

Physics-informed neural networks for coupled Allen-Cahn and Cahn-Hilliard phase field problems

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Physics-informed neural networks (PINNs) have emerged as a promising tool for effectively resolving diverse partial differential equations (PDEs). However, their application to complex nonlinear systems, such as the coupled Allen-Cahn (AC) and Cahn-Hilliard (CH) equations [1,2] governing phase field interface dynamics, remains challenging due to inherent nonlinearities. To address these challenges, PF-PINNs [3], a robust, enhanced framework tailored for solving coupled AC-CH phase field problems, was developed.

The PF-PINNs framework includes three key features. First, a scale-adaptive normalization-denormalization technique bridges disparities in temporal and spatial scales inherent to real-world physical problems, enabling stable training across diverse domains. Second, a dynamic interface sampling strategy is developed to efficiently resolve the diffusion of initial interfaces and adaptively track their evolution during neural network training. Third, a balanced loss optimization scheme combines neural tangent kernel (NTK) inspired adaptive weighting with a random-batch approach to equilibrate competing loss terms arising from the coupled governing equations. Essential framework features are depicted in Figure 1.

To validate the framework, numerical experiments were conducted on electrochemical corrosion problems, a representative application of AC and CH phase field modeling. The results demonstrate PF-PINNs accuracy and computational efficiency, with close agreement to reference solutions generated using the FEniCS finite element solver (see Figure 2). These benchmarks underscore the framework versatility in addressing a broad spectrum of phase field challenges, positioning PF-PINNs as a transformative tool for interface modeling in materials science, and beyond.

References

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- [2] J. W. Cahn, J. E. Hilliard, Free Energy of a Nonuniform System. I. Interfacial Free Energy, *The Journal of Chemical Physics* 28 (2) (1958) 258–267.
- [3] N. Chen, S. Lucarini, R. Ma, A. Chen, and C. Cui, Pf-Pinns: Physics-Informed Neural Networks for Solving Coupled Allen-Cahn and Cahn-Hilliard Phase Field Equations, *Journal of Computational Physics* (2024). Under review, available at SSRN 4761824.

Figures

Figure 1. Schematic of the PF-PINNs framework

Figure 2. Two-dimensional semi-circular pitting corrosion evolution. Contours of phase-field variable obtained from PF-PINNs framework, FE solution, and their absolute error at two representative time points.