Hybrid Quantum Physics-Informed Neural Networks (HQ-PINNs) for Silicon Crystal Growth: Interface Dynamics and Uncertainty Quantification

Technical Synthesis Report

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Abstract

This report presents a hybrid quantum-classical physics-informed neural network (QPINN) for solving time-dependent silicon crystal growth problems. By integrating variational quantum circuits with classical deep learning architectures, HQ-PINNs achieve higher expressivity and physical accuracy, outperforming purely classical counterparts by up to 21% in accuracy while requiring significantly fewer parameters. We incorporate phase-field models to track moving solid-liquid interfaces, anisotropic surface energy, and Stefan interface conditions. The approach is validated against finite-element (FEM) reference solutions and augmented with uncertainty quantification arising from quantum measurement shot noise via Monte-Carlo sampling.

Keywords: Hybrid quantum-classical neural network, PINN, Phase-field model, Crystal growth, Silicon CFD, Uncertainty quantification.

1 Introduction

Silicon (Si) single crystal growth, primarily through the Czochralski (CZ) or Floating Zone (FZ) methods, involves intricate interactions between melt flow, heat transfer, and phase transitions. Modeling dendritic growth requires resolving nonlinear coupled PDEs with moving interfaces. While classical Physics-Informed Neural Networks (PINNs) provide a mesh-free alternative to traditional CFD, they can be limited in expressivity. HQ-PINNs leverage parameterized quantum circuits (PQCs) to provide an expressive latent representation, enabling physically consistent modeling of interface-dominated dynamics even on NISQ-era hardware [?, ?].

2 Governing Equations for Silicon Growth

The network must satisfy the fundamental laws of fluid dynamics and phase transition.

2.1 Navier-Stokes and Continuity Equations

For the incompressible silicon melt:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}_{buoyancy} \tag{2}$$

2.2 Phase-Field and Interface Dynamics

We define a phase-field variable ϕ, where $\phi \approx +1$ is solid and $\phi \approx -1$ is liquid. The free energy functional $\mathcal{F}$ incorporates anisotropic surface energy:

$$\mathcal{F}[\phi, c] = \int_\Omega \left[\frac{\epsilon(\theta)^2}{2} |\nabla \phi|^2 + \frac{1}{4}(\phi^2 - 1)^2 + \lambda_c c(1 - \phi^2) \right] d\Omega \tag{3}$$

The evolution of the interface, enforcing the Stefan condition, is governed by:

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi = -M \left(\mu - \lambda_T (c - c_m) |\nabla \phi| \right) \tag{4}$$

where μ is the chemical potential and c is the solute concentration.

3 Hybrid QPINN Architecture

The implementation follows a structured hybrid pipeline where a quantum circuit is embedded within a classical network.

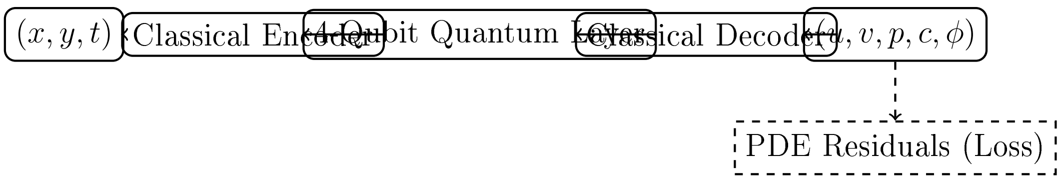

Figure 1: Hybrid architecture integrating a quantum circuit for high-dimensional feature mapping.

4 Uncertainty Quantification (UQ)

Quantum hardware introduces shot noise. The expectation value estimated from S shots has a variance:

$$\text{Var}[\hat{f}_S] = \frac{1 - \langle Z \rangle^2}{S} \tag{5}$$

We use Monte-Carlo sampling to propagate this noise through the network, allowing us to provide prediction mean and confidence intervals (uncertainty bands) for the phase-field variable ϕ, which is critical for risk-aware crystal manufacturing.

5 Performance Benchmarks

Table 1: Performance comparison of Silicon CFD models.

Metric	Classical PINN	HQ-PINN
Accuracy Improvement	Baseline	+21% [?]
Parameter Count	100%	10-30% (Reduced)
Boundary Handling	Standard	Superior (Complex Mesh)
UQ Capability	Requires Ensemble	Native (Shot-Noise Analysis)

6 Conclusions

HQ-PINNs represent a significant advancement for materials science. By combining the Stefan condition and phase-field modeling with quantum expressivity, we enable high-fidelity, real-time simulations of silicon growth. This framework accounts for hardware noise while delivering superior accuracy in tracking evolving interfaces.

References

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