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

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1. Clear Explanation & Novelty

Problem Context:

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.

Algorithm Rationale:

- Amplitude Encoding is used to map classical field data (e.g., velocity fields) into quantum states with low qubit overhead (`log₂(N)` qubits).
- 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:

- 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):**
   - 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`).

Noise Resilience Demonstrated:

- The noisy run with `8192` shots and custom noise still produced meaningful results.
- **Comparison metrics** (vs ideal):
    - KL divergence
    - Total Variation
    - Fidelity

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.