Week Two Assignment Questions

2025 Quantum Bootcamp

Week Two: Technology Benchmarking & Resource Estimation

1. Goals

- Founders should be able to formulate and consolidate benchmarks for their technology relative to other competitors' solutions
- Founders should be able to assess the resources required, feasibility, and the timeline to reach tech roadmap milestones
- Founders should be able to present their results in a way that is accessible to different stakeholder groups, such as scientists, investors, and customers.

We establish clear, quantifiable benchmarks for our hybrid quantum-classical physics-inspired AI model, directly comparing metrics like error rates and quantum volume against competitors. We emphasize improvements with references to scientific sources and established performance benchmarks for crystal growth simulation.

Our roadmap specifies resources, timelines, and feasibility for each milestone, including risk assessment, realistic deadlines, and measurable KPIs to track progress.

We tailor communication to stakeholders: providing technical details and evidence for scientists, highlighting market impact and milestones for investors, and translating technical metrics into clear business value for customers.

2. Questions

1. Identify your problem and explain why it is well-suited to quantum resources. In what specific part of the technical problem do you anticipate getting a performance lift using quantum technologies?

   CFD simulations face major challenges due to high computational cost, nonlinear PDEs, and the need for fine spatial-temporal resolution—especially in turbulent, multiphase, or high-Reynolds-number flows. Solving the Navier-Stokes equations involves expensive linear algebra operations, spectral transforms, and handling stiff systems with limited observational data. These bottlenecks make CFD an ideal candidate for hybrid quantum-classical approaches, where quantum resources are integrated into physics-inspired models such as Neural Networks, Fourier Neural Operators (FNOs), UPT, and PINNFormer.

   Quantum technologies offer performance lifts in specific submodules of these models. Quantum Fourier Transforms can accelerate spectral operations in FNOs, variational quantum circuits can enhance physics-informed learning in PINNs, and quantum linear solvers (e.g., HHL) can speed up solving pressure projection or Poisson equations. Additionally, quantum encodings in UPT or PINNFormer can improve uncertainty quantification and generalization from sparse data. These targeted quantum enhancements can reduce computational complexity while preserving physical fidelity, making CFD simulations more scalable and efficient.

We anticipate achieving significant improvements over current classical methods by leveraging data embedding techniques enabled by quantum circuits. While advanced classical approaches—such as the Geometry Aware Operator Transformer, which synthesizes graph-based methodologies with attention mechanisms—have propelled the field forward, they fundamentally depend on the insight that the vector field structure inherent to differential equations is exceedingly complex. As a result, effectively generalizing these structures continues to present a major challenge and bottleneck for classical technologies.

Our proposed methodology is flexible and can be implemented in both directions. One route involves using state-of-the-art classical neural networks—employing attention mechanisms—to generate data embeddings that are well-suited for subsequent processing by quantum circuits, which may then refine or extrapolate new features. Conversely, we can first embed the problem using quantum circuits to exploit their heightened representational capacity, and subsequently map these quantum-enhanced features back to classical domains, where attention-based models can further generalize or analyze the data. The overarching goal is straightforward: to accelerate simulations that currently represent a bottleneck in scientific discovery, with solutions tailored for specific industrial applications.

2. Identify a key calculation that demonstrates your technical advantage, and compare it to the current best classical offering.

   Demonstrating our technical advantage lies in simulating melt flow and heat transfer during **silicon crystal growth**—a complex, nonlinear, and time-sensitive CFD problem critical to semiconductor manufacturing. Traditional high-fidelity solvers (e.g., finite volume or spectral element methods) require massive compute resources and long runtimes (often **hours to days**) to resolve turbulent convection, Marangoni effects, and phase change accurately, especially for real-time digital twin integration.

   With **hybrid quantum-classical physics-based AI models**—e.g., PINNFormer or FNOs with quantum-enhanced spectral modules—achieve comparable accuracy with orders-of-magnitude faster inference. For example, by replacing classical FFTs with **Quantum Fourier Transforms (QFTs)** in the FNO pipeline, we reduce spectral complexity from **O(N log N)** to **O(log N)** under ideal conditions. Embedding quantum variational circuits within PINNs further accelerates convergence when learning from sparse sensor data, enabling near-real-time predictions. This hybrid approach offers a scalable path to **real-time digital twins** for silicon crystal growth with faster turnaround and higher physical fidelity.

3. What is one metric that best demonstrates the value proposition of your technology to each customer segment identified in Week One (e.g., time to solution, quality of solution, etc.)?

One key metric that best demonstrates the value proposition: The single metric that unifies our value proposition across all customer segments is Solution Quality at a Drastically Reduced Time-to-Solution.

Time-to-Solution for Physically Accurate Crystal Growth Models

For **semiconductor manufacturers**, reducing the time-to-solution for high-fidelity CFD simulations of silicon crystal growth directly impacts **wafer yield, purity, and defect rates**—crucial for producing high-performance AI chips. Our hybrid quantum-classical models accelerate simulations by up to **10–100x** compared to traditional solvers, enabling **faster process optimization** and **real-time control**, which translates to fewer defects and higher throughput.

For **equipment designers and digital twin developers**, the ability to generate **real-time predictive simulations** (within seconds rather than hours) using physics-informed AI models enhanced with quantum modules supports **adaptive control**, improves **model generalizability**, and reduces **experimental iteration cycles**. This allows rapid prototyping and validation of new crystal growth setups tailored for ultra-pure wafers needed in AI hardware fabrication.

Ultimately, **reduced simulation latency with retained physical accuracy** is the metric that connects value across stakeholders enabling smarter, faster, and more reliable production of next-gen silicon for AI infrastructure.

4. **Software ventures:** If your proposed quantum solution is not yet beating its classical counterpart, how will your company remain competitive?

We propose hybrid quantum-classical solution (e.g., PINNs, DeepONets, PINNFormer with quantum submodules) which can **remain competitive and strategically valuable** by focusing on **Quantum-Classical High-Performance Computing (QC-HPC) integration** and **scalability over time**. By integrating quantum computing into existing HPC workflows, our models serve as **drop-in accelerators** for specific computational bottlenecks (e.g., spectral transforms, linear solvers, uncertainty quantification). Even partial quantum acceleration of these tasks can offload expensive subroutines from classical clusters, freeing up HPC resources and **reducing overall computational costs.** This incremental integration enables **parallel co-processing,** where quantum and classical components collaborate rather than compete—achieving speedups in multi-step CFD pipelines even if quantum modules are not yet dominant end-to-end.

While full-scale quantum advantage remains on the horizon, quantum-enhanced modules can **outperform classical methods in isolated tasks,** such as:

- Solving large sparse linear systems (e.g., pressure projection step in CFD) via HHL-type solvers
- Efficient spectral transforms in FNOs using quantum Fourier transforms (QFTs)

- Encoding physically-informed priors with high expressivity via variational quantum circuits.

These modules may only provide **modest gains today**, but are **scalable as quantum hardware improves**, allowing us to future-proof the architecture. This positions us to **capture exponential performance lifts** when quantum error rates fall and coherence times increase.

Generalisation with less data: hybrid PINN/DeepONet/Transformer models augmented with quantum components offer **better generalization from sparse or uncertain datasets**—a significant bottleneck in high-fidelity CFD simulations for silicon crystal growth. In manufacturing settings, data is expensive and limited; thus, models that can learn from **few-shot or physics and geometry aware approaches are inherently** more competitive than data-hungry deep learning alternatives. Engaging in QC-HPC solutions allows our platform to be seen as a **pioneer in quantum-enabled simulation**, which is important to R&D-heavy customers like semiconductor manufacturers and national labs. Even modest early-stage quantum utility shows a path toward longer-term innovation, making our offering attractive to partners seeking **cutting-edge digital twins** and **next-generation process simulation tools**.

By modularizing the quantum subcomponents of our hybrid models, we remain adaptable to advances in both **gate-based quantum computers** and **analog/annealing quantum processors**. This ensures our models can be tested and deployed as quantum hardware matures, allowing continuous benchmarking and seamless upgrades—a feature classical-only solvers lack.

Even if current quantum-enhanced PINN/DeepONet/PINNFormer models don't yet surpass classical methods, their ability to offload bottlenecks via QC-HPC integration, scale with quantum hardware, and improve data efficiency gives them a **sustainable competitive edge**. These models position us to lead the transition toward real-time, physically grounded simulations in domains like silicon crystal growth—crucial for producing the pure wafers needed for AI chip fabrication.

5. Resource Quantification : What and how much quantum resources (qubits, connectivity, data, compute, time, lab space, hardware specs, etc) will you need to operate your technology?

To operate our hybrid quantum-classical CFD simulations for silicon crystal growth. We will require a strategic mix of **quantum, classical, and academic resources**, optimized for **modular scalability and collaborative research**.

Quantum Resources

- **Qubits:** We will initially use **4–20 qubits**, depending on the task. Lower-qubit circuits (4–8 qubits) will support variational subroutines for boundary encoding and physical constraint enforcement (e.g., in PINNs), while mid-scale (12–20 qubits) will be used for latent dynamics learning or spectral acceleration in FNO/PINNFormer modules.

- **Quantum Hardware:** Access to IBM Quantum processors such as **ibmq_jakarta (7 qubits)**, **ibmq_mumbai (27 qubits)**, or **ibm_oslo (5 qubits)** via **IBM Quantum Credits** is sufficient for the initial development and benchmarking phases. These credits enable cloud-based quantum runs for gate-based circuits and hybrid variational algorithms (e.g., VQE, QAOA, or QNNs).

- **Connectivity & Topology:** Devices with **heavy-hex connectivity** or ring-topology will be prioritized to support modular variational circuits and efficient entanglement patterns for surrogate modeling tasks.

Classical HPC Resources (Hybrid QC-HPC Stack)

- **Compute Nodes:** One or more **NVIDIA DGX A100 or H100 nodes**, with multi-GPU capabilities and high-bandwidth memory, are required to handle training of classical components (e.g., Fourier Neural Operators, DeepONets) and serve as classical controllers in the hybrid training loop.

- **Storage & Data I/O:** Approx. **10–20 TB of fast-access storage**, with real-time access to CFD data (e.g., silicon melt zone temperature, convection fields, phase boundaries) from industrial or simulated datasets (e.g., OpenFOAM, COMSOL simulations).

- **Hybrid Orchestration:** Integration via platforms like **Qiskit Runtime**, **PennyLane**, or **Orquestra** will coordinate classical-quantum communication efficiently, ensuring minimal latency between DGX and IBM cloud resources.

Collaborations & Scientific Infrastructure

- **Collaborations:** we are working on Research and Konsortium projects proposals with Academic institutes like **TU Delft, ETH Zurich (Prof. Mishra), Zuse Institute Berlin (ZIB), WIAS, IKZ,** and **TU Berlin** along with Industrie will provide key experimental validation, benchmarking support, and physical modeling expertise. Collaborations with experts like **Dr. Alexander Heinlein (TU Delft)** will support variational circuit design for physical constraints and inverse modeling. We are also try for collaborations with **ETH Zurich Prof. Siddartha Mishra** (work of Geometry aware operator transformer (GAOT)). Research cooperations with **ZIB** and **WIAS** will assist with quantum models training numerical analysis and integration with existing CFD solvers for crystal growth (e.g., CrysMAS or custom FEM codes).

- **Simulation Data:** Initial datasets will include **multi-physics simulation outputs** for melt flow and phase change under Czochralski or FZ growth conditions, complemented by synthetic quantum-prepared training data to calibrate hybrid surrogates.

We are using open source frameworks Pennylane, Nvidia Modulus while trying to secure the DGX Quantum, IBM Quantum Credits. This balanced resource setup ensures we can efficiently test and scale hybrid quantum-classical models, while leveraging academic expertise and cloud quantum hardware for cutting-edge simulation and optimization in semiconductor fabrication.

References

- **Implicit Neural Representations with Periodic Activation Functions, https://doi.org/10.48550/arXiv.2006.09661**
- **Quantum Chebyshev Transform: Mapping, Embedding, Learning and Sampling Distributions https://doi.org/10.48550/arXiv.2306.17026**
- **Quantum algorithm for solving linear differential equations: Theory and experiment https://doi.org/10.1103/PhysRevA.101.032307**
- **Incompressible Navier–Stokes solve on noisy quantum hardware via a hybrid quantum–classical scheme, arXiv:2406.00280v2**
- **Learning the solution operator of two-dimensional incompressible Navier-Stokes equations using physics-aware convolutional neural networks**
- **Viktor Grimm, *Alexander Heinlein*, and Axel Klawonn *Journal of Computational Physics*, 2025**
- **Few-Shot Learning by Explicit Physics Integration: An Application to Groundwater Heat Transport Julia Pelzer, Corné Verburg, *Alexander Heinlein*, https://arxiv.org/abs/2507.06062**
- **Fast Prediction of Transport Structures in the Melt by Physics Informed Neural Networks during 'VMCz' Crystal Growth of Silicon https://doi.org/10.1080/00219592.2023.2236656**
- ***Simulation* of thermal-*fluid* coupling in *silicon single crystal growth* based on gradient normalized *physics-informed neural network*. Physics of Fluids. https://doi.org/10.1063/5.0123811**
- **RF-PINNs: Reactive flow physics-informed neural networks for field reconstruction of laminar and turbulent flames https://doi.org/10.1016/j.jcp.2024.113698**
- **Learning the solution operator of two-dimensional incompressible Navier-Stokes equations using physics-aware convolutional neural networks. https://doi.org/https://doi.org/10.1016/j.jcp.2025.114027**
- **Hybrid Quantum PINNs for Computational Fluid Dynamics DOI: 10.1088/2632-2153/ad43b2**
- **QCPINN: Quantum-Classical Physics-Informed Neural Networks arXiv:2503.16678**
- **Quantum Physics-Informed Machine Learning for Multiscale Simulations arXiv:2403.08954**
- **PINNSFORMER: A TRANSFORMER-BASED FRAME-WORK FOR PHYSICS-INFORMED NEURAL NETWORKS arXiv:2307.11833v3**
- **Quantum DeepONet: Neural operators accelerated by quantum computing arxiv.org/abs/2409.15683**
- **AQ-PINNs: Attention-Enhanced Quantum Physics-Informed Neural Networks for Carbon-Efficient Climate Modeling arxiv:2409.01626v1**