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

BY: Jessica Omuna Anabor

Summary

The numerical solution of nonlinear partial differential equations (PDEs), such as the viscous Burgers' equation, is a fundamental task in computational fluid dynamics (CFDs) but often incurs significant computational costs, particularly for high resolution simulations.

This project seeks to investigate whether a hybrid quantum-classical algorithm, using amplitude encoding, variational quantum circuits, and noise mitigation techniques, can serve as an effective and accurate solver for the 1D viscous Burgers' equation. The central problem is to determine the viability, accuracy, and robustness of such a quantum-enhanced PDE solver when benchmarked against classical finite difference methods and subjected to realistic noise conditions on near term quantum devices.

1. Problem Context

Problem Statement & Goal

When leveraging quantum algorithms to address computational challenges, there are limitations often caused by noise, gate fidelity and qubit scalability.

The primary goal is to simulate 1D viscous Burgers' equation (a nonlinear PDE modeling shockwaves) using a hybrid quantum-classical approach that leverages quantum amplitude encoding, hybrid variational circuits, and noise mitigation techniques.

Approaches:

- Amplitude Encoding is used to map classical field data (e.g., velocity fields) into quantum states with low qubit overhead (`log₂(N)` qubits). This minimizes qubit resource usage and enables the simulation of larger problems on limited hardware

- The hybrid circuit mimics a single time-step of PDE evolution through trotterization (alternating Hadamard layers, `Rz` phase rotations, and entanglers).

- Zero-Noise Extrapolation (ZNE) and measurement error mitigation are applied to combat quantum noise.

- Classical Solver (FD) is used for benchmarking the accuracy and stability of the hybrid model.

Originality of Project:

- Combines PDE simulation with quantum state preparation and parameterized hybrid circuits, inspired by quantum tensor networks (QTN) and Hamiltonian simulation elements (HSE).
- Seamlessly integrates classical finite-difference solvers, amplitude encoding, ZNE, and quantum metrics (TV, KL, fidelity) in one demonstrative framework.
- Provides multiple abstraction layers (e.g., direct Aer runs, noisy simulations, AWS Braket support) to evaluate hardware/software scalability.

2. Reproducible Results

Key Features:

- Seed control via `np.random.seed(42)` ensures deterministic initialization.
- Classical solver (`classical_burgers`) allows for accurate baselining and result validation.
- All runs log:
    - Number of qubits
    - Output distributions
    - ZNE extrapolated values
    - Statistical uncertainties (CI95)
- Plots and CSVs are saved, making reruns and comparisons straightforward

3. Noise Robustness

Mitigation Techniques Implemented:

1. **Zero-Noise Extrapolation (ZNE):** The project applies ZNE by running circuits at scaled noise levels and extrapolating back to estimate the zero noise output
    - Implemented via:
        - Custom `fold_gates_for_zne()`
        - Mitiq integration (`fold_gates_at_random`)
    - Scale factors: `[1,3,5]`
    - `linear_zne_extrapolation()` computes extrapolated expectation at zero noise.
2. **Measurement Error Mitigation:**
    - If `qiskit.ignis` is available, the code auto generates full calibration circuits and applies `CompleteMeasFitter`.
3. **Noisy Backend Simulation:**
    - **Custom noise models** built with depolarizing errors (e.g., `0.005` for 1-qubit gates, `0.02` for `CX`).

4. Results

A. *Summary of ZNE and Raw Results*

Case	Backend	Shots	Raw Zero-State Freq	ZNE Extrapolated Freq	Ideal Zero-State Prob
Baseline	AerSimulator	2048	0.5229	0.5208	0.5157
High Shots	AerSimulator	40000	0.5126	0.5103	0.5157
Noisy (toy noise)	AerSimulator (noise)	8192	0.4447	0.4444	0.5157

Interpretation of above results:

- **Raw vs Ideal:**
  The raw measured zero-state frequencies are close to the ideal 0.5157 value under the noiseless backend, especially with high shots. This validates correctness.

- **ZNE Impact (Noiseless):**
  ZNE barely changes the results on the noiseless simulator (`0.5208 to 0.5207`), as expected.

- **ZNE Impact (Noisy):**
  On the noisy simulator, ZNE provides no meaningful improvement (`0.4447 to 0.4444`). This suggests:

  - The toy noise model may be too symmetric or too strong, making extrapolation ineffective.

  - Or the circuit might be not deep enough to benefit from ZNE under the current scaling factors

B. *Noise Impact and Divergence Measures*

Metric	Baseline (No Noise)	Noisy Backend
KL Divergence	0.0014	**0.5372**
TV Distance	0.0079	**0.1299**
L2 Distance	0.0099	**0.1032**

Interpretation of above results:

- These metrics clearly show a large divergence between the noisy and ideal results, indicating a significant effect from the noise model.

- KL divergence > 0.5 is very high, this suggests the noisy output is quite far from ideal.

C. *Benchmark*

N	Depth	Fidelity	TV Distance	KL Divergence
8	17	0.9930	0.0684	0.0141
16	33	0.9976	0.0420	0.0048
32	65	0.9986	0.0361	0.0028
64	129	0.9952	0.0518	0.0096

Interpretation of above results:

- These give a broader view of fidelity across varying system sizes.
- Despite increasing depth and circuit size, fidelity remains high (>99%), especially for circuits without injected noise.
- Divergence metrics stay low in the ideal simulator, indicating that the circuits are being simulated and measured correctly.