Idea: **Development of Real time digital twins by accelerating Computational Fluid Dynamics (CFD) simulations for crystal growth (Silicon Single Crystal) with Physics-inspired geometry aware classical and hybrid quantum-classical approaches**

The Problem: The growth of high-quality silicon single crystals—critical for semiconductors, optics, and advanced materials—relies on processes like Czochralski and Bridgman methods, driven by complex, multiscale fluid dynamics, heat transfer, and phase-change phenomena. Accurate modeling requires high-fidelity CFD simulations, but these are computationally prohibitive, often taking days or weeks on HPC systems. This latency prevents real-time monitoring, control, and optimization, forcing manufacturers to rely on costly, empirical trial-and-error approaches.

Current solutions fail due to:

- Speed – Simulations are too slow for in-situ decision-making.
- Fidelity – Reduced-order models compromise physical accuracy.
- Generality – Models lack adaptability to different geometries and materials.

This challenge persists because research academia focuses on narrow physics, startups avoid high-risk quantum-classical approaches, and big tech prioritizes generic platforms over domain-specific innovation. The integration of domain-driven physics, heterogeneous computing, and hybrid AI–quantum models remains an untapped opportunity for transformative real-time digital twins in crystal growth.

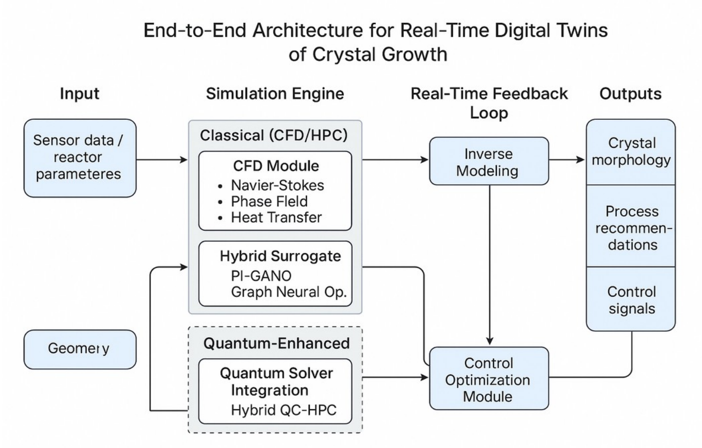
High-Impact Innovation Program: Development of real-time digital twin for silicon single-crystal growth by fusing **quantum computing**, **AI**, and **physics-based modeling**.

Core Components:

- **Hybrid Quantum–Classical Backends**: Heterogeneous HPC–QC systems (e.g., NVIDIA DGX Quantum, QPU–CPU–GPU stacks) running classical CFD solvers alongside quantum-accelerated modules for pressure solves, optimization, and inverse problems.
- **Physics-Informed, Geometry-Aware AI**: Surrogates such as PI-GANO and GAOT integrate Navier–Stokes, heat transfer, and solidification kinetics with mesh-aware graph neural operators for accurate, generalizable flow–thermal predictions.
- **Quantum-Accelerated Solvers**: Variational Quantum Linear Solvers (VQLS), VQE, and variational time-stepping methods for PDEs, coupled with Hamiltonian encodings, to speed up sparse linear solves and nonlinear PDE dynamics relevant to melt flow and phase change.
- **Inverse Control & Optimization**: Quantum optimization loops adjust process parameters (e.g., pull rate, rotation speed, thermal gradient) in real time to minimize defects and maintain target crystal shapes.

Platform Architecture:

1. **Hybrid Simulation Backend** – GPU-based CFD for geometry and streaming flow; QPU-accelerated routines for linear solves and optimization.
2. **Surrogate Modeling Layer** – PI-GANO/GAOT modules trained on multiphysics CFD data for orders-of-magnitude faster inference.
3. **Quantum-Accelerated Control** – VQA-based loops for parameter tuning and steady-state target tracking.
4. **Multi-Modal Data Integration** – Real-time sensor fusion with adaptive surrogate retraining to handle drift and geometry variation.



Innovations:

- Physics-informed loss functions embedding PDE residuals directly into training (PINNs, GN-PINNs, RF-PINNs, PI-GANO, GAOT).
- Geometry-aware mesh graph encodings with node features like curvature, local gradients, and resolution.
- Quantum iterative PDE solvers (Jacobi/Gauss–Seidel, HHL-based) for CFD subproblems.
- Transferable architecture applicable to multiple crystal growth processes.

What needs to become possible?

1. **Ultra-fast, high-fidelity simulation** of 3D, non-linear, multiphase CFD systems in real-world reactor geometries.
2. **Model generalization** across materials, scales, and reactor designs with minimal retraining.
3. **Differentiable, inverse-model capabilities** for real-time process control, optimization, and AI co-design of reactors.

Path to prototype

- Develop and validate a hybrid physics-based AI surrogate for 2D crystal growth (e.g., simplified Czochralski) with quantum modules for sparse linear solvers.
- Integrate hybrid quantum-classical solvers into the HPC stack. Scale to 3D geometries Build a simulation-as-a-service layer that supports real-time data ingestion and feedback
- Validation across different semi conducting materials (GaN, SiC, Si, Perovskites).
- Demonstrate closed-loop control in a physical lab reactor via the digital twin, achieving >10x reduction in modeling time and increased process efficiency.

Why now?

- **Quantum-classical hardware integration is emerging**, notably NVIDIA DGX Quantum and IonQ's quantum networking stack.
- **Neural operators** and physics-aware GNNs have reached maturity and demonstrated orders-of-magnitude speedups in surrogate modeling.
- **Materials science is bottlenecked by compute-bound simulation**—and global demand for semiconductors and clean energy devices is skyrocketing.

Societal, economic, and geopolitical pressures are aligning around **sovereign materials infrastructure**—real-time digital twins are a critical enabler.

Scale & Impact: This Idea demands a convergent, multidisciplinary effort—bringing together quantum physicists, AI researchers, CFD specialists, HPC engineers, and crystal growth experts. It requires access to quantum hardware (QPU time), HPC infrastructure, and test-bed crystal growth reactors, alongside deep collaboration with academic labs, quantum platform providers (e.g., NVIDIA, Rigetti, IQM), and materials manufacturers.

A **€50M, 3-year investment** will enable:

- Multi-site coordination with integrated data and cloud infrastructure
- Recruitment of top talent across disciplines
- Leasing of quantum and HPC resources
- Development of an open-source digital twin platform (software, APIs, datasets)

Transformative Milestones:

- **1000× faster** simulations than traditional CFD for benchmark scenarios
- **Real-time, closed-loop control** in an operational growth chamber (TRL6+)
- **Cross-process transferability** to at least different crystal growth approaches
- A **universal, open digital twin stack** deployable across industries such as semiconductors, photovoltaics (Solar Cells), and fusion materials

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