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 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.

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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 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 for weakly-dissipative flow problems that eliminate the possibility of using a second-order central scheme. However, first-order schemes are also numerically dissipative, and 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 [5]. $b_j^1 \in \{0,1\}$ represents the binary state of qubit

j. By convention, the most significant bit is on the left, b_1^1 while the least significant bit is on the right, b_N^1.

2 Quantum Algorithm

2.1 Matrix product state encoding

The initial condition is encoded as a matrix product state (MPS) owing to the ability for MPSs to reduce the resource cost of state preparation [19]. Due to the local nature of the discontinuous initial condition u_0, MPS bond dimension is 2, regardless of the number of qubits, and thus lossless compression is readily achieved. Moreover, any MPS with a bond dimension of two can be exactly implemented in a quantum circuit without approximation [12]. Also, this particular data encoding strategy means that MPS compression occurs by finding correlations across similar length scales [5].

Ostensibly, the cost of preparing any general matrix product states on a quantum computer scales linearly with the number of qubits [16] via the sequential generation or single-layer scheme. Such a linear-depth preparation is always possible. Recently, there have been reductions of the preparation cost from linear, to logarithmic, to constant-depth [6, 12, 13, 8, 18].

However, this particular discontinuous initial velocity vector u_0 can be encoded with only a single layer of $N-1$ Hadamard gates on the highest $N-1$ qubits i.e., qubits $1, 2, \ldots, N-1$. This represents the minimum possible, constant depth MPS encoding scheme, without any of the higher error two-qubit gates that usually occur with universal state preparation schemes [17].

2.2 Matrix product operator embedding via LCU

This section concerns the treatment of the linear Laplacian in Equation (1). To preserve the Hermitian property of the Laplacian, it is discretised with a second-order accurate central finite difference scheme. The matrix product operator (MPO) representation of the discretised Laplacian scheme is created using ladder operators, as given by [4, 14, 15]. Such a scheme is guaranteed to have a bond dimension of 3, suggesting there exists an efficient quantum gate representation. The Dirichlet boundary conditions are embedded in the operator at this stage [11, 14].

The practical implementation of this generally non-unitary discretised operator involves linear combination of unitaries (LCU) [3]. Given that the MPO of this Hermitian operator is known classically in terms of the ladder operator, a decomposition into simplified Pauli strings via the Hadamard transform is readily possible [10]. Generally, the number of ancilla qubits required for this LCU decomposition is $\mathcal{O}(N)$ to encode $\mathcal{O}(2^N)$ terms in the LCU decomposition. However, the Laplacian is a sparse near-tridiagonal or banded circulant matrix, which yields more efficient LCU circuits that have gate complexity $\mathcal{O}(\text{poly}(N))$ and constant ancilla scaling[2].

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

The nonlinear convection term is implemented on the quantum circuit without variational methods. Firstly, the first derivative associated with the nonlinear convection term is discretised with a first-order upwind finite difference scheme. Then, its matrix product operator (MPO) representation is created in terms of ladder operators and thus Pauli strings. An ancilla registry is prepared containing a copy of the amplitude-encoded velocity state vector $|u(x,t)\rangle$, reminiscent of the quantum nonlinear processing unit (QNPU) [7]. Then, apply the MPO of the first-order upwind scheme using LCU on the ancillae qubits [9]. Either through mid-circuit measurement of the copied ancilla registry to postselect the all $|0\rangle$ state or through extra control ancillae, a Hadamard product operator is applied to the quantum circuit to implement the nonlinear term.

2.4 Hamiltonian simulation

To evolve the velocity in time, a Hamiltonian for the quantum implementations of all terms on the right-hand side of Equation (1) is found [9]. Standard Hamiltonian simulation methods, such as the Trotter-Suzuki method, can be used to evolve the velocity forwards in time.

2.5 Implementation details

This solver uses the Pennylane package [1].

3 Results

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