

Diffuse Approximate Method for Casting Simulations

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Summary

This document introduces a mesh-free computational procedure for simulation of coupled heat, mass, momentum, and solute transport in solidification systems. The physical model takes into account the pure liquid, nucleation and movement of the globulitic solid phase, formation of the rigid porous solid matrix, and complete solid within mixture continuum theory. The computational procedure is based on explicit Diffuse Approximate Method (DAM) with nine-noded support, second order polynomial trial functions, and Gaussian window weighting functions. Treatment of velocity and pressure fields is described in detail.

Introduction

Metal castings are fundamental to practically all other manufacturing industries [1]. Although the manufacturing path from the melt to the finished shape is most direct, it involves coupled physical phenomena of great complexity which have to be simultaneously controlled. Castings are usually of complex shape which represents an additional difficulty. Therefore, numerical modeling and simulation is increasingly applied in casting. The field has expanded very rapidly in recent years owing both to the continuing exponential growth in hardware performance and the ongoing developments of physical models [2] and numerical techniques [3,4,5]. A common defect that occurs in casting is macrosegregation [6], an inhomogenous distribution of alloy elements on the scale of the product. It is caused by solute transport, primarily due to flow of solute-enriched liquid and movement of solute-depleted solid grains. The macrosegregation modeling can be based on the two-phase or one-phase model of the solidification system. The one phase model is used in this work, derived from the averaging of the microscopic equations for the solid and the liquid phase, defining macroscopic mixture quantities [7] and relations between macroscopic and microscopic quantities [8]. Despite the powerful features of well established numerical methods such as the finite difference (FDM), finite volume (FVM), the finite element (FEM), the spectral (SM), and the boundary element methods (BEM), there are often substantial difficulties in applying them to realistic phase-change situations [9]. A common drawback of the mentioned methods is the need to create a polygonisation, either in the domain and/or on its boundary. This type of meshing is often the most time consuming part of the solution process and is far from being fully automated. In recent years, a new class of methods has been developed which do not require polygonisation but use a set of nodes to approximate the solution. The

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rapid development of these type of methods and their classification is elaborated in the very recent monographs [9,10]. Because of the clear advantages of these methods in geometrically involved situations a great incitement for their introduction in casting simulations exists [11].

Governing Equations

Consider a two-component solidification system with a material that can exist either in the solid S or in the liquid phase L , confined to domain Ω with boundary Γ . The volume fractions of these two phases add up to unity ${}^v f_L + {}^v f_S = 1$. The macroscopic mass conservation of the system is governed by

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \vec{v}) = 0, \quad \rho = {}^v f_S \rho_S + {}^v f_L \rho_L, \quad \vec{v} \rho = {}^v f_S \rho_S \vec{v}_S + {}^v f_L \rho_L \vec{v}_L, \quad (1,2,3)$$

with the mixture density ρ and velocity \vec{v} are defined from phase densities and velocities. The macroscopic momentum conservation of the system is governed by

$$\begin{aligned} \frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = & -\nabla P + {}^v f_L \nabla \cdot \boldsymbol{\tau}_L + \nabla \cdot (\rho \vec{v} \vec{v} - {}^v f_S \rho_S \vec{v}_S \vec{v}_S - {}^v f_L \rho_L \vec{v}_L \vec{v}_L) \\ & + \left({}^v f_S \nabla \cdot \boldsymbol{\tau}_S + {}^v f_S \rho_S \vec{f}_S + {}^v f_L \rho_L \vec{f}_L \right) c^+ \{ {}^v f_S^c - {}^v f_S \} + \left(\rho_L \vec{f}_L + \vec{g}_L \right) c^+ \{ {}^v f_S - {}^v f_S^c \} \end{aligned} \quad (4)$$

$$\nabla \cdot \boldsymbol{\tau}(\mu, \vec{v}) = \mu \nabla^2 \vec{v} + \nabla \cdot (2\mu \mathbf{v}) - \frac{2}{3} \nabla \cdot [\mu (\nabla \cdot \vec{v}) \cdot \mathbf{I}] \quad (5)$$

where P represents the pressure, $\boldsymbol{\tau}_\varphi$ the Newtonian extra stress tensor, \vec{f}_φ the body force, \vec{g}_φ the inter-phase force on phase φ , and c^+ the linearised Heaviside function over interval $2\delta x$

$$c_+ \{x\} = \begin{cases} 1; & x \geq +\delta x \\ (x + \delta x) / (2\delta x); & \delta x > x > -\delta x \\ 0; & x \leq -\delta x \end{cases} \quad (5)$$

Note that the first term of the last row in equation (4) sets-in in the so called slurry region with ${}^v f_S < {}^v f_S^c$ where solid grains are free to move, and the last term of equation (4) sets-in in the mushy zone, where solid phase with ${}^v f_S > {}^v f_S^c$ moves with the system velocity $\vec{v}_S = \vec{v}_{SYS}$. ${}^v f_S^c$ represents the rigid solid fraction limit. The stress tensors are calculated from the following logic

$$\boldsymbol{\tau}_s = \boldsymbol{\tau}_s(\mu_s, \vec{v}_s), \boldsymbol{\tau}_L = \boldsymbol{\tau}_L(\mu_L, \vec{v}_L(\vec{v}, \vec{v}_s)), \mu_s = \frac{\mu_L}{f_s} \left(1 - \frac{f_s}{f_s^c}\right)^{-2.5 f_s^c} - \frac{f_L}{f_s} \mu_L \quad (6,7)$$

the interphase force is modeled by the Darcy law with the Kozeny-Karman permeability with δ_K denoting a small number

$$\vec{g}_L = -\frac{\mu_L}{K} \frac{\rho}{\rho_L} (\vec{v} - \vec{v}_{sys}), \quad K = K_0 \frac{(1 - f_s)^3}{f_s^2 + \delta_K} \quad (8,9)$$

The body force is modeled by the Bussinesq approximation with \vec{a} denoting acceleration, $\rho_{0\varphi}$, T_0 and $f_{0\varphi}$ the reference density, temperature and mass fraction of species ℓ in phase φ , and $\beta_{\varphi T}$, $\beta_{\varphi \ell}$ denoting the respective thermal and concentration expansion coefficients.

$$\rho_{\varphi} \vec{f}_{\varphi} = \rho_{0\varphi} \vec{a} \cdot [1 - \beta_{\varphi T}(T - T_0) - \beta_{\varphi \ell}(f_{\varphi} - f_{0\varphi})] \quad (10)$$

The energy conservation of the system is governed by

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{v} h) = \nabla \cdot (k_{eff} \nabla T) + \nabla \cdot (\rho \vec{v} h - f_s \rho_s \vec{v}_s h_s - f_L \rho_L \vec{v}_L h_L) \quad (11)$$

where T represents mixture temperature, k_{eff} the effective heat conduction, and h represents the mixture enthalpy, defined from the phase enthalpies and fractions. c_{φ} , T_0 and T_L stand for the specific heats, the reference temperature and the solidus temperature, respectively.

$$\rho h = f_s \rho_s h_s + f_L \rho_L h_L, \quad h_s = \int_{T_0}^T c_s dT, \quad h_L = \int_{T_0}^T c_L dT + \int_{T_0}^{T_s} (c_s - c_L) dT + L \quad (12,13)$$

The macroscopic conservation of species ℓ in the system is governed by

$$\begin{aligned} \frac{\partial}{\partial t}(\rho^m f) + \nabla \cdot (\rho \vec{v}^m f) &= \nabla \cdot (\rho \vec{v}^m f - f_s \rho_s \vec{v}_s^m f_s - f_L \rho_L \vec{v}_L^m f_L) \\ + \nabla \cdot (\rho_{\ell} D_{eff} \nabla^m f) - \nabla \cdot (\rho_{\ell} D_{eff} \nabla^m f - f_s \rho_s \ell D_s \nabla^m f_s - f_L \rho_L \ell D_L \nabla^m f_L) \end{aligned} \quad (14)$$

where f represents mixture concentration of species ℓ , defined from phase mass fractions f_{φ}

$$\rho_{\ell}^m f = {}^v f_s \vec{v}_s \rho_s^m f_s + {}^v f_L \vec{v}_L \rho_L^m f_L \quad (15)$$

${}_{\ell} D_{eff}$ represents the effective species and ${}_{\ell} D_{\phi}$ phase diffusion coefficients. The macroscopic equations are closed by the following microscopic assumptions. The relative movement of the solid phase with respect to the liquid phase is described by assuming a linear drag force

$$\vec{v}_s = \begin{cases} \vec{v}_L + \frac{1 - {}^v f_s}{18\mu_{eff}} (\rho_s - \rho_L) d_s^2 \vec{a}; & {}^v f_s < {}^v f_s^c \\ \vec{v}_{sys}; & {}^v f_s \geq {}^v f_s^c \end{cases} \quad (16)$$

The solid grains move with the grain transport equation and grow as

$$\frac{\partial}{\partial t} n + \nabla \cdot (\vec{v}_s n) = \frac{n_{max}}{\sqrt{2\pi}\Delta T_{\sigma}} \exp\left(-\frac{1}{2}\left(\frac{\Delta T - \Delta T_n}{\Delta T_{\sigma}}\right)^2\right), \quad d_s = \left(\frac{3 {}^v f_s}{4\pi n}\right)^{\frac{1}{3}} \quad (17,18)$$

where ΔT_n represents the mean nucleation undercooling corresponding to the maximum of the distribution, ΔT_{σ} is the standard deviation of the distribution, n_{max} is the maximum density of nuclei given by the integral of the total distribution from zero undercooling to infinite undercooling, and $\Delta T = T_L - T$, with T_L standing for the liquidus temperature.

The three parameters strongly depend on the grain refiner and melt composition. The total liquid volume fraction is related to the local temperature according to the lever rule (18). For calculation of the solute concentration in the liquid phase the relation (19) is used, with k representing the equilibrium partition ratio and T_f the melting temperature

$${}^v f_L = \frac{\rho}{\rho_L} \left(1 - \frac{1}{1-k} \frac{T - T_L}{T - T_f}\right), \quad {}^m f_L = \frac{{}_{\ell} f}{1 + (1 - {}^m f_L)(k - 1)} \quad (19,20)$$

Solution over time-step includes calculation of mixture velocity and pressure fields, temperature and concentration fields from the macroscopic equations, and phase fractions, concentrations, velocities and enthalpies from the microscopic equations.

Solution Procedure

The described set of equations is solved by the explicit DAM. This mesh-free method has been introduced by Nayroles [12] and further developed by Sadat [13,14]. The solution of nonlinear scalar transport equation by this method is given in our accompanying paper [16]. Here we focus on a novel solution of the velocity and pressure

fields through an fully explicit procedure. This is very important in present context since the explicit nature of the calculations preserves the small algebraic equation systems used for calculation of each of the unknowns. The DAM is based on the approximation of the unknown function value Φ_n and its derivatives in point \bar{p}_n by the moving least squares method which uses the values of Φ_i at I points $\bar{p}_i; i = 1, 2, \dots, I$, situated in the vicinity of and including \bar{p}_n . One can write the following approximation of the function and its first and second order partial derivatives

$$\Phi(\bar{p}) \approx \sum_{k=1}^K \alpha_k \psi_k(\bar{p} - \bar{p}_n) \quad \frac{\partial}{\partial p_\zeta} \Phi(\bar{p}) \approx \sum_{k=1}^K \alpha_k \frac{\partial}{\partial p_\zeta} \psi_k(\bar{p} - \bar{p}_n) \quad (21,22)$$

$$\frac{\partial^2}{\partial p_{\zeta\xi}} \Phi(\bar{p}) \approx \sum_{k=1}^K \alpha_k \frac{\partial^2}{\partial p_{\zeta\xi}} \psi_k(\bar{p} - \bar{p}_n); \quad \zeta, \xi = x, y; \quad (23)$$

Functions ψ_k have been chosen as polynomials $\psi_1 = 1, \psi_2(\bar{p}) = p_x, \psi_3 = p_y, \psi_4(\bar{p}) = p_x p_y, \psi_5(\bar{p}) = p_x^2, \psi_6 = p_y^2$, i.e. $K = 6$. The coefficients α_k can be calculated from the minimization of the following functional

$$\mathfrak{S}(\alpha_n) = \sum_{i=1}^I \omega_n(\bar{p}_i - \bar{p}_n) \left[\Phi_i - \sum_{k=1}^K \alpha_k \psi_k(\bar{p}_i - \bar{p}_n) \right]^2 \quad (24)$$

with ω_n representing a suitable weighting function [15]. The pressure field is solved by taking the divergence of the momentum equation and considering the mass conservation

$$\nabla \cdot \frac{\partial}{\partial t}(\rho \vec{v}) = \frac{\partial}{\partial t} \nabla \cdot (\rho \vec{v}) = -\frac{\partial^2 \rho}{\partial t^2} = -\nabla \cdot [\nabla \cdot (\rho \vec{v} \vec{v})] - \nabla^2 P + \nabla \cdot (\nabla \cdot \boldsymbol{\tau}) + \nabla \cdot \vec{f} \quad (25)$$

The pressure is calculated from a false transient of the following equation towards the steady-state

$$\frac{\partial}{\partial t} P = -\nabla^2 P - \nabla \cdot [\nabla \cdot (\rho \vec{v} \vec{v})] + \nabla \cdot (\nabla \cdot \boldsymbol{\tau}) + \nabla \cdot \vec{f} + \frac{\partial^2 \rho}{\partial t^2} \quad (26)$$

with Neumann boundary conditions obtained by multiplication of the momentum equation with the normal derivative

$$\frac{\partial P}{\partial n_r} = \left[-\frac{\partial}{\partial t}(\rho \vec{v}) - \nabla \cdot (\rho \vec{v} \vec{v}) + \nabla \cdot (\nabla \cdot \boldsymbol{\tau}) + \nabla \cdot \vec{f} \right] \cdot \vec{n} \quad (27)$$

Let us assume the initial velocity and pressure fields are known. The initial pressure is calculated from a three-level time-step procedure

$$P_0 = P'_0 + \left[-\nabla^2 P'_0 - \nabla \cdot [\nabla \cdot (\rho_0 \vec{v}_0 \vec{v}_0)] + \nabla \cdot (\nabla \cdot \boldsymbol{\tau}_0) + \nabla \cdot \vec{f}_0 + \frac{\rho_{-2} - 2\rho_{-1} + \rho_0}{\Delta t^2} \right] \Delta t \quad (28)$$

where P_0^i represents the value from previous iteration, and ρ_{-1}, ρ_{-2} represent the value of density at time $t_0 - \Delta t, t_0 - 2\Delta t$. The pressure equation boundary conditions are discretised as

$$\frac{\partial P}{\partial n_r} = \left[\frac{-\rho_0 \vec{v}_0 + \rho_{-1} \vec{v}_{-1}}{\Delta t} - \nabla \cdot (\rho_0 \vec{v}_0 \vec{v}_0) + \nabla \cdot (\nabla \cdot \boldsymbol{\tau}_0) + \nabla \cdot \vec{f}_0 \right] \cdot \vec{n} \quad (29)$$

After calculation of the pressure field at time t_0 , the new velocity field at time $t_0 + \Delta t$ is calculated from

$$\vec{v} = \left[\frac{\rho_0 \vec{v}_0}{\Delta t} - \nabla \cdot (\rho_0 \vec{v}_0 \vec{v}_0) - \nabla P_0 + \nabla \cdot \boldsymbol{\tau} + \vec{f} \right] \frac{\Delta t}{\rho} \quad (30)$$

Afterwards, the solid phase movement (16) is calculated, followed by the solution of the grain transport (17,18), and the solution of the energy and species conservation equations. The microscopic equations are solved at the end of one internal timestep iteration. After a sufficiently small difference between results of the two successive internal timestep iterations is achieved, the next timestep is attempted. The computational details regarding solution of the scalar transport equations are given in an accompanying paper [15].

Conclusions

The present paper introduces DAM for numerical evaluation of highly complex solidification models. Attempts of solving such models were previously made only more established numerical methods. Probably for the first time it copes with solution of the momentum and pressure equations in the DAM context in fully explicit way, preserving the small systems of equations that need to be solved for each node. The method appears efficient, because it does not require a solution of the large systems of equations like for example the RBFCM [11]. Instead, small (in our case 6x6) systems of linear equations have to be solved in each timestep for each node, representing the most natural and automatic domain decomposition. The numerical examples with solution of the temperature, velocity and concentration fields in DC cast aluminum alloys and their match with the FVM will be shown at the conference.

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