A Note on Phase Field (PF) Method

Jin Young Choi, Tianju Xue

February 3, 2023

1 Background

Phase-field (PF) method is a physics-based computational approach used to solve problems at interfaces, such as grain boundaries in metal. We implemented a PF model for solving grain evolution that occurs during the melting/solidification of laser-based metal additive manufacturing processes.

2 Equations

2.1 PF Equations

A parameter $\eta_i(r,t)$ describes grains with different orientations, where $(i = 1, 2, \ldots, n)$, and n is number of grain orientations. η_i is 1 in the i^{th} orientation and 0 in other orientations, and continuously changes from 1 to 0 at the boundaries [1].

The governing equation for the microstructure evolution is a time-dependent Ginzburg-Landau equation:

$$\frac{\partial \eta_i(r,t)}{\partial t} = -L_g \frac{\partial F(\zeta, \eta_i, T)}{\partial \eta_i(r,t)} \tag{1}$$

where L_g is a kinetic coefficient for interfacial mobility at grain boundaries, and has a form:

$$L_g = L_0 \exp\left\{-\frac{Q_g}{RT}\right\} \tag{2}$$

L_0 is a constant coefficient, Q_g is the activation energy and R is the gas constant.

The total free energy F is given as:

$$F = \int_V f_{\text{grain}} + f_{\text{grad}}\, dV \tag{3}$$

The local grain energy f_{grain} is:

$$f_{\text{grain}} = m_g[\sum_{i=1}^{n}(\frac{(\eta_i)^4}{4} - \frac{(\eta_i)^2}{2}) + \gamma \sum_{i=1}^{n}\sum_{j\neq i}(\eta_i)^2(\eta_j)^2 + \frac{1}{4} + (1-\zeta)^2 \sum_{i=1}^{n}(\eta_i)^2] \tag{4}$$

where m_g is a pre-coefficient, γ is a model parameter, f_{grain} reaches the minimum when $[\eta_1, \eta_2, ..., \eta_n] = [1, 0, ..., 0], [0, 1, ..., 0], ..., [0, 0, ..., 1]$, and ζ is related to L/S state defined by:

$$\zeta = \frac{1}{2}(1 - \tanh\left(\theta \frac{T}{T_{\text{liquidus}}} - 1\right)) \tag{5}$$

where θ is a constant assigned so that ζ tends to be 0 in the liquid phase and 1 in the solid phase.

The gradient energy f_{grad} is:

$$f_{\text{grad}} = \frac{\kappa_g}{2}(\boldsymbol{\nabla}\eta_i)^2 \tag{6}$$

where κ_g is a gradient term coefficient for the grain boundary.

The PF model also includes the grain boundary anisotropy. We recommend interested readers to check [1] for the equations, [2] and [3] for how the parameters are determined.

2.2 Temperature Equation

The PF model uses one-way temperature coupling as input. We use Rosenthal's solution for a steady-state temperature profile with a moving point source [2].

$$T(X,R) = T_0 + \frac{Q}{2\pi\kappa_T}(\frac{1}{R})\text{exp}[-\frac{V_p}{2\alpha}(R+X)] \tag{7}$$

where, $R = \sqrt{X^2+Y^2+Z^2}$, and X, Y, and Z are positional coordinates.

Alternatively, we implemented a CFD-PF coupling which uses the JAX-CFD simulations to calculate a more physical temperature field. Check out our note on JAX-CFD for more information on the CFD model.

References

[1] M. Yang, L. Wang, and W. Yan, "Phase-field modeling of grain evolutions in additive manufacturing from nucleation, growth, to coarsening," *Npj Computational Materials*, vol. 7, no. 1, pp. 1–12, 2021.

[2] A. F. Chadwick and P. W. Voorhees, "The development of grain structure during additive manufacturing," *Acta Materialia*, vol. 211, p. 116862, 2021. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1359645421002421

[3] N. Moelans, B. Blanpain, and P. Wollants, "Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems," *Phys. Rev. B*, vol. 78, p. 024113, Jul 2008. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevB.78.024113