Matrix product states for simulating nonlinear Burgers' equation

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This paper presents a quantum algorithm that solves a canonical classical nonlinear partial differential equation, Burgers' equation, suitable for execution on a quantum computer. Matrix product states (MPS) are used to efficiently encode the velocity variable. Linear terms are efficiently represented as matrix product operators (MPOs). The typically challenging nonlinear convection term is made more suitable for near-term (NISQ) quantum computers through mid-circuit measurement, or through recycled ancillae qubits, thereby avoiding hard-to-scale variational techniques. Hamiltonian simulation drives the evolution of the velocity in time.

Nonlinear partial differential equations are known to be computationally intensive to solve, with for contemporary exascale supercomputers. It is hoped that a quantum algorithm that leverages superposition, entanglement, and quantum parallelism may enable larger simulations of nonlinear partial differential equations that are intractable classically.

1 Governing equations

The equation of interest in the present work is the one-dimensional Burgers' equation.

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}; \tag{1}$$

where ν is the dynamic viscosity, the boundary conditions are $u(x=0,t) = u_l, u(x=1,t) = u_R$, and the initial condition is $u(x,t=0) = u_0(x)$. $\forall x \leq 0.5, u_0 = 1$ and $u_0 = 0$ for all other values of x. The expected behaviour is that of a discontinuous shock being convected towards the positive x-direction while experiencing viscous dissipation over time. This suggests that the discontinuous shock will become broader over space as time progresses.

The linear term mentioned in the previous section is the Laplacian, $\nu\frac{\partial^2 u}{\partial x^2}$. It is important to note that it is a Hermitian operator, and so any discretisation should retain the this property for both correctness and for exploitation in creating a suitable operator on a quantum computer.

The nonlinear convection term is $-u\frac{\partial u}{\partial x}$. Due to the expected positive x-direction convection direction from the initial conditions, a finite difference method may need to use an upwind discretisation scheme.

All differential operators in Equation (1) are discretised using the finite difference method. The Laplacian term is discretised with a second-order accurate central finite difference scheme while the nonlinear term is discretised with a first-order accurate upwind finite difference scheme. A first-order scheme is selected due to the well-known numerical instabilities associated with using fully-dispersive schemes on weakly-dissipative flow problems that eliminate the possibility of using a second-order central scheme. However, first-order schemes are also numerically dissipative, so can smooth out sharp features. As a compromise between truncation error and numerical stability, a first-order upwind scheme was selected. Note that other schemes are possible such as higher-order biased schemes, Lax-Wendroff, or Lax-Friedrichs schemes.

The spatial domain is discretised into 2^N uniform grid points $x \in [0,1]$, where N is the number of qubits. The i^{th} grid point has the physical location $x_i = \frac{q^1}{2^N-1}$, where $q_i^1 = (b_1^1 b_2^1 \dots b_N^1)$ is the index represented using binary encoding [1].

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2 Quantum Algorithm

2.1 Matrix product state encoding

2.2 Matrix product operator embedding via LCU

2.3 Near-term nonlinear operator embedding via mid-circuit measurement or recycled ancillae

2.4 Hamiltonian simulation

References

[1] Nikita Gourianov, Peyman Givi, Dieter Jaksch, and Stephen B. Pope. Tensor networks enable the calculation of turbulence probability distributions. *Science Advances*, 11(5):eads5990, 2025.