Project 3:Quantum Algorithm as a PDE Solver for Computational Fluid Dynamics (CFD)

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WISER Quantum Project

Project Statement:

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About Project

Designing resource-lean, quantum-enhanced PDE solvers to tackle the 1-D viscous Burgers' equation, a fundamental CFD benchmark.

What problem we are addressing?

•**Classical CFD struggles at scale** – High-fidelity solvers face prohibitive computational demands due to fine grid requirements and stiff non-linear PDEs.

•**Burgers' equation as testbed** – Captures key nonlinearity and diffusion dynamics of fluid motion while remaining analytically solvable.

Why does it matter?

- **Scalability limits cut accuracy** for complex flow simulations.
- **Quantum algorithms like** QTN and HSE compress fluid states efficiently, promising faster, more compact simulations.

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Objectives: Enabling Quantum Breakthroughs in CFD

- **Design** quantum algorithms optimized for nonlinear PDEs in fluid dynamics.
- **Benchmark** solvers on Burgers' equation to capture complex flow behaviors.
- **Overcome** classical computational limits with scalable quantum methods.
- **Validate** solutions rigorously against classical and analytical results.
- **Integrate** quantum solvers into conventional CFD workflows for real-world use.
- **Pioneer** pathways toward quantum advantage in other fields like aerospace and climate simulations.

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Problem Statement: 1D viscous burger equation

Governing equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}, \quad x \in [0,1], \quad t > 0$$

Initial condition:

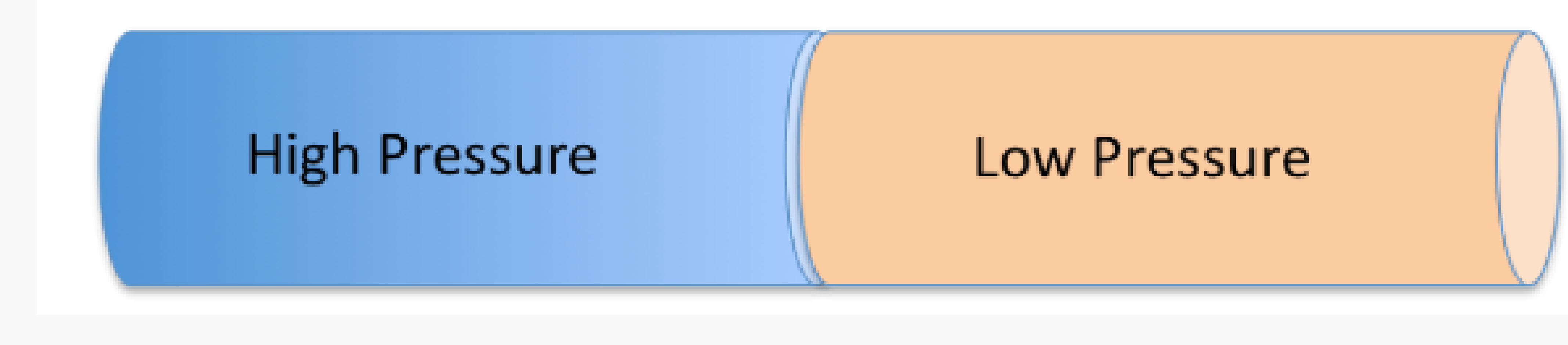
$$u(x,0) = \begin{cases} 1, & x \leq 0.5 \\ 0, & x > 0.5 \end{cases}$$

Boundary Equation:

$$u(0,t) = 1, \quad u(1,t) = 0, \quad \forall t > 0$$

Wave Phenomena:

- A shock wave propagates into the low-velocity region, causing an abrupt change in velocity.
- A rarefaction wave moves into the high-velocity region, representing a smooth spreading of the flow.
- A contact discontinuity separates the two flow regions, across which velocity and pressure remain continuous.



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1. Algorithm Design — Analytic Approach

1. Analytic Benchmark Algorithm (Cole–Hopf Transform)

Steps:

1. **Defined** the viscous Burgers' equation:

$$u_t + u\,u_x = \nu\,u_{xx},$$

with Riemann initial condition

$$u(x,0) = \begin{cases} 1, & x \le 0.5, \\ 0, & x > 0.5, \end{cases}$$

and Dirichlet boundary conditions $u(0,t) = 1$, $u(1,t) = 0$.

2. **Applied** the Cole–Hopf transform:

$$u = -2\nu \frac{\partial}{\partial x} \log \phi,$$

which converted the nonlinear PDE into the linear heat equation

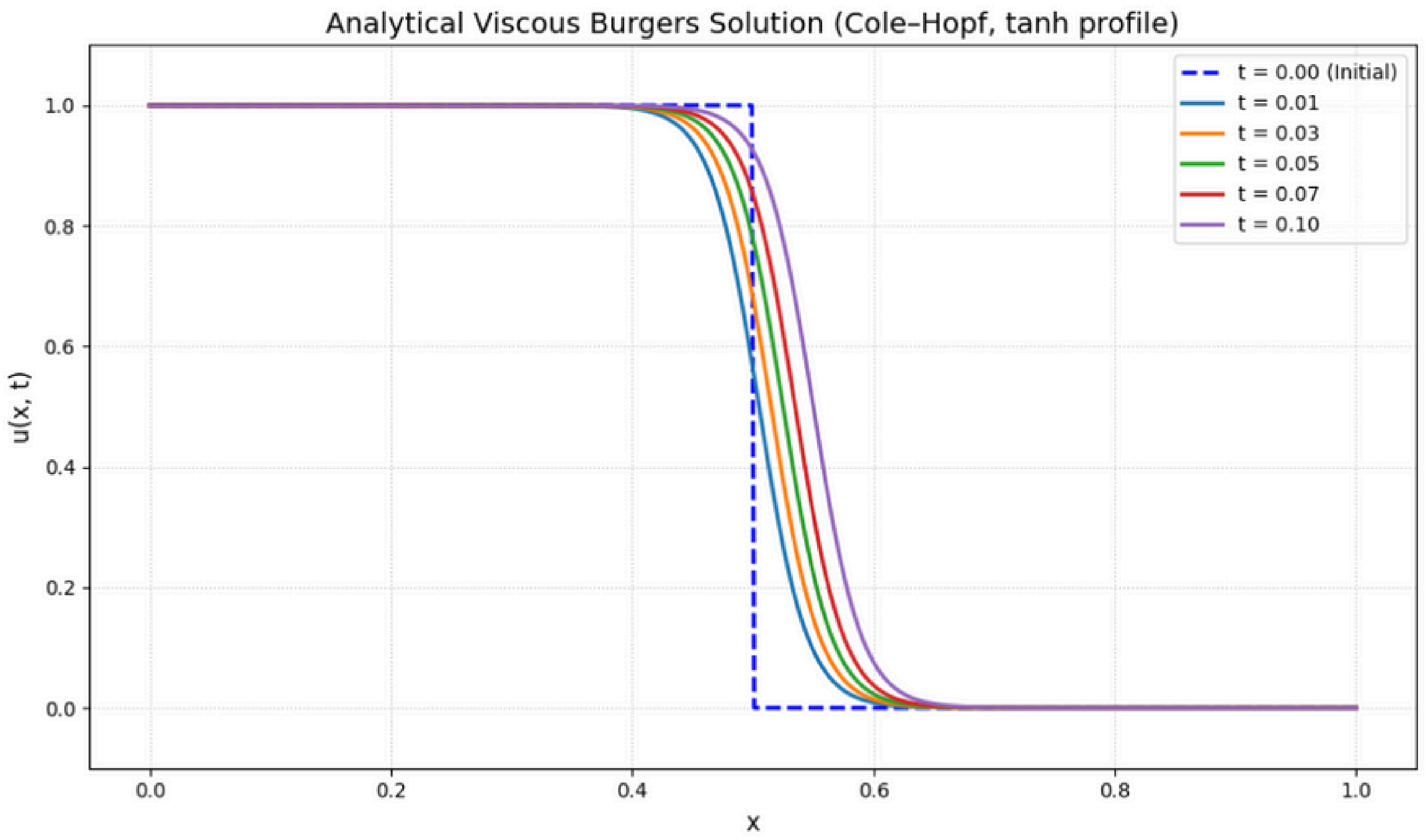
$$\phi_t = \nu \phi_{xx}.$$

3. **Solved** the heat equation for ϕ with the corresponding transformed initial and boundary conditions.

4. **Recovered** the solution $u(x,t)$ from ϕ.

5. **Obtained** the travelling viscous shock solution:

$$u(x,t) = \frac{1}{2} - \frac{1}{2}\tanh\left(\frac{x - x_0 - \frac{1}{2}t}{4\nu}\right),$$



Analytical solution using Cole–Hopf Transform.

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Algorithm Design — Numerical Approach

2. Numerical Solver Algorithm (Finite-Volume Godunov Method)

Setup: We discretized the domain into $N = 200$ cells with $\Delta x = 0.005$, and set the viscosity $\nu = 0.01$. We selected the timestep as

$$\Delta t = \min\left(0.2\frac{\Delta x}{\max|u|}, 0.5\frac{\Delta x^2}{\nu}\right) = 0.001,$$

with $\mathrm{CFL} = 0.2$ and final time $t = 0.1$.

Algorithm steps per timestep:

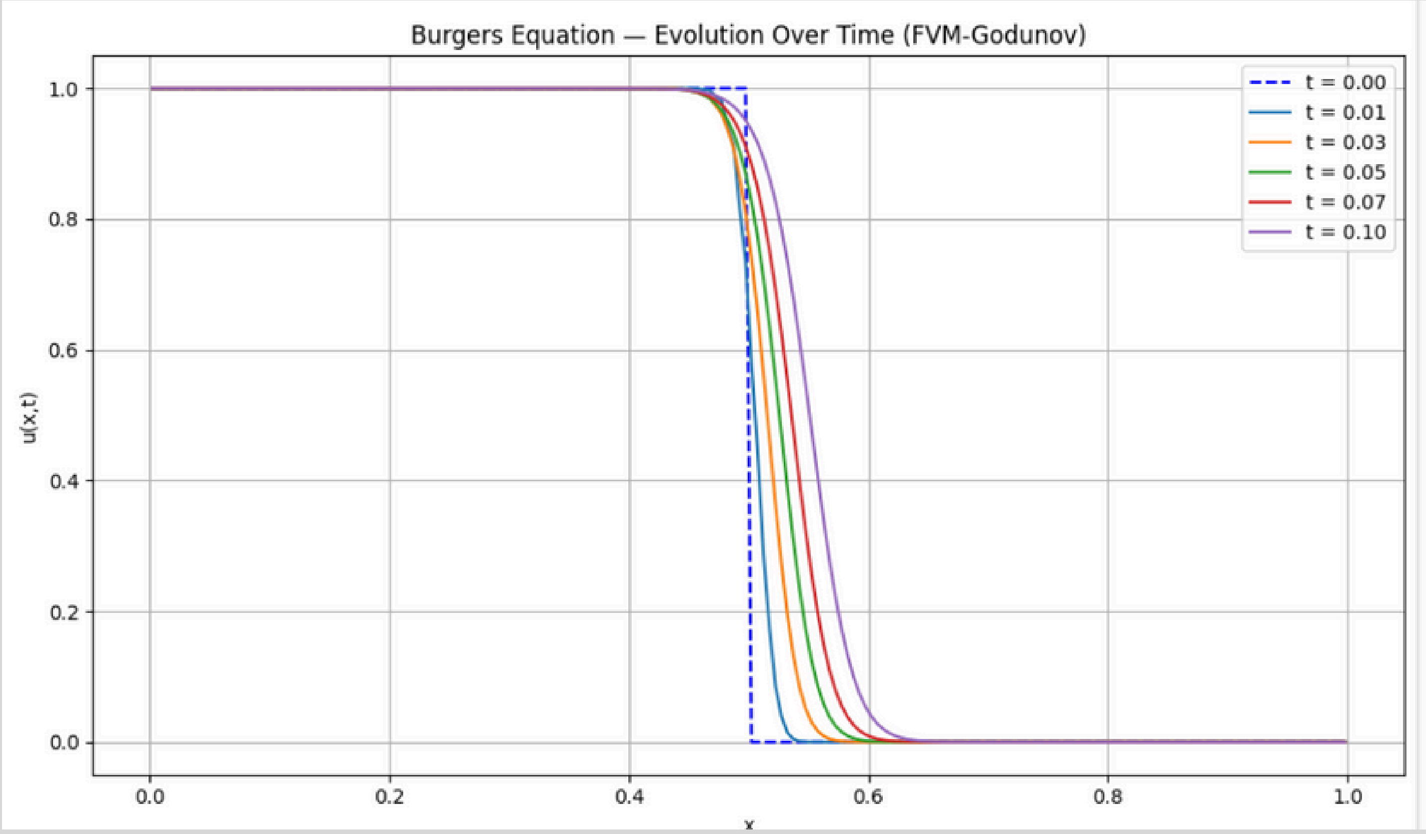
1. **Computed** interface states u_L and u_R at each cell face.
2. **Evaluated** the Godunov flux $F_{i+1/2}$ for the convex flux $f(u) = \frac{u^2}{2}$ using the scalar Riemann solver logic.
3. **Calculated** the diffusion term with second-order central differences:

$$D_i = \nu\frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}.$$

4. **Updated** the solution explicitly:

$$u_i^{n+1} = u_i^n + \Delta t\left(-\frac{F_{i+1/2} - F_{i-1/2}}{\Delta x} + D_i\right).$$

We recorded snapshots at times $t = \{0.01, 0.03, 0.05, ..\}$.



Numerical solution using FVM-Godunov method

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Quantum Tensor Network

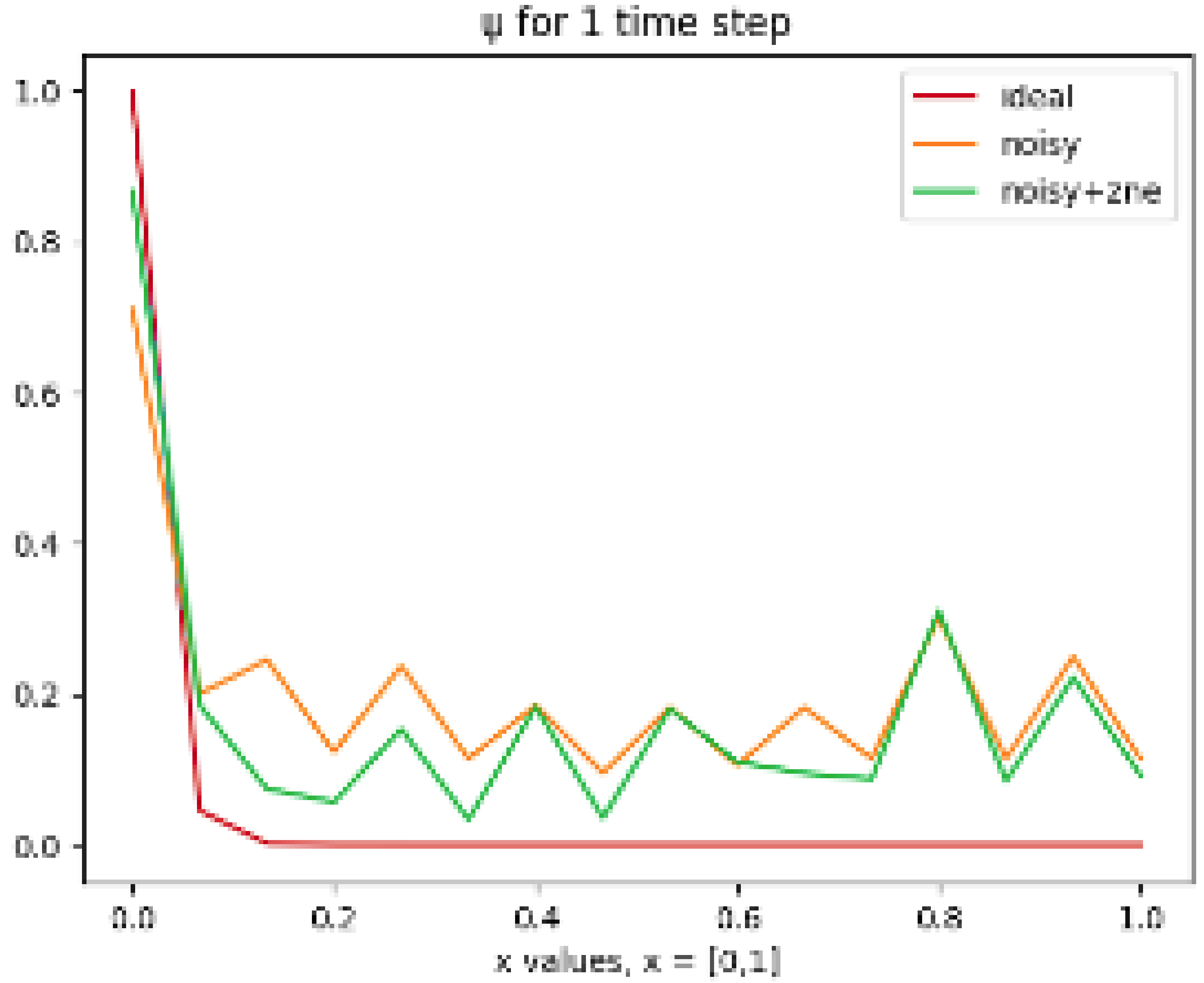

Figure 3: $\psi(x,t) = A(t) \cdot \exp\left(\frac{1}{2\nu} \int u(x,t)\,dx\right)$ on the noisy simulator with and without ZNE error mitigation.

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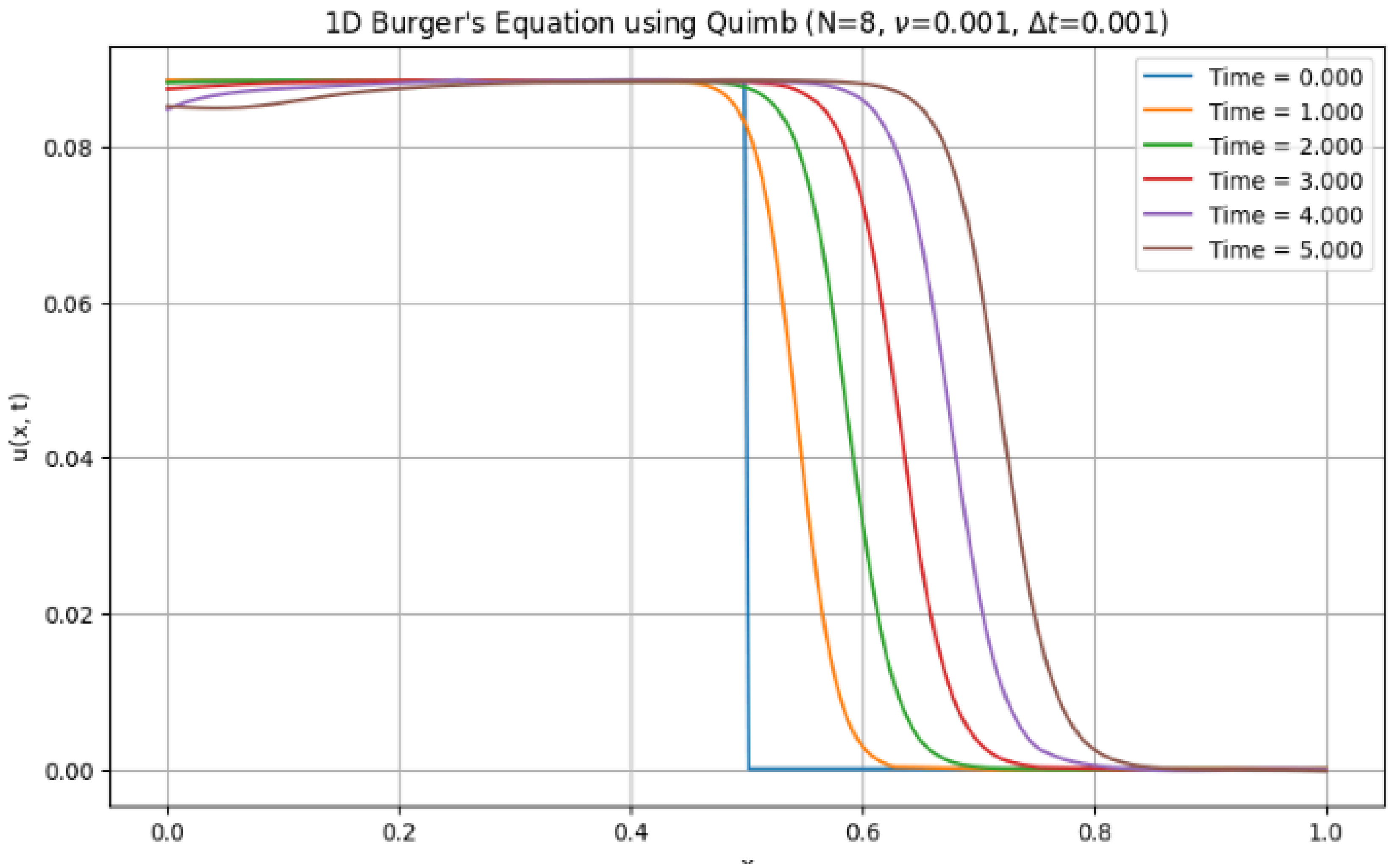
1 QTN:

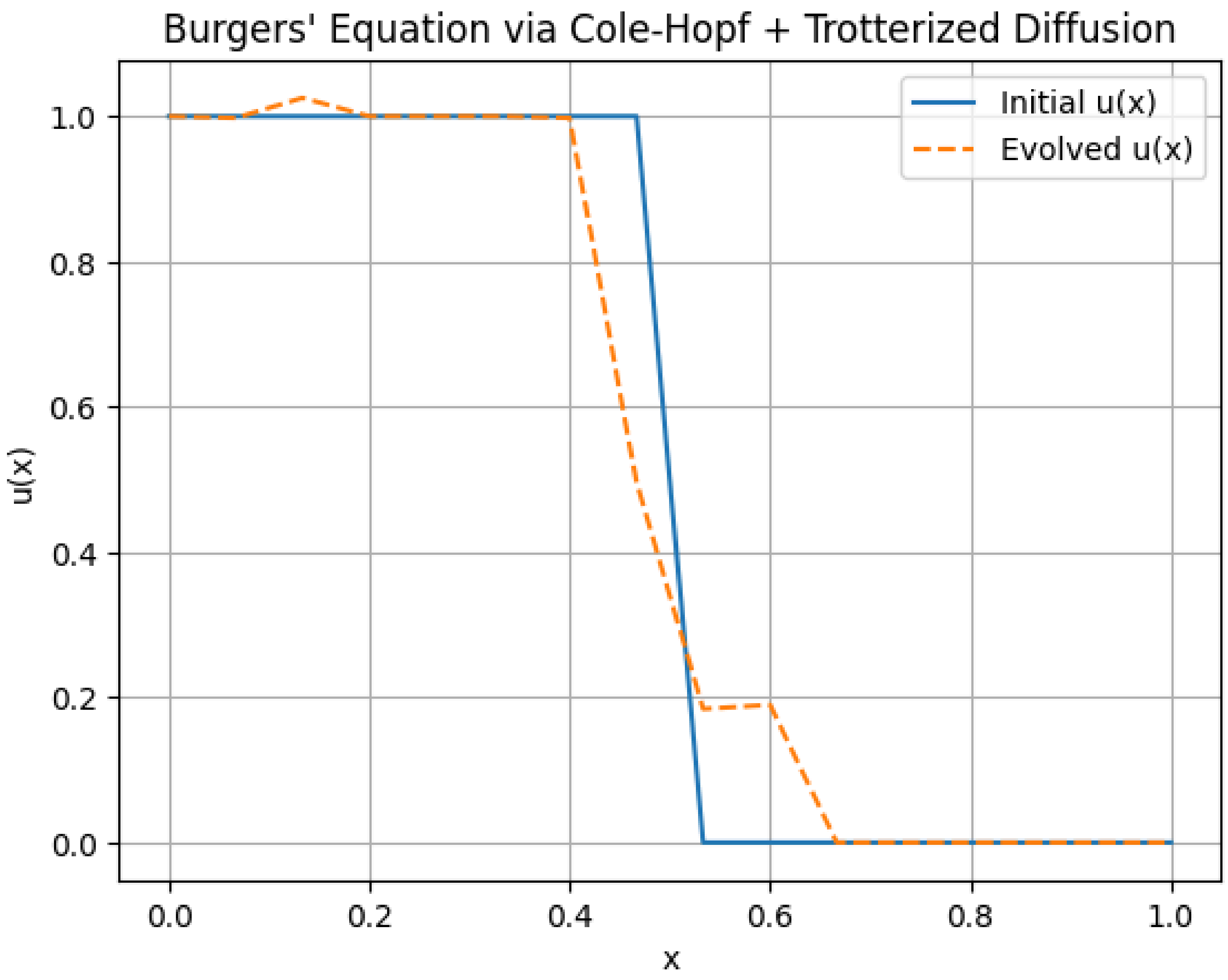
1.1 Methodology:

The solution implements two approaches for the QTN challenge: a quantum-inspired classical method (using quimb, no gates) and a true quantum version with trotterization (using gates/circuits). One mimics quantum techniques classically, while the other runs on actual quantum computation. The quantum solution includes the following steps:

- The algorithm starts first by a riemann step function of the velocity vector u. $\begin{cases} 1 & \text{if } 0 \leq x \leq 0.5 \\ 0 & \text{if } 0.5 < x \leq 1 \end{cases}$
- u is transformed to psi using the Cole-Hopf transformation, this makes the nonlinear burger's equation linear. $\psi(x,t) = A(t) \cdot \exp\left(\frac{1}{2\nu} \int u(x,t)\,dx\right)$
- The qmprs package is then used to build the MPS, matrix product state, circuit representation of ψ.
- Trotterization is performed on the MPS circuit encoding of ψ.
- The statevector is built. On the noisless simulator it is easily accessed by qiskit built-in functions, while on the noisy simulator and real QPU, the statevector is built from the measurement counts.
- The final statevector represents the evolved ψ vector, we transform it into the evolved u vector by the following formula: $u(x,t) = -2\nu \frac{\partial_x \psi}{\psi}$

Quantum inspired solution MPS QTN + Trotterization





Noiseless vs. Noisy Quantum QTN Results — Key Insights

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Noisy Simulation

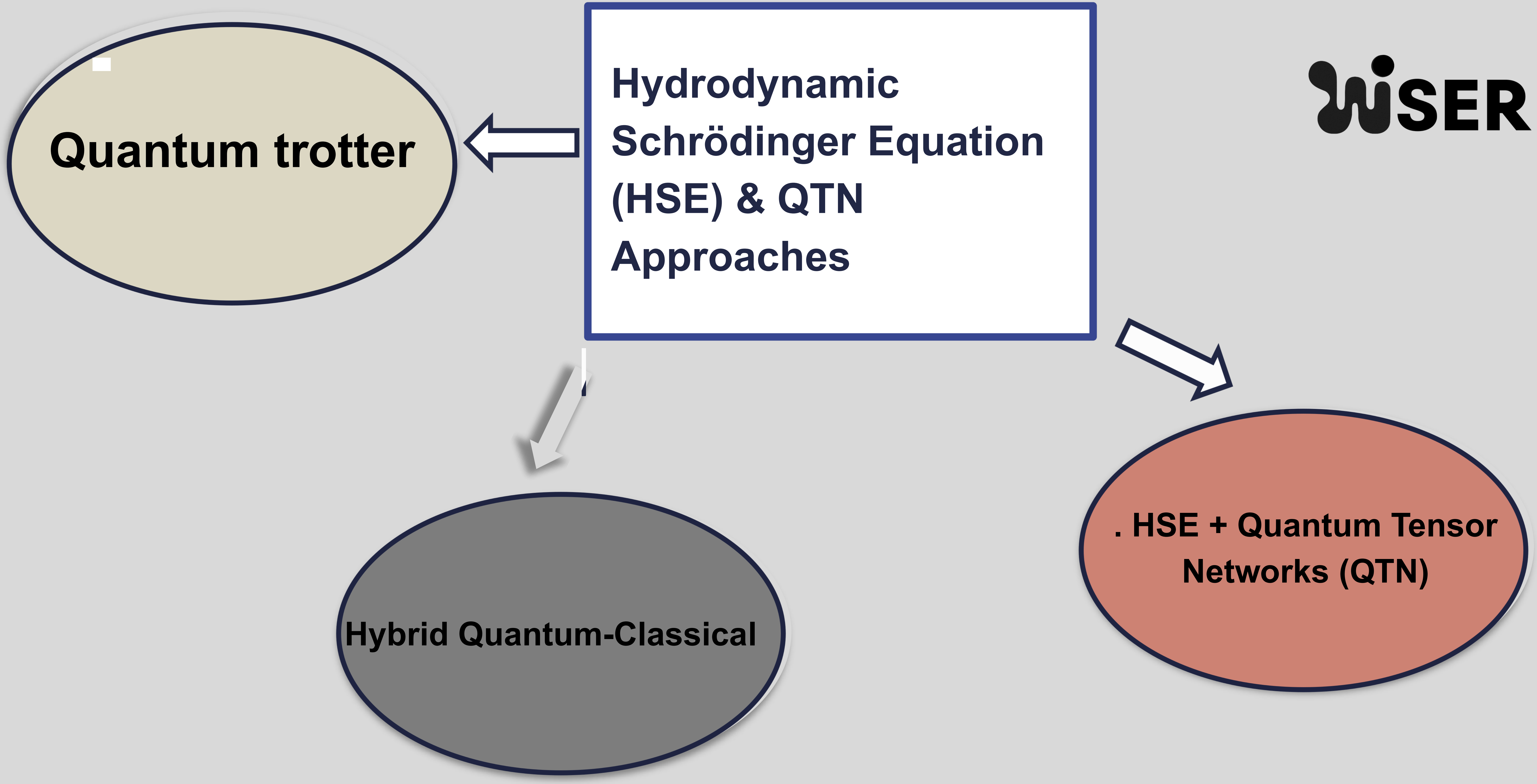
Vs

- 4-qubit, 1–3 steps, FakeManilaV2 backend.
-
- ZNE: Best (~23% gain at step 1, less after).
-
- DD: No gain, slightly worse.
- Noise impact grows with steps.

Noiseless + Scaling

- Classical Best: Godunov FVM (L2=0.288) — slowest (108.8 s).
- Worst: Quantum inspired (L2≈174) — fastest (0.03 s).
- More qubits → exponential grid & depth growth.
- Higher qubits in Trotter → more gates, slower, less accurate.

algorithm


Hydrodynamic Schrödinger Equation (HSE) & QTN Approaches
Quantum trotter
Hybrid Quantum-Classical
. HSE + Quantum Tensor Networks (QTN)

Hydrodynamic Schrodinger equation Method

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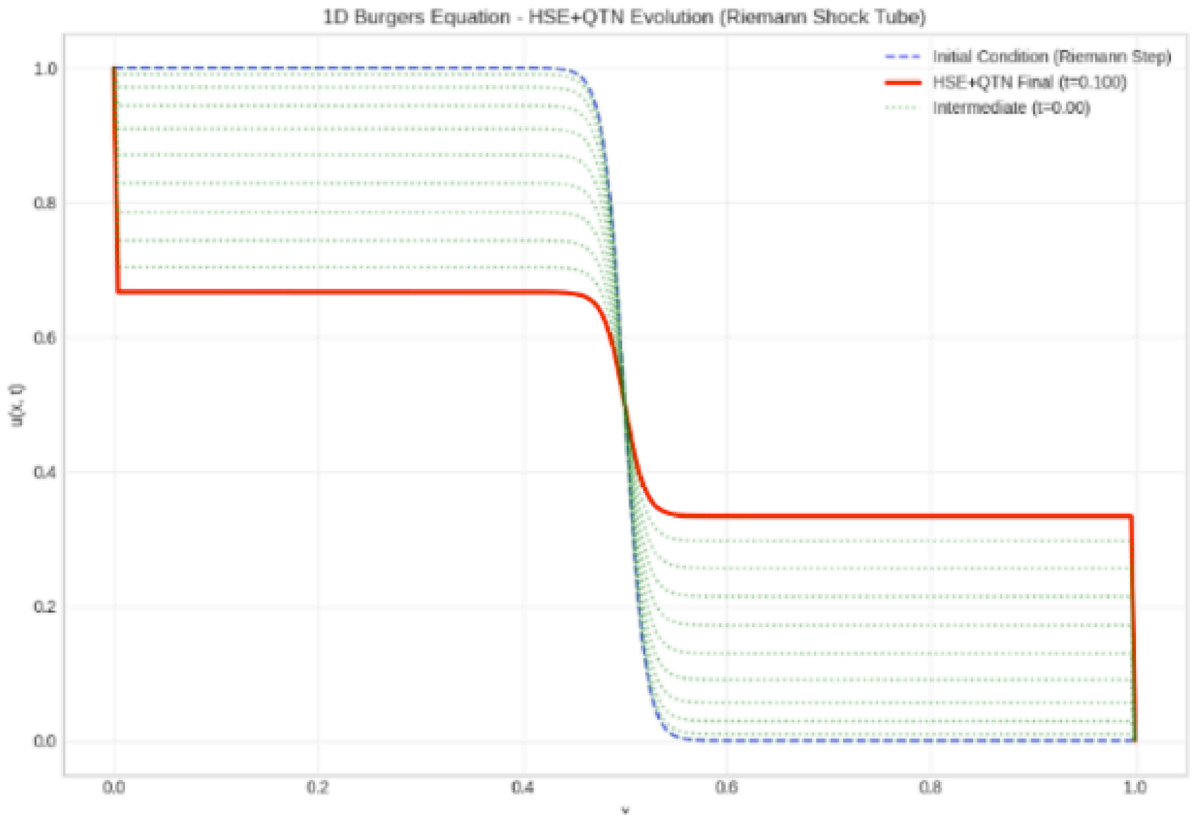
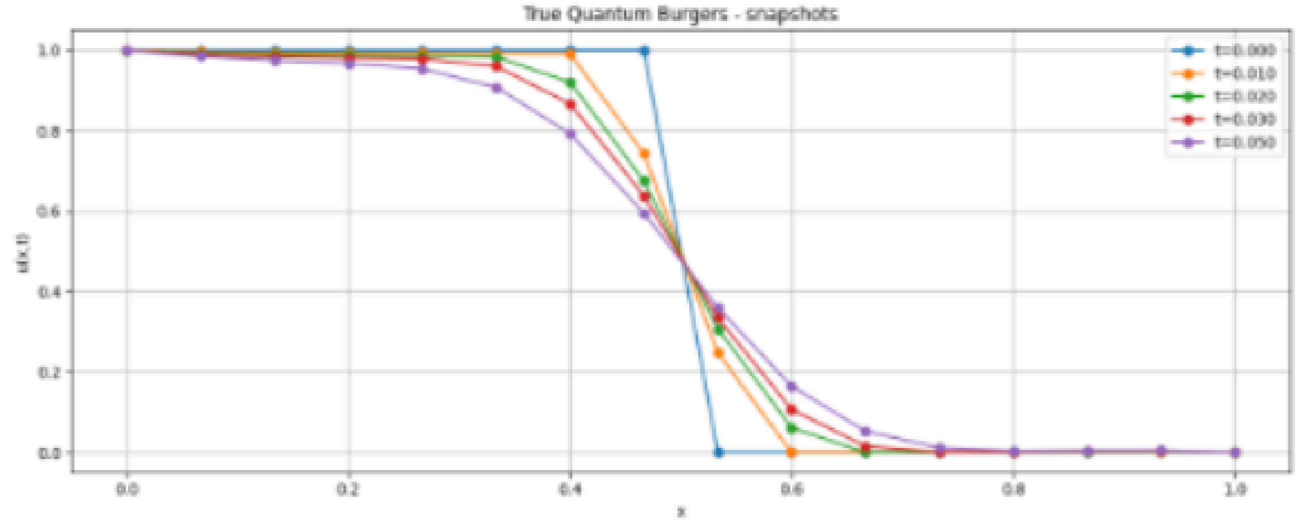
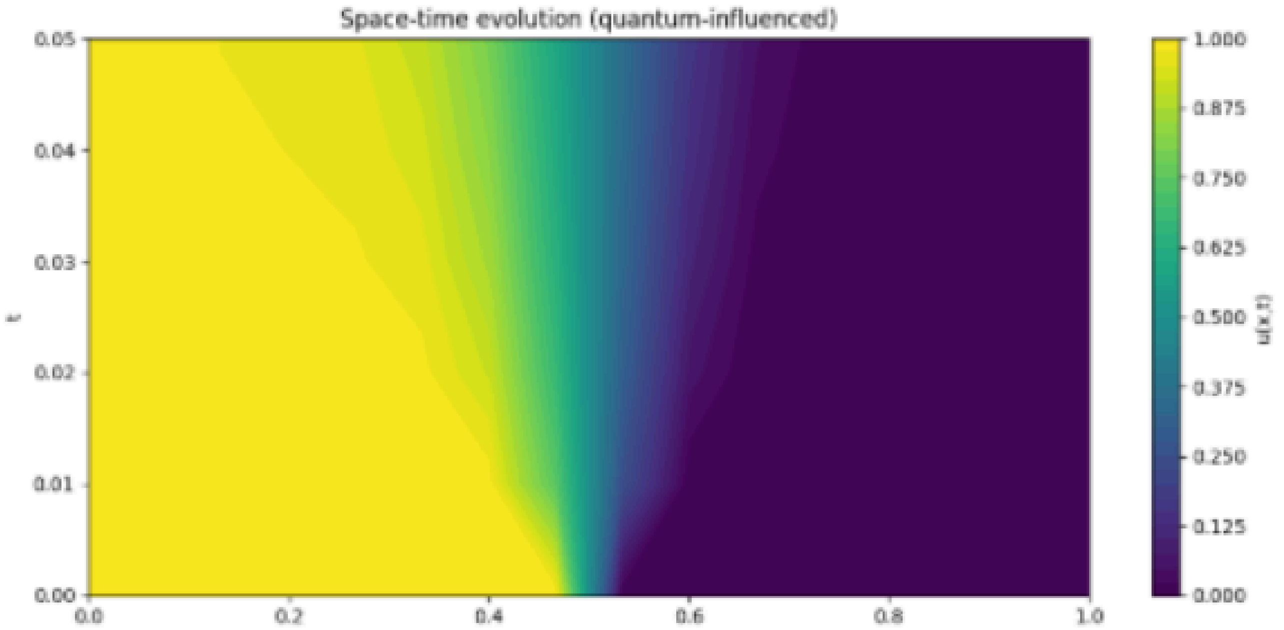
1. **HSE+QTN:** Transforms Burgers' equation into a quantum wavefunction form, compresses it using tensor networks for efficient simulation of shocks.



1. Solving Burgers' equation using a hybrid quantum-classical approach, via quantum circuits and measurement decoding.





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Impact and Future Scope

Impact

Improved accuracy and efficiency for complex quantum simulations.

why quantum

To simulate complex systems and scale beyond classical computing limits.

Future Scope

- **Improving Trotterization**
- **Reducing cumulative errors**

Related publications

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Tushar Pandey, Amir Ali Malekani Nezhad. QMPRS: Quantum Matrix Product Reduced Synthesis, 2025.
DOI: 10.5281/zenodo.15437417.

Johnnie Gray. "quimb: a python library for quantum information and many-body calculations." Journal of Open Source Software, vol. 3, no. 29, 2018, p. 819.
DOI: 10.21105/joss.00819.

IBM. Silicon Quantum Computing announces the world-first integrated circuit manufactured at the atomic scale.

URL: https://qiskit-community.github.io/qiskit-algorithms/tutorials/13_trotterQRTE.html.

R. D. Peddinti et al. "Quantum-inspired framework for computational fluid dynamics." Communications Physics, vol. 7, Article 135, 2024.
DOI: 10.1038/s42005-024-01623-8.

Thank You

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