

# A Note on Phase Field (PF) Method

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## 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  $(i = 1, 2, \dots, n)$ , and  $n$  is number of grain orientations.  $\eta_i$  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:

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

The total free energy  $F$  is given as:

$$F = \int_V f_{\text{grain}} + f_{\text{grad}} dV \quad (2)$$

The local grain energy  $f_{\text{grain}}$  is:

$$f_{\text{grain}} = m_g \left[ \sum_{i=1}^n \left( \frac{(\eta_i)^4}{4} - \frac{(\eta_i)^2}{2} \right) + \gamma \sum_{i=1}^n \sum_{j \neq i} (\eta_i)^2 (\eta_j)^2 + \frac{1}{4} + (1 - \zeta)^2 \sum_{i=1}^n (\eta_i)^2 \right] \quad (3)$$

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

$$\zeta = \frac{1}{2} \left( 1 - \tanh \left( \theta \frac{T}{T_{\text{liquidus}}} - 1 \right) \right) \quad (4)$$

where  $\theta$  is a constant assigned so that  $\zeta$  tends to be 0 in the liquid phase and 1 in the solid phase.

The gradient energy  $f_{\text{grad}}$  is:

$$f_{\text{grad}} = \frac{\kappa_g}{2} (\nabla \eta_i)^2 \quad (5)$$

where  $\kappa_g$  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].

$$T(X, R) = T_0 + \frac{Q}{2\pi\kappa_T} \left(\frac{1}{R}\right) \exp\left[-\frac{V_p}{2\alpha}(R + X)\right] \quad (6)$$

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>