Direct Handling of Sharp Interfacial Energy for Microstructural Evolution

Efraín Hernández–Rivera[1,2], Veena Tikare[2] and Sylvia Saltzstein[2] (man.)

[1]Dept Nuclear Engineering & Radiological Sciences, University of Michigan, Ann Arbor MI
[2]Advanced Nuclear Energy Progs, 6225, Sandia National Lab/US DOE, Albuquerque NM

Expected graduation: Dec 2014

SAND2014-15978D

Introduction

Many microstructural evolution processes have been simulated by the Cahn–Hilliard (CH) based phase field model. The CH equation was originally developed to model spinodal decomposition [1] of glass with interfacial energy introduced by a gradient in the composition of the glass. Since then, many have adapted this to simulate a wide range of microstructural evolution mechanisms with "order parameters" introduced by *Khachaturyan* [2] to represent many other materials characteristics, such as grains and precipitates with a gradient in the parameters representing the interfaces.
We introduce a simplification to the previously demonstrated hybrid Potts–phase field (hPPF) [3], which relates interfacial energies to microstructural sharp interfaces. The model defines interfacial energy by a Potts–like discrete interface approach of counting unlike neighbors, which we use to compute local curvature. The model is compared to the hPPF by studying interfacial characteristics and grain growth behavior. The models give virtually identical results, while the new model allows the simulator a more direct approach to model interfacial energy.

Microstructure Representation

- Divided into distinct order parameters
  - Discrete: grain id (orientation) and phases
    - Features with a sharp interfaces
  - Continuum: concentration

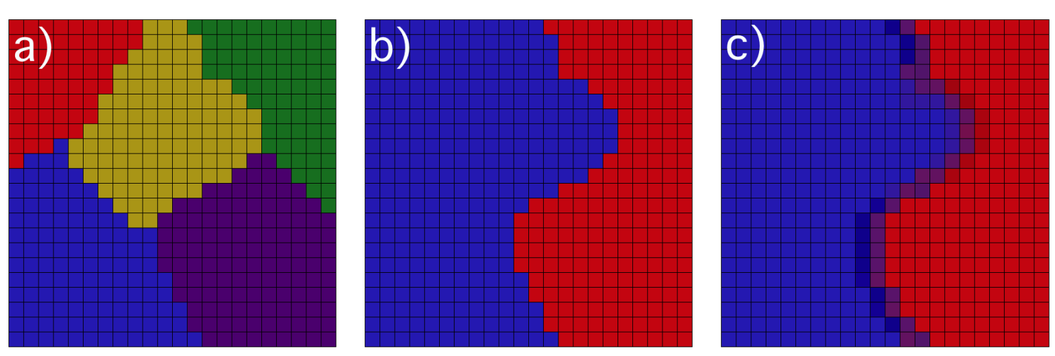

Figure 1 : Schematic showing the different types of order parameters and their inter–relationship. The order parameters used to model the microstructural evolution include: (a) grain id, (b) phase, and (c) concentration.

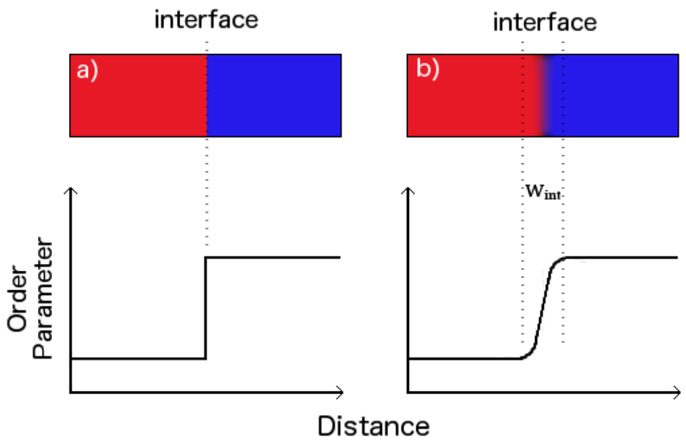

Figure 2 : Microstructural evolution has been model with both diffuse and sharp interfaces. Our hybrid model incorporates both types into an efficient description of microstructural evolution.

Energetics, Kinetics and Thermodynamics

- The free energy functional, i.e. equation of state (EoS), is defined by volumetric and interfacial energy terms

$$F = \int_{\mathcal{V}} f_0 dV + \int_{\mathcal{S}} \gamma dS = \int_{\mathcal{V}} f_0 dV + \frac{\gamma_{CH}}{2} \int_{\mathcal{V}} |\nabla C|^2 dV + \gamma_{Potts} \int_{\mathcal{S}} dS \quad (1)$$

Energetics, Kinetics and Thermodynamics (cont.)

- Using Potts interfacial energy, the EoS can be discretized

$$F_{d,i} = \sum_{i=1}^{N} \left(f_0(q_i, C_i) + J \sum_{j=1}^{n} (1 - \delta_{s(i)s(j)}) \right) \quad (2)$$

where f_0 is the bulk free energy and J is the interaction energy of adjacent elements

- The chemical potential for the compositional evolution is given by the variational derivative of the EoS w.r.t. concentration

$$\frac{\delta F}{\delta C} = \gamma \frac{\delta S}{\delta C} = \gamma \frac{\delta V}{\delta C} \frac{\delta S}{\delta V} = \gamma \Omega \frac{8\pi R \delta r}{4\pi R^2 \delta r} = \frac{2\gamma\Omega}{R} \equiv \gamma\Omega\kappa \quad (3)$$

which tells us that the chemical potential is proportional to the curvature

- This allows use to rewrite the commonly used CH equation with an equivalent one that defines the compositional evolution in terms of curvature

$$\frac{\partial C}{\partial t} = \nabla \cdot \left[\nabla \left(\frac{\partial f_0}{\partial C} - \nabla^2 C \right) \right] \quad \rightarrow \quad \frac{\partial C}{\partial t} = \nabla \cdot \left[\nabla \left(\frac{\partial f_0}{\partial C} + \kappa \right) \right] \quad (4)$$

Discrete Curvature

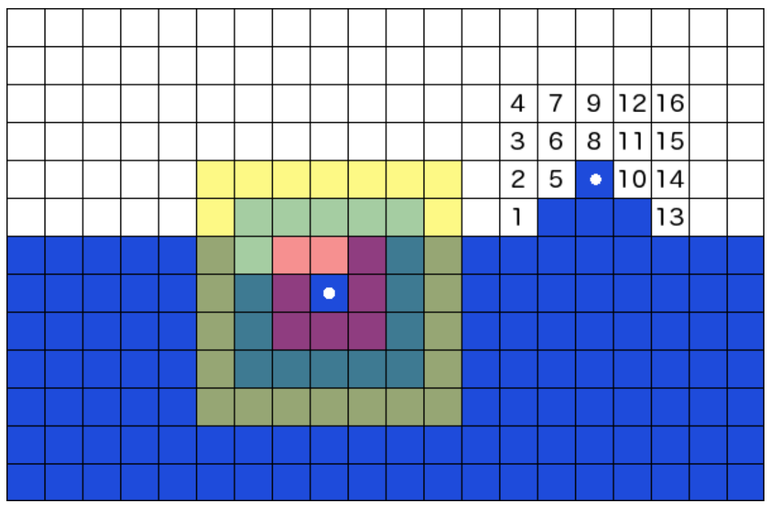

Figure 3 : Diagram of the approach used to calculate the local curvature. Each colored square surrounding the white dot on the lower left depicts a different curvature measurement.

$$\kappa_i = \frac{\sum_{j=1}^{n_s} (1 - \delta_{q(i)q(j)}) - n_{base}}{n_s} \quad (5)$$

where n_s is the number of sites within the colored squares and n_{base} is the reference number of sites that yield $\kappa = 0$ for a flat surface

Phase Transformation

- Grain growth and phase coarsening is simulated by minimizing the EoS by means of the standard Metropolis algorithm
  - Following Boltzmann statistics

$$P_i = \begin{cases} 1, & \Delta F_d \leq 0 \\ \exp\left(-\frac{\Delta F_d}{k_B T}\right), & \Delta F_d > 0 \end{cases} \quad (6)$$

where $\Delta F_d = F_{d,i}^{trial} - F_{d,i}^{initial}$ is the change in the EoS between the attempted and the initial configurations

Mail: ehernan@sandia.gov
efrainhr@umich.edu

Direct Handling of Sharp Interfacial Energy for Microstructural Evolution

E. Hernández–Rivera, V. Tikare and S. Satlzstein (man.)

Results

- Equilibrium concentration

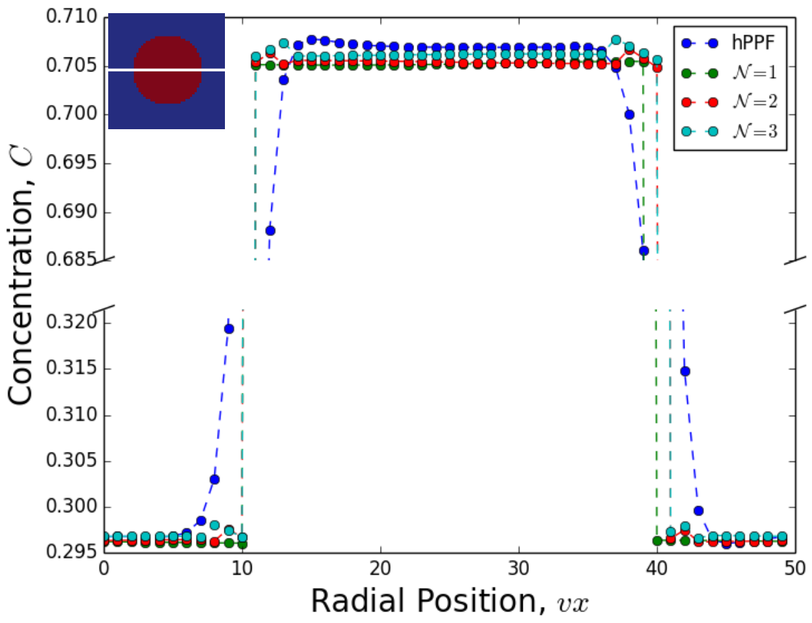

Figure 4 : Concentration profile for the matrix–precipitate (insert) system after quasi–equilibrium has been reached. The concentration is taken across the center of the precipitate, as shown by the white line in the insert. The concentration for all cases are similar, especially as the interface width is increased, and is highlighted by the high resolution of the y–axis.

- Grain growth

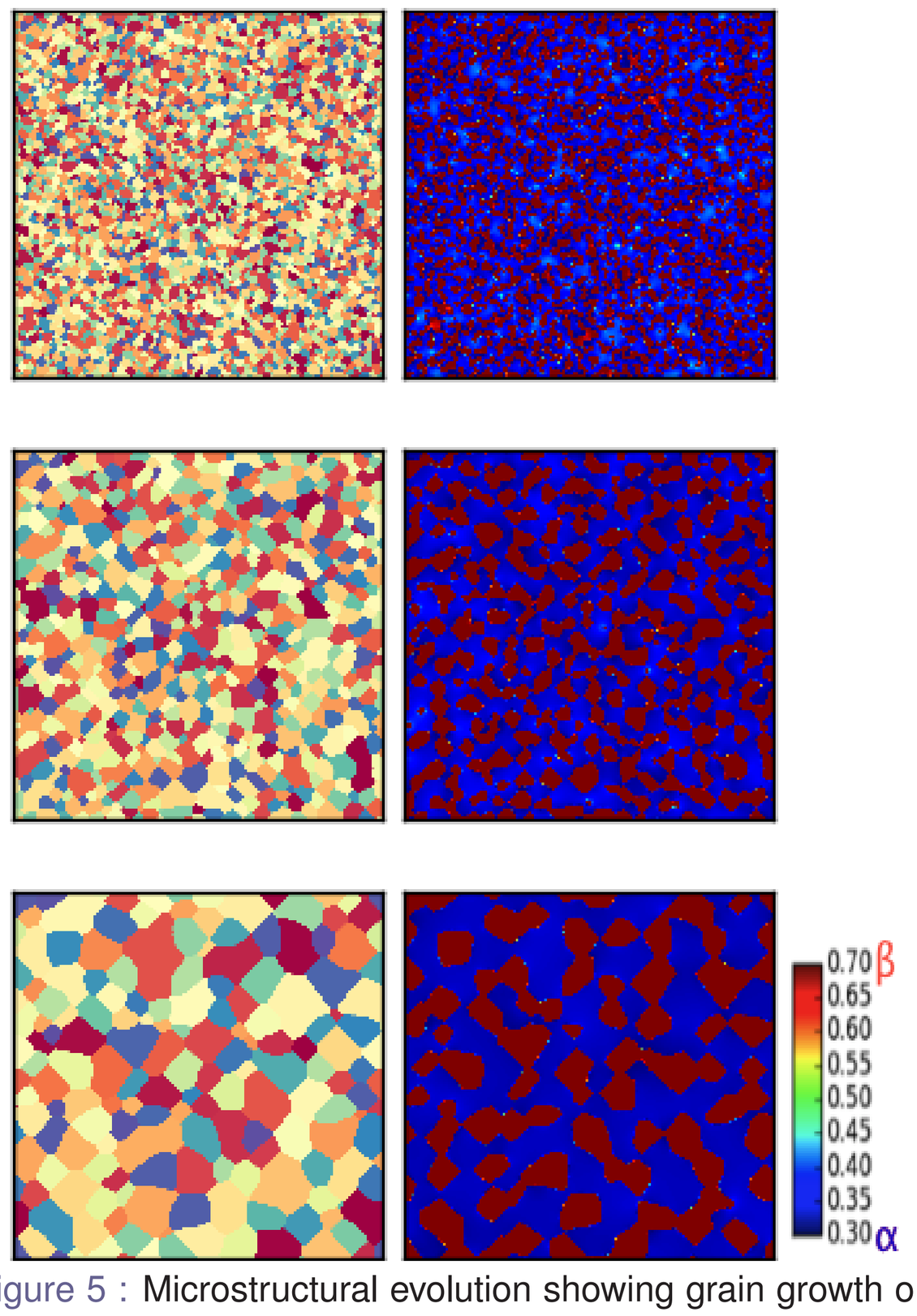

Figure 5 : Microstructural evolution showing grain growth on the left, and concentration evolution and coarsening of the α (blue) and β (red) phases on the right for the $\mathcal{N} = 1$ case. We show the spin and concentration distributions for: (top to bottom) $t = 464$, 4640 and 46416 *MCS*.

Results (cont.)

- Grain growth (cont.)

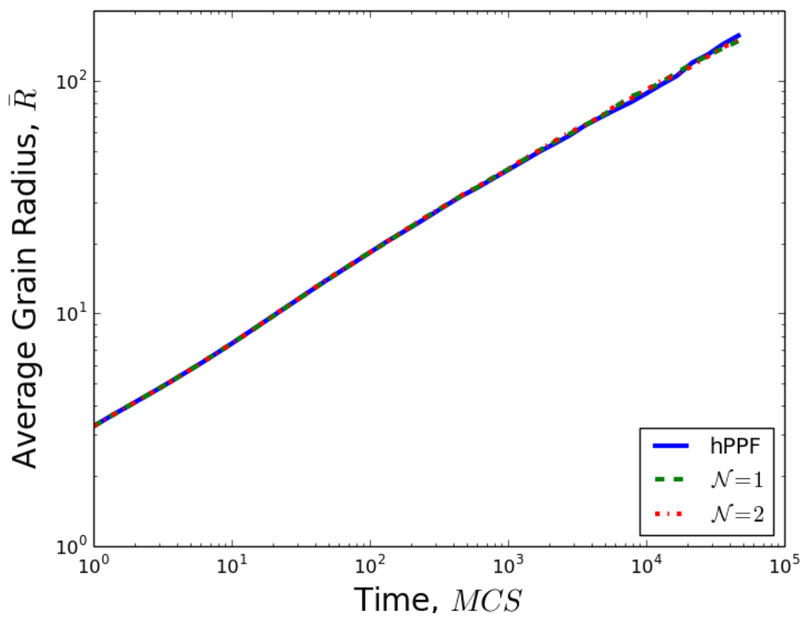

Figure 6 : Grain growth curves for hPPF and our simplified model with shells $\mathcal{N} = 1$ and 2. We can see that all three curves are virtually identical.

Table 1 : Summary of the grain growth exponential inverse, $1/n$, for the hPPF model and a series of discrete curvature calculations with varying $\mathcal{N}$.

hPPF	$\mathcal{N}$		$\mathcal{N}_{3D} = 1$
	1	2	
0.350	0.337	0.345	0.386

Conclusion & Future Work

- We have shown that our discretized curvature approach is accurate and robust for simulation of microstructural evolution
  - Grants a direct method for calculating the thermodynamic state
- Successfully applied to continuum thermodynamic and kinetic equations to simulate microstructural evolution by capillarity

Future work

- Use a more mathematical and physical approach to calculating the curvature

$$\kappa_i = \nabla \cdot \hat{n}_i = \nabla \cdot \left(\frac{\sum_{j=1}^{n} d_{ij}(1 - \delta_{q(i)q(j)})}{||d_{ij}(1 - \delta_{q(i)q(j)})||} \right) \tag{7}$$

Acknowledgment

Sandia National Laboratories is a multi–program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE–AC04–94AL85000.

References

1. J.W. Cahn, Acta Met., 9, 795 (1961)
2. A.G. Khachaturyan, *The Theory of Structural Transformations in Solids*, Wiley & Sons (1983)
3. E.R. Homer, V. Tikare and E.A. Holm, Compt. Mats. Sci., 69, 414 (2013)

Mail: ehernan@sandia.gov
efrainhr@umich.edu