

## A MULTI-SCALE/MULTI-PHYSICS MODELING FRAMEWORK FOR SOLIDIFICATION SYSTEMS

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### ABSTRACT

Models of solidification need to account for multiple physical processes that occur at multiple length scales. A general solidification modelling framework is outlined which can be used to systematically handle the multi-scale/multi-physics nature of a given process. This framework is illustrated by considering specific models, a model of an alloy casting, and a model of dendrite growth in an under cooled melt. The paper concludes by quantifying the computer requirements for an integrated solidification model that would span across the length scales of interest.

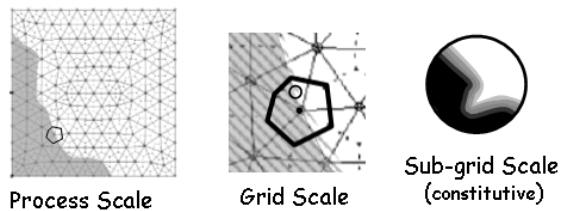
### NOMENCLATURE

$g$	solid fraction
$H$	dimensionless enthalpy
$T$	temperature
$\varepsilon$	anisotropic strength
$\kappa$	curvature
$\theta$	interface angle

### INTRODUCTION

Solidification of metal alloys is a multi-scale/multi-physics process. A complete model of a given system could involve phenomena at the process scale ( $\sim m$ ), e.g., the fluid flow in a continuous caster, closely coupled with phenomena occurring at length scales associated with the solid liquid interface, e.g., a mass diffusion (micro-segregation) in a secondary dendrite arm space ( $\sim 10 \mu m$ ). The objective of this paper is to outline a general framework that can be used to develop multi-scale/multi-physics models of solidification systems. The essential feature in the framework is the identification of three distinct length scales; the Process Scale that defines the domain of the problem, the Grid Scale where nodal values of process variables are defined and stored, and the Sub-grid Scale where phenomena at scales below the grid resolution are incorporated into the analysis via the use of volume averaging and the development of constitutive relationships. The operation of this framework is illustrated by considering two solidification models. The first is a heat and mass transfer model of the solidification of an alloy. This model is aimed at tracking the fate and transport of the solute components (segregation) in a casting. The second model looks at the evolution of microstructure, in particular an equi-axed crystal growing in an undercooled melt. Together, these models span nine

decades of length scales. The paper concludes by investigating the possibility of combining these models into a single integrated solidification model. The focus in this investigation is a quantification of the computational requirement.



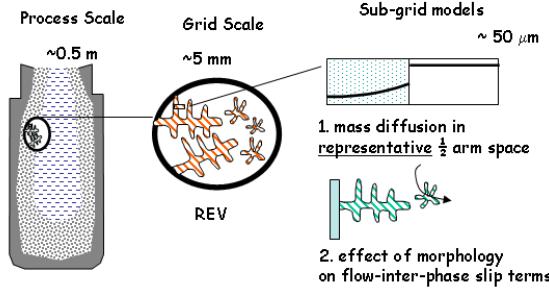
**Figure 1:** A general modelling framework for multi-scale/multi-physics processes.

### A MULTI-SCALE/MULTI-PHYSICS FRAMEWORK

In very broad terms the multi-scale/multi-physics features in a solidification system focus on the treatment of the interfaces (transitions) between phases and/or phenomena; features that often operate at a local scale which is significant smaller than the process scale of industrial interest. Hence, a successful model has to be able to account for the influence of process scale on the local scale and visa-versa. In this light, a numerical modelling framework can be envisaged that is build on three distinct length scales, see Figure 1. The Process Scale defines the domain of the problem. At this scale the domain of interest is covered by an appropriate grid of elements defined by a discrete set of node points. On this grid, algebraic equations are developed that relate values of the independent variables stored at a given node to values at neighbouring nodes and the domain boundaries. The Grid Scale is defined by a specified volume associated with a node point. The conditions in the grid-scale volume are accounted for by the nodal value of the independent variable which, at this scale, is regarded as a representative or averaged value. The averaging process used to define the nodal values is informed by the Sub-grid Scale and in this process account is made of the phenomena that occur at, across, or adjacent to phase interfaces and transitions. In addition to the independent variables, through homogenization and volume averaging, the sub-grid scale can also be used to arrive at grid scale representative values for process parameters and coefficients. This simple minded framework may not work exactly in every case but, as illustrated by two specific examples below, it does provide a useful framework for building models that can span a wide range of length scales.

## COUPLED HEAT AND MASS TRANSFER MODEL

The first specific example of multi-scale/multi-physics model is a coupled model of the heat and mass transfer during solidification of an alloy, see Figure 2.



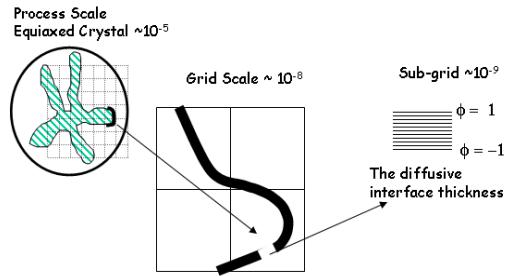
**Figure 2:** A coupled model of the heat and mass transfer during solidification of an alloy.

The process scale is a casting, a static ingot casting is shown in the Figure but the model developed can be readily extended to continuous or DC casting geometries. The objective is to track the evolution the solid fraction, thermal, and solute fields. This is achieved by solving the heat and mass transport equations for nodal values of temperature and solute concentration. This solution needs to be consistent with the thermodynamics that couple the solute concentrations and temperature and take account of advective transport of the liquid melt and solid grains in the casting. When averaging over the nodal volume at the grid scale (the REV), the local morphology of the solid phases is account for in the construction of sub-grid models. Two examples are (i) a model that couples the thermal and solute fields through tracking the segregation and diffusive transport of the solute components at the solid liquid interface and (ii) a model leading to a constitutive relationship for the momentum exchange between the solid phases and the liquid melt. Full descriptions of this type of modelling can be found in the work of Bennion and Incropera (1987), Beckermann and Viskanta (1989), Voller et al. (1989), Beckermann and Wang (1995), and Swaminathan and Voller (1997). To provide a little more detail consider the recent work by Voller et al (2004) and Voller (2006a). These authors advocate a mixed explicit/implicit time stepping technique. In a time step the conserved quantities of mixture enthalpy and mixture solute within each REV are directly obtained from an explicit time integration of the heat and mass transfer equations. To move to the next time step, nodal values for solid fraction, temperature and, solute concentrations need to be extracted from these quantities. Appropriate values are obtained by enforcing consistency between the mass balance in a representative length scale of the solid-liquid morphology and the liquidus surface of the phase diagram. In seeking this consistency, the calculated variables are constrained to maintain the current nodal values of the mixture enthalpy and solute concentrations. Following this step, with a solid fraction now in hand, appropriate sub-grid interphase drag terms can be calculated and the two-phase momentum equations solved for the liquid and solid velocities; standard modifications of the implicit SIMPLE algorithm can be used. Voller et al (2004) and Voller (2006a) have verified this explicit /implicit approach by comparing with available semi-analytical solutions and an experimentally

validation for an inverse segregation has been reported by Ferreira et al (2004).

## MICROSTRUCTURE MODEL

The heat and mass transfer model presented in the previous section requires sub-grid models that account for morphology. As the model stands a simple morphological model based on a representative length scale is used. While such an approach works well for considerations connected to the interface scale redistribution of the solute components (microsegregation) it might be inadequate to account for interphase drag terms. In addition, a correct averaging of a grid scale coefficients such as a mass or thermal diffusivities could require a more complete description of the microstructure in the REV. The way to go in this case, is to develop a model of the microstructure development. A good starting point is a model of a single equi-axed grain in an undercooled melt. The process scale, see Figure 3, is a box of initially undercooled liquid slightly larger than the final grain size.



**Figure 3:** A model of crystal growth in an undercooled melt/

Examples of sub-grid models are constitutive models that accounts for surface anisotropy and, if a phase field model is used, the interpolations of thermal properties and the phase field marker across the diffuse interface (Karma and Rappel, 1998). The development of models of this system has been a real growth industry in the solidification modelling community and many sophisticated approaches based on level-set techniques (Chen et al., 1997, and, Kim et al., 2000) and phase field formulations have been developed (Boettger et al., 2002). As pioneered by Tacke (1990) and Tacke and Harnisch (1991) and followed up more recently by Voller and Murfield (2005), Pal et al. (2006), Chatterjee and Chakraborty (2006) and Voller (2006b), a reasonable model, however, can also be obtained with a modest enthalpy formulation. In this approach, as detailed by Voller and Murfield (2005) and Voller (2005b) the enthalpy equation

$$\frac{\partial H}{\partial t} = \nabla^2 T \quad (1)$$

is solved explicitly, where assuming an appropriate scaling, the dimensionless enthalpy is defined as

$$H = T + (1 - g) \quad (2)$$

the sum of the temperature and liquid fraction. An explicit solution of (1) will provide a value of  $H$  at each node point in the domain. A point wise procedure can then be used to extract a temperature and liquid fraction to be used

at the next time step of the calculation. This extraction has to be carried out so that it is consistent with sub-grid models that provide relationships for the curvature undercooling (Gibbs–Thomson condition). For example, in a pure material, following the definitions in Kim et al (2000), at a phase change node  $0 < g < 1$  the temperature is given by

$$T = -\kappa(1 - 15\varepsilon \cos 4\theta) \quad (3)$$

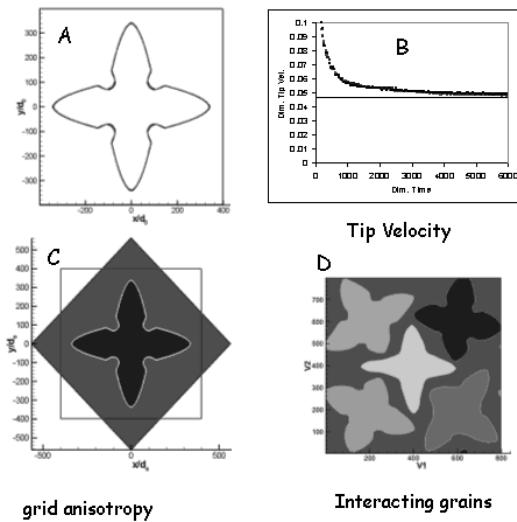
where the curvature

$$\kappa = -\nabla \cdot \left[ \frac{\nabla g}{|\nabla g|} \right] \quad (4)$$

and interface angle

$$\theta = \tan^{-1} \left( \frac{g_x}{g_y} \right) \quad (5)$$

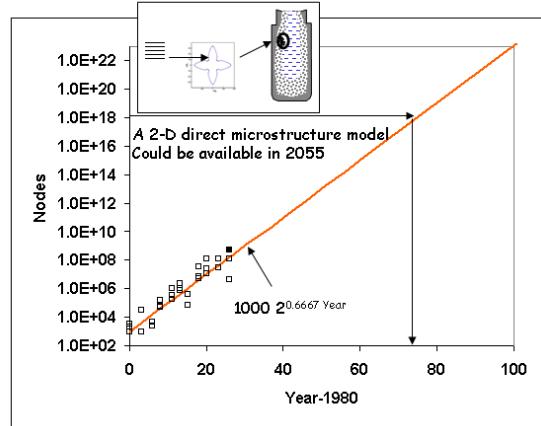
can, on appropriate discretizations, be calculated from the nodal solid-fractions; the parameter  $\varepsilon \sim 0.05$  is the anisotropic strength. Hence, the procedure for extracting temperature  $T$  and liquid fraction ( $1 - g$ ) from enthalpy  $H$  reduces to the solution of the non-linear equations (2)-(4) at each phase change node; readily achieved through iteration. This surprisingly simple model can lead to solutions of dendrite crystals that (i) are consistent with other models, panel A in Figure 4 shows a time shot prediction of a four fold symmetry dendrite, (ii) have the correct long time behaviour for the tip velocity (see panel B), (iii) are relatively free of grid anisotropy, panel C compares predictions made with the axis of symmetry at  $0^\circ$  and  $45^\circ$ , and (iv) can be extended to predict multiple grains growing at various angles of preferred growth (see panel D). The last result is a worthwhile one since it provides a framework for calculating averaged (homogenized) quantities of mass and thermal diffusivities that are based on realistic solid-liquid morphologies (DasGupta et al., 2006).



**Figure 4:** Simulation results for dendritic growth with four fold symmetry into an undercooled melt. Conditions match those of Kim et al (2000).

## HOW WIDE A SCALE RANGE?

The development of the microstructure model was motivated by the need to accurately characterize the solid-liquid morphology in the grid volumes of the heat and mass transfer model. Now that it has been established that it is possible to develop microstructure models, can we close the loop and build a heat and mass transfer model based on a seamless simulation from the process down to the smallest microstructural length scale. In other words, can we have a solidification model of heat and mass transfer at the industrial process scale ( $\sim m$ ) that resolves down the interface capillary scale ( $\sim nm$ ); a simulation (in 2D) that will require  $10^{18}$  node points. Is this feasible? Recently, Voller and Porté-Agel (2002) undertook a study where the time evolution of grid sizes used by researchers attending the conference series “Modeling of Casting, Welding and Advanced Solidification Processes” were quantified. Figure 5 presents an update of the results through 2006. The plot provides the three largest grid sizes (number of nodes) from each of the eleven proceedings of this conference. Not surprisingly, this result shows a scaling consistent with the popular form of Moore’s law; the grid size doubles every 18 months. In this way, it is seen that a grid of  $10^{18}$  will not be feasible until the year 2055.



**Figure 5:** Time evolution of grid size (number of nodes) used in solidification simulations.

## CONCLUSION

Models of heat and mass transfer in solidification systems are now well established. The concept of a modelling framework based on the three length scales of process, grid, and sub-grid allows for a comprehensive treatment that accounts for all the relevant scales. The weakest point in this model is the need to assume something about the nature of the morphology in the grid volume. This problem could be overcome by the application of direct modelling of the microstructure within a heat and mass transfer model. Indeed tools are in place where microstructure models can be built from sub-grid models that operate on the nano-meter scale. Unfortunately, however, a projection of future computer power indicates that it may be some time before models with the required range of scales can be attempted. In the mean time researchers should focus on developing the heat and mass transfer models of solidification with emphasis on

modelling the general two-phase nature of the solidification morphology. At the same time they should look toward “value added” models of microstructure that will be able to indirectly inform the heat mass transfer models in the absence of being able to contribute directly.

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