Accelerating CFD Simulations for Silicon Single Crystal Growth via Hybrid Quantum Physics-Informed Neural Networks (HQ-PINNs)

Technical Report

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Abstract

The manufacturing of high-quality silicon single crystals, primarily via the Czochralski (CZ) method, requires precise control over fluid dynamics and heat transfer. Traditional Computational Fluid Dynamics (CFD) methods are computationally expensive for real-time optimization. This report details the implementation of Hybrid Quantum Physics-Informed Neural Networks (HQ-PINNs), which combine the expressive power of variational quantum circuits with the physical consistency of PINNs. HQ-PINNs demonstrate up to 21% higher accuracy and significant parameter efficiency compared to classical counterparts, offering a transformative approach to semiconductor process modeling.

1 Introduction

Silicon crystal growth is a complex multi-physical process involving melt convection, heat transport, and phase-change kinetics. Physics-Informed Neural Networks (PINNs) have emerged as a viable surrogate for traditional CFD, but classical architectures often struggle with high-dimensional non-linearities and large-scale optimization.

Hybrid Quantum PINNs (HQ-PINNs) integrate quantum layers into the neural network architecture. By leveraging quantum entanglement and high-dimensional Hilbert spaces, these models capture complex fluid patterns with fewer parameters, accelerating the prototyping and optimization of growth conditions for large-diameter semiconductor crystals [**?**, **?**].

2 Governing Equations for Silicon Growth

In a 2D CFD simulation of silicon melt, the HQ-PINN must satisfy the fundamental conservation laws. The governing PDEs for the incompressible melt flow and temperature distribution are:

2.1 Mass and Momentum Conservation

The Navier-Stokes equations for the melt velocity field $\mathbf{u}$ and pressure p are:

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

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

where ρ is the density, μ is the dynamic viscosity, and $\mathbf{f}_b$ represents buoyancy forces (typically modeled via the Boussinesq approximation).

2.2 Energy Transport and Phase Change

Heat transfer in the melt and the solid crystal is governed by:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \alpha \nabla^2 T \tag{3}$$

At the crystal-melt interface, the Stefan condition must be enforced to account for latent heat release:

$$L\rho_s v_n = [k_s \nabla T_s - k_l \nabla T_l] \cdot \mathbf{n} \tag{4}$$

where L is the latent heat of fusion, v_n is the growth velocity, and k is the thermal conductivity of the solid (s) and liquid (l) phases.

3 HQ-PINN Architecture

The hybrid architecture consists of three functional stages designed to process spatial coordinates (x, y, t) and output physical variables $(\mathbf{u}, p, T)$.

3.1 Classical Preprocessing

A classical feedforward network (typically 2 layers with 50 neurons each using $Tanh$ activation) transforms raw coordinates into a feature vector ξ. This prepares the data for the limited dimensionality of current quantum hardware.

3.2 Quantum Variational Layer

The feature vector is encoded into a quantum state $|\psi\rangle$. For 2D crystal growth, the **Cascade Topology** is often preferred for its balance of expressivity and entanglement:

- **Encoding:** Angle embedding using R_x or R_y gates.
- **Variational Ansatz:** Trainable rotation gates ($R_z(\theta)$) and entangling CNOT gates in a ring-like configuration.
- **Measurement:** Expectation values of Pauli operators $\langle Z_i \rangle$ are extracted as enhanced features.

3.3 Hybrid Loss Function

The model is trained by minimizing a composite loss function $\mathcal{L}_{total}$:

$$\mathcal{L}_{total} = w_{pde}\mathcal{L}_{PDE} + w_{bc}\mathcal{L}_{BC} + w_{data}\mathcal{L}_{data} \tag{5}$$

The physics-based loss $\mathcal{L}_{PDE}$ is computed using automatic differentiation (AD) to evaluate the residuals of the Navier-Stokes and Energy equations at collocation points throughout the 2D domain.

4 Implementation Workflow

The deployment for Silicon CFD follows these technical steps:

1. **Domain Discretization:** Selection of collocation points in the crucible geometry, focusing on the boundary layer near the crystal interface.
2. **Hybrid Framework:** Integration of *PyTorch/TensorFlow* with *PennyLane* or *Qiskit* for gradient-based optimization.

3. **Optimization:** Use of the Adam optimizer; quantum gradients are calculated via the **parameter-shift rule**.

4. **Symmetry Enforcement:** For silicon ingots, rotational or hexagonal symmetry constraints can be appended to the loss function to ensure physical validity.

5 Advantages and Performance

HQ-PINNs offer specific benefits for the semiconductor industry:

Feature	**Classical PINN**	**HQ-PINN**
Accuracy	Baseline	Up to 21% improvement [**?**]
Parameter Count	High	Low (due to quantum expressivity)
Non-linearity	Sigmoidal/ReLU	Quantum Hilbert Space Mapping
Complex Geometries	Moderate scaling	Superior boundary handling [**?**]

Table 1: Comparison of Classical and Hybrid Quantum PINNs in CFD contexts.

6 Conclusion

Hybrid Quantum Physics-Informed Neural Networks represent a critical advancement in accelerating CFD for silicon single crystal growth. By embedding the governing laws of fluid dynamics directly into a hybrid quantum-classical learner, manufacturers can achieve high-fidelity simulations with reduced computational overhead, directly supporting the production of larger, defect-free silicon wafers.

References

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