

A Variational Quantum Approach for the 1D Viscous Burgers' Equation

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

In this document, we present a theoretical framework of our approach for solving the one-dimensional viscous Burgers' equation using a hybrid quantum-classical algorithm. The methodology is founded on approximating the solution with a Chebyshev polynomial basis, where the expansion coefficients are encoded in the measurement probabilities of a parameterized quantum state. This method allows to capture both nonlinear wave steepening and viscous diffusion effects. The optimization is driven by minimizing a physics-informed loss function that incorporates the partial differential equation residual, initial conditions, and boundary constraints. This approach leverages the expressiveness of variational quantum circuits for function representation while maintaining numerical stability and accuracy through the spectral properties of Chebyshev polynomials. We built a hybrid quantum-classical framework for nonlinear PDEs relevant to quantum computational fluid dynamics

1 The Burgers' Equation

The 1D viscous Burgers' equation is a fundamental nonlinear partial differential equation (PDE) that models the interplay between nonlinear convection and viscous diffusion. It is expressed as:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \quad (1)$$

where $u(x, t)$ is the velocity field, ν is the kinematic viscosity, $x \in [0, 1]$ is the spatial domain, and $t > 0$ is the temporal domain.

For this problem, we consider a Riemann step initial condition (IC) and Dirichlet boundary conditions (BCs):

- **Initial Condition:**

$$u(x, 0) = \begin{cases} 1 & x \leq 0.5 \\ 0 & x > 0.5 \end{cases} \quad (2)$$

- **Boundary Conditions:**

$$u(0, t) = 1 \quad \text{and} \quad u(1, t) = 0, \quad \forall t > 0 \quad (3)$$

This setup models the evolution of a shock wave, making it an excellent test case for numerical solvers designed to handle sharp gradients and nonlinear dynamics.

2 Mathematical and Computational Framework

Our strategy is to formulate the PDE problem as a variational optimization task, where a parameterized function ansatz is trained to satisfy the governing equation and its associated conditions.

2.1 Function Approximation via Chebyshev Polynomials

We approximate the solution $u(x, t)$ using a truncated series of tensor-product Chebyshev polynomials of the first kind, $T_n(z)$. This basis is chosen for its excellent approximation properties and numerically stable computation of derivatives. The ansatz takes the form:

$$u_{approx}(x, t; \mathbf{c}, \lambda) = \lambda \sum_{k=0}^{M-1} c_k T_{k_x}(2x - 1) T_{k_t}(2t/T_{max} - 1) \quad (4)$$

where:

- $\{c_k\}$ are the expansion coefficients to be determined.

- λ is a learnable global scaling parameter.
- $M = 2^{n_x+n_t}$ is the total number of basis functions, defined by the number of qubits n_x and n_t allocated to the spatial and temporal dimensions, respectively.
- T_{k_x} and T_{k_t} are Chebyshev polynomials. The arguments $(2x - 1)$ and $(2t/T_{max} - 1)$ map the physical domain $[0, 1] \times [0, T_{max}]$ to the canonical domain $[-1, 1]^2$ where the polynomials are defined.

The derivatives required by the Burgers' equation can be computed analytically by differentiating the series term-by-term. For a single basis function $\Phi_k(x, t) = T_{k_x}(2x - 1)T_{k_t}(2t/T_{max} - 1)$, the derivatives are:

$$\frac{\partial \Phi_k}{\partial t} = T_{k_x}(2x - 1) \frac{dT_{k_t}}{dt}(2t/T_{max} - 1) \quad (5)$$

$$\frac{\partial \Phi_k}{\partial x} = \frac{dT_{k_x}}{dx}(2x - 1)T_{k_t}(2t/T_{max} - 1) \quad (6)$$

$$\frac{\partial^2 \Phi_k}{\partial x^2} = \frac{d^2 T_{k_x}}{dx^2}(2x - 1)T_{k_t}(2t/T_{max} - 1) \quad (7)$$

2.2 Variational Quantum Eigensolver (VQE) Approach

The core of the hybrid method is to use a Variational Quantum Eigensolver (VQE) to generate the coefficients $\{c_k\}$. A Parameterized Quantum Circuit (PQC), or ansatz, denoted $U(\theta)$, is used to prepare a quantum state $|\psi(\theta)\rangle$ on $n_q = 1 + n_x + n_t$ qubits.

$$|\psi(\theta)\rangle = U(\theta)|0\rangle^{\otimes n_q} \quad (8)$$

The coefficients are then extracted from the measurement outcomes of this state. An ancillary qubit is used to encode the sign of the coefficients, allowing for both positive and negative values. The probability of measuring a computational basis state $|k\rangle$ is $p_k = |\langle k|\psi(\theta)\rangle|^2$. The Chebyshev coefficients are constructed as:

$$c_k = p_k - p_{k+M}, \quad \text{for } k \in \{0, 1, \dots, M - 1\} \quad (9)$$

Here, the total Hilbert space of n_q qubits is partitioned to represent the indices k and $k + M$. The circuit parameters θ become the trainable variables of the optimization problem.

3 The Physics-Informed Loss Function

The training process minimizes a composite loss function \mathcal{L} that quantifies the discrepancy between the ansatz u_{approx} and the true physical behavior. The loss is evaluated over a grid of N_c discrete collocation points (x_i, t_j) within the domain. It comprises three distinct terms.

3.1 PDE Residual Loss

This term penalizes violations of the Burgers' equation at interior collocation points.

$$\mathcal{L}_{PDE} = \frac{1}{N_c} \sum_{i,j} \left(\frac{\partial u_{approx}}{\partial t} + u_{approx} \frac{\partial u_{approx}}{\partial x} - \nu \frac{\partial^2 u_{approx}}{\partial x^2} \right)_{(x_i, t_j)}^2 \quad (10)$$

3.2 Initial Condition Loss

This term enforces the Riemann step profile at time $t = 0$.

$$\mathcal{L}_{IC} = \frac{1}{N_x} \sum_i (u_{approx}(x_i, 0) - u(x_i, 0))^2 \quad (11)$$

3.3 Boundary Condition Loss

This term enforces the Dirichlet conditions at the spatial boundaries $x = 0$ and $x = 1$.

$$\mathcal{L}_{BC} = \frac{1}{N_t} \sum_j [(u_{approx}(0, t_j) - 1)^2 + (u_{approx}(1, t_j) - 0)^2] \quad (12)$$

The total loss function is a weighted sum of these components, where η_{IC} and η_{BC} are hyperparameters that balance the contribution of each term.

$$\mathcal{L}(\theta, \lambda) = \mathcal{L}_{PDE} + \eta_{IC} \mathcal{L}_{IC} + \eta_{BC} \mathcal{L}_{BC} \quad (13)$$

4 Theoretical Advantages of the Hybrid Approach

The proposed method offers several theoretical benefits:

- **Spectral Accuracy:** Chebyshev expansion provides exponential convergence for smooth solutions

- **Implicit Regularization:** Quantum state preparation imposes implicit smoothness constraints
- **Parameter Efficiency:** n -qubit system encodes $O(2^n)$ basis functions
- **Exact Derivatives:** Analytic differentiation avoids approximation errors
- **Physical Consistency:** Loss function structure preserves conservation properties

Conclusion

This theoretical framework establishes a rigorous foundation for solving non-linear PDEs using hybrid quantum-classical methods. By synergistically combining Chebyshev spectral methods with variational quantum algorithms, we achieve:

- **Compact representation** of solutions in high-dimensional function spaces through quantum state encoding
- **Exact computation** of spatial and temporal derivatives via analytic Chebyshev recurrence relations
- **Physics-constrained optimization** through composite loss functions that enforce PDE compliance

The method transforms PDE solving into a high-dimensional optimization task while preserving fundamental physical constraints. The variational quantum approach with Chebyshev polynomial expansions provides an efficient pathway for solving nonlinear systems like the 1D Burgers' equation, with direct extensibility to more complex fluid models including full Navier-Stokes equations.

Future research will focus on three critical extensions:

- Implementation for 3D fluid systems requiring higher-qubit architectures
- Adaptive basis selection techniques for dynamic solution refinement
- Error analysis frameworks addressing noise resilience in NISQ-era devices

By maintaining spectral accuracy through Chebyshev expansions while leveraging quantum state expressivity, this approach provides a robust computational

paradigm for tackling complex differential equations on emerging quantum hardware. The physics-informed loss function ensures mathematical consistency with underlying conservation laws, positioning the method as a versatile tool for computational fluid dynamics in the quantum era.

References

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