]

\[
= A^{-1}PW_{m}T^1 + \ldots + A^{-1}PW_{m}T^m - A^{-1}PW(e_1 + \cdots + e_m)T^0
\]

\[
= -m_j T^0 + \sum_{i=1}^{m} m_j T^i
\]

where \( e_i \) are the vectors of the canonical basis.

According to the above analysis, the derivative of the unknown function for each node \( x^0 \) in the calculation domain can be represented by a linear combination of the function values of its neighboring nodes. Substituting equation (13) into equation (6) yields the following expression

\[
L_m[T] = \frac{\lambda}{C(T)} \left( \bar{m}_j T^0 + \sum_{i=1}^{m} \bar{m}_j T^i \right) = U(T) \left( \bar{m}_0 T^0 + \sum_{i=1}^{m} \bar{m}_j T^i \right)
\]

where \( U(T) = \lambda / C(T) \) is a nonlinear coefficient and the coefficients \( \bar{m}_0 \) and \( \bar{m}_j \) can be obtained from equation (13). The nonlinear equations can be obtained by repeating the same process for each node in the computational domain.

### 3.2. Discrete time domain by Crank-Nicolson scheme

The Crank-Nicolson scheme, also known as the six-point symmetric format, is essentially the arithmetic averaging of the forward difference format and the backward difference format. In this paper, the six-point symmetric format can be obtained by

\[
\frac{(T^{n+1})^0 - (T^n)^0}{\Delta t} = \frac{1}{2} \left( L^2_n \left[T^n\right] + L^2_{n+1} \left[T^n\right] \right)
\]

Substituting equation (14) into equation (15), the following recursive relation is obtained
\[
(T^n)^{n+1} - \frac{\Delta t}{2} U^{n+1}(T) \left[ m_0 \cdot (T^n)^{n+1} + \sum_{i=1}^{n} m_i \cdot (T^i)^{n+1} \right] = (T^n)^n + \frac{\Delta t}{2} U^n(T) \left[ m_0 \cdot (T^n)^n + \sum_{i=1}^{n} m_i \cdot (T^i)^n \right] \quad (16)
\]

Then, a system of nonlinear algebraic equations can be obtained, which was then solved by the MATLAB function ‘fsolve’ step by step in this paper. As the first time step (i.e. \( n=0 \)), the function value at the next time-step \( n=1 \) can be determined by the initial and boundary conditions equation (3-5). Then, all the values for each time can be obtained by repeating the process until the prescribed time step.

4. Numerical example and results
A square casting domain is considered in the following numerical example. The cross-section area of casting is \( 0.04 \times 0.04 \text{[m}^2\text{]} \). The following thermophysical parameters of material are assumed: \( \lambda = 35 \text{[W/(mK)]} \), \( c_s = 5.175 \text{[MJ/(m}^3\text{K)]} \) for \( T < 1470\degree C \), \( c_p + L / (T_L - T_s) = 61.4 \text{[MJ/(m}^3\text{K)]} \) for \( T \in [1470,1505) \), \( c_L = 5.74 \text{[MJ/(m}^3\text{K)]} \) for \( T \geq 1505\degree C \), the pouring temperature \( T_P = 1550\degree C \).

In our numerical implementation, a regular node distribution (see figure 2) in the square domain is considered with the time increment selected as \( \Delta t = 1\text{s} \). Two types of boundary conditions are considered: (I) all the boundary temperatures are fixed as \( T_b = 1465\degree C \); (II) the upper surface temperature is set as room temperature, and the remaining surfaces are regarded as adiabatic boundaries.

The isotherms in the casting domain under the BC (I) are shown in the figures 3-4 for different time steps. It can be seen from these figures that the trend of the phase-change interface varying with time. The liquid-mush interface (\( T = 1550\degree C \)) is moving inward. The solid-mush interface (\( T = 1470\degree C \)) appears at the time \( t=90\text{s} \). The temperatures at all nodes gradually approach to the boundary temperature.

![Figure 2. Nodes distribution in the square domain.](image)

![Figure 3. The isotherms in the casting domain at (a) \( t=10\text{s} \) (b) \( t=30\text{s} \) under BC(I)](image)
The temperature field and the isotherms under the BC (II) are illustrated in the figure 5. It is can be observed from these figures that the heat transfer of the casting from the upper boundary.

**Figure 4.** The isotherms in the casting domain at (a) $t=50s$ (b) $t=90s$ under BC(I)

**Figure 5.** Temperature field at (a) $t=5s$ and (b) $t=10s$ and the isotherms at (c) $t=5s$ and (d) $t=10s$ under BC(II).
5. Conclusion
The hybrid GFDM combined the meshless GFDM for space domain with classical Crank-Nicholson scheme for time domain has been successfully developed for heat transfer analysis of phase change during solidification processes in this paper. The numerical examples show the high efficiency and accuracy of this meshless method for this kind of Stefan problem. It will be further explored for residual stress analysis of these solidified structures in the future work.

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