Project Proposal: Predicting Dendritic Growth in Solidification Processes Using Surrogate Models

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Abstract

Dendritic solidification is a fundamental process in materials science, influencing the microstructure of metals, alloys, and energy storage systems. Although phase field models provide accurate simulations, their high computational cost limits their feasibility. This project proposes a machine learning-based surrogate model to predict dendritic growth patterns while efficiently preserving physical fidelity. Training data will be generated using a *FiPy*-based phase-field model, capturing the evolution of the phase field (ξ) and undercooling (ΔT). Additionally, we will explore optimization techniques to determine the optimal dendrite morphology for different fractal growth patterns, tailoring microstructures for specific applications.

1 Introduction

Dendritic growth plays a crucial role in materials science, affecting the microstructure of metals, alloys, and energy storage systems. The morphology of dendritic structures significantly influences mechanical properties, thermal behavior, and electrochemical performance. In particular, controlling dendritic growth is essential for optimizing solidification processes in metallurgy and mitigating undesired phenomena such as dendrite-induced failure in rechargeable batteries [1, 2]. Among the various computational approaches used to model dendritic growth, *phase-field modeling* (PFM) has emerged as a powerful tool for simulating microstructure evolution. Phase-field methods enable the representation of complex interface dynamics without explicitly tracking interfaces [3]. However, these models are computationally expensive due to their need for fine spatial and temporal resolution to capture interface, temperature [2].

Given the high computational cost of phase-field simulations, machine learning (ML) offers a promising alternative for accelerating predictions while maintaining physical fidelity, i.e., ML models are trained on high-fidelity simulation data to approximate the relationship between input parameters and dendritic growth patterns [4, 5]. This project aims to develop an ML-based surrogate model to predict dendritic growth patterns in solidification processes. Training data will be generated using a FiPy-based phase-field model, specifically utilizing the anisotropy example [6], to simulate the evolution of the phase field (ξ) and undercooling (ΔT). Additionally, we will explore optimization strategies to identify optimal dendrite morphologies for different applications, ensuring that our model is not only computationally efficient but also physically consistent.

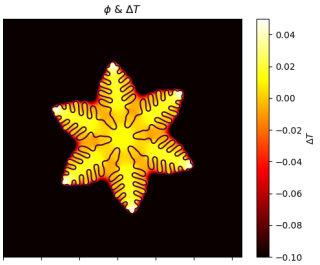

Figure 1: Dendritic growth simulation with phase-field ξ and temperature ΔT

2 Data Description

The data is simulated in a two-dimensional domain under isothermal solidification with anisotropic surface energy. It will be solved using the finite volume method on uniform mesh with periodic or Dirichlet boundary conditions.

Fields and Outputs: The simulation produces the following spatio-temporal fields including the $\xi(t, x, y)$, which is a scalar field representing the state of the ma-

terial, where $\xi = 1$ denotes solid and $\xi = 0$ denotes liquid. In addition to $\Delta T(t, x, y)$, which is a scalar field representing the deviation of the local temperature from the equilibrium solidification temperature.

Input Parameters: The simulations are parameterized by several inputs including initial undercooling ΔT_0, anisotropy strength c, seed size, anisotropy orientation function $\beta(\psi)$ of orientation angle ψ.

Dataset Structure: The dataset is structured into pairs of input-output mappings suitable for training machine learning models: **Inputs** $\mathbf{x} = [\Delta T_0, c, N, \text{seed type}, \ldots]$, **Outputs** $\xi(t, x, y)$ at a fixed time (e.g., final morphology) or as a time series. In total, the dataset includes N_{sim} (to be decided later) simulation runs, each comprising a sequence of 2D fields stored at selected time steps. The data is preprocessed to ensure consistent scaling, dimensionality, and formatting for downstream ML pipelines.

3 Process and Timeline

Week	Task
1	Run simulations and preprocess data.
2	Select and implement surrogate models.
3-4	Train models, validate, and tune hyperparameters.
5	Analyze results and conduct error analysis.
6	Write final report documenting methodology and results.

4 Methodology

4.1 Numerical Solution of PDEs

To be able to collect the data, one has to calculate the temperature field and the respective phase field, which can be done by discretizing the conduction diffusion equation (1) coupled with the phase field equation (2), represented in the equations below:

$$\frac{\partial \Delta T}{\partial t} = D_T \nabla^2 \Delta T + \frac{\partial \xi}{\partial t}, \tag{1}$$

$$\tau \frac{\partial \xi}{\partial t} = \nabla \cdot (D \nabla \xi) + \Big(\xi - 0.5 - \frac{\kappa_1}{\pi} \arctan(\kappa_2 \Delta T)\Big)(1 - \xi) \tag{2}$$

Such that τ is the relaxation time parameter, k_i being the thermodynamic driving force, and the diffusivity is given by:

$$\mathsf{D} = \alpha^2 (1 + c\beta) \begin{bmatrix} 1 + c\beta & -c\frac{\partial \beta}{\partial \psi} \\ c\frac{\partial \beta}{\partial \psi} & 1 + c\beta \end{bmatrix}. \tag{3}$$

where α is a scaling parameter.

4.2 Surrogate Model Development

To reduce the computational cost, we will design a surrogate model to estimate dendritic growth from input parameters. The surrogate model will allow rapid predictions of dendritic growth behavior without requiring full numerical solutions.

Let $\mathcal{F}_\theta$ denote the surrogate model that maps simulation parameters $\mathbf{x}$ to the final dendritic morphologies $\xi(t, x, y)$, as defined in Section 2:

$$\xi(t, x, y) \approx \mathcal{F}_\theta(\mathbf{x}), \tag{4}$$

where θ denotes the trainable parameters of the model. We will explore many potential surrogate modeling techniques, including:

- **Gaussian Processes:** for flexible function approximation with uncertainty quantification.
- **Regression Models:** linear regression, polynomial regression, PCA/modal decomposition. simple and interpretable baselines that can capture low-dimensional or linear trends.
- **Neural Networks:** PINNs, LSTMs for time-dependent patterns, and CNNs for spatial structures.

5 Evaluation Strategy

5.1 Metrics

Relative L_2 Error A normalized measure to evaluate how well the surrogate model captures the global structure of the dendritic growth patterns.

5.2 Validation

To evaluate the surrogate model, we will split the generated dataset into training and testing sets, ensuring fair assessment of generalization (extrapolation) performance. We will also apply k-fold cross-validation to assess model stability across different data partitions.

References

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