Multiscale modeling of alloy solidification[1]

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A multiscale model based on a database approach is presented to investigate alloy solidification. Appropriate assumptions are introduced to describe the behavior of macroscopic temperature, macroscopic concentration, liquid volume fraction and microstructural features. These assumptions lead to a macro-scale model with two unknown functions: liquid volume fraction and microstructure features. These functions are computed using information from the solution of selected micro-scale problems. This work addresses the selection of the sample problems relevant to the interested problem and the utilization of data from the micro-scale solution of the selected sample problems. A computationally efficient model, which is different from both the micro-scale model and macro-scale model, is utilized to find relevant sample problems. In this work, the computationally efficient model is a sharp interface model that does not account for nucleation and treats the solidification material as a pure material. Similarities between the sample problems and the interested problems are explored by assuming that the liquid volume fraction and microstructure features are functions of solution features extracted from the solution of the computationally efficient model. The solution features of the computationally efficient model are defined as the interface velocity and thermal gradient in the liquid at the time the sharp interface passes through. An analytical solution of the computationally efficient model is utilized to select sample problems relevant to solution features obtained at any location of the interested problem domain. The microscopic solution of selected sample problems is then utilized to evaluate the two unknown functions (liquid volume fraction and microstructure features) in the macro-scale model. Interpolation is utilized in the feature space to greatly reduce the number of sample problems needed and to make the database approach a computationally efficient one. The efficiency of the proposed multi-scale framework is demonstrated with numerical examples that consider a large number of solidifying crystals. A computationally intensive fully-resolved micro-scale analysis is also performed to evaluate the accuracy of the multiscale framework.

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