Simulating Fluid Dynamics on a Quantum Computer

Brief: Quantum computing may offer the potential for a large computational speedups in fluid dynamics problems by encoding and propagating a fluid density efficiently in the Hilbert space of a quantum state. One way of applying this is known as the quantum lattice Boltzmann method (QLBM), and works by applying a form of quantum walk to a fluid density. In this challenge problem, we will explore this idea by walking through a simple implementation of the QLBM algorithm for the one-dimensional advection-diffusion equation.

LMB Background:

The 1D linear advection-diffusion equation with a constant diffusion coefficient *D* is given by

$$\frac{\partial\phi}{\partial t} + \frac{\partial(u\phi)}{\partial x} = D\frac{\partial^2\phi}{\partial x^2} \tag{1}$$

where ϕ is the concentration, *t* is the time, *x* is the coordinate, and *u* is the fluid velocity. Equation 1 can be solved numerically using the lattice Boltzmann method (LBM). The LBM formalism describes the flow of individual particle densities $f_i(x,t)$ on discretized x and t. The macroscopic density ϕ is then given by

$$\phi(x,t) = \sum_i f_i(x,t). \tag{2}$$

The distributions f_i march in space and time according to

$$f_i(x + e_i\Delta t, t + \Delta t) = \left(1 - \frac{\Delta t}{\tau}\right) f_i(x,t) + \frac{\Delta t}{\tau} f_i^{eq}, \tag{3}$$

where e_i is the particle velocity, Δt is the time step, τ is the relaxation time, and f_i^{eq} is the local equilibrium distribution function given by

$$f_i^{eq} = w_i\phi(x,t)\left(1 + \frac{e_i.\vec{u}}{c_s^2}\right), \tag{4}$$

where w_i is the weighing factor for the link *i*, $\vec{u}$ is the advection velocity vector, and c_s is the speed of sound. For simplicity, we set $\Delta t = \tau$, and using Eqs. (3) and (4) we get

$$\phi(x,t) = \sum_i k_i\phi(x - e_i\Delta t, t - \Delta t), \tag{5}$$

where the parameters k_i are given by

$$k_i = w_i \left[1 + \frac{e_i u_i}{c_s^2}\right]. \quad 6$$

The Quantum implementation of LBM involves four steps: initialization, collision, streaming, and addition [1,2]. This challenge walks through each of the four steps to implement the QLBM algorithm to solve Eq. (1) for dimensional flow.

1. **Initialization**
   The initialization step encodes the distribution *ϕ(x,0)* into a quantum state. This can be achieved by using two quantum registers |q> for spatial dimension encoding, and |d> for the encoding the distribution functions. Consider a 1D lattice with M cells and Q microscopic velocities.
   a. How many qubits in the register |q> are needed to encode ϕ(x,0)?
   b. How many qubits in the register |d> are needed to encode distribution functions?
   c. Suppose M = 64, Q = 3, and the initial distribution is zero everywhere except at the point source x_s = 32, where ϕ(x_s,0) = 1.0. Using qiskit, write a function that returns a quantum circuit that initializes ϕ(x,0).

2. **Collision**
   For uniform velocity field, the collision step amounts to preparing the state in the direction register |d> [2]

   $$|k> = \frac{1}{\sqrt{2^{nd}}} \sum_i k_i |i>_d , \quad 7$$

   where *nd* is the number of qubits in the |d> register, and constants k_i are given by Eq. (6).
   a. Consider the 1D case described in the initialization part above (part c) with weight coefficients w = [2/3,1/6,1/6], particle speeds [0,1,-1], advection speed u = 0.2, and the speed of sound c_s=1. Using qiskit, write a function that initializes the state ϕ(x,0) and applies the collision operator.

3. **Streaming**

The distribution functions f_i are propagated in the directions corresponding velocities e_i in the streaming step. In the streaming step, each of the distributions f_i is shifted in the direction along link *i* with speed e_i. Consider the 1D case with velocity vectors 0,1,-1 for the distributions f_0,f_1, and f_2 respectively and periodic boundary conditions. The streaming operator will shift f_1 to the right, and f_2 to the left. This can be implemented on a quantum circuit applying the right and left operators R, L on the qubit register |q>. The R operator performs the operations R|i> = R|i+1>, and the L operator performs the operations L|i> = |i-1> with periodic boundary conditions.

   a. What is the product RL?
   b. Using qiskit, write a function that implements the operators R, and L for n qubit states |i>. **Hint:** what does circuit look like for 2 and 3 qubits?
   c. After collision, the R and L operators are applied to shift the right distribution. As a result, the operators must be applied conditioned on the direction register. Suppose the distribution functions f_0,f_1, and f_2 are encoded by the states |00>, |01>, and |10> respectively in the register |d>. Use qiskit to write a function that applies the streaming step after the collision step.

4. **Addition**

The addition step calculates the macroscopic density according to Eq. (2). This is achieved by applying Hadamard gates on the qubits in the |d> register and post selection. Which state on the |d> register will give us the desired state $\phi(x,t=1)$?

5. **Simulation**

   a. Using $\phi(x,t=1)$ from the addition step above as the input state, repeat the steps above to get $\phi(x,t=2)$.
   b. Repeat the steps above to simulate fluid flow for 20 steps.
   c. Plot the states $\phi(x,0)$, $\phi(x,1)$, $\phi(x,2)$, and $\phi(x,20)$.

References

1. L. Budinski, Quantum algorithm for the advection–diffusion equation simulated with the lattice Boltzmann method, Quantum Inf. Process. 20 (2) (2021) 1–17.

2. A. Tiwari, J. Iaconis, J. Jojo, S. Ray, M. Roetteler, C. Hill, and J. Pathak, Algorithmic advances towards a realizable quantum lattice Boltzmann method, arXiv preprint arXiv:2504.10870 (2025).