Developing Quantum Computing Algorithms for Modeling Heat Transfer with Phase Change

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Goal

CFD is historically the most compute-heavy field. Despite all the resources allocated to it, simulations still require compromises in fidelity to run in a reasonable amount of time. Quantum computing promises to accelerate these algorithms exponentially, by creating superpositions of states and solving them simultaneously.

- LBM works well on quantum computers because of its locality
- Cooling processes that lead to grain formation are not well understood
- Quantum spin states affect grain boundaries
- Quantum mechanics are well-suited for simulation on QC

Conclusions

Our algorithm promises to greatly speed up transport simulations and allow us to simulate these systems at a higher fidelity. This promises insights into grain formation and properties.

Acknowledgements

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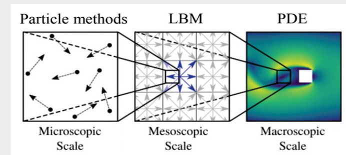
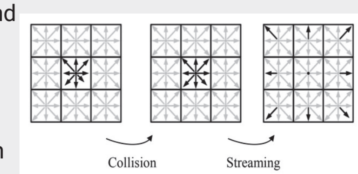
Quantum LBM

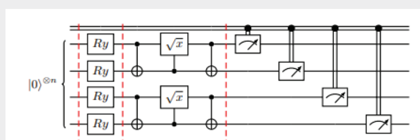
Traditional LBM

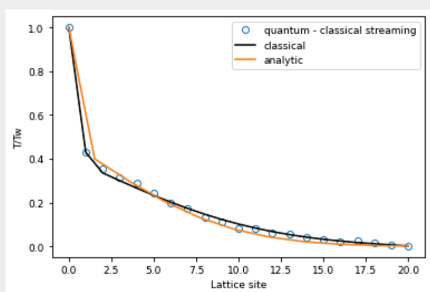
- The lattice Boltzmann method (LBM) solves the Boltzmann transport equation at the mesoscale
- Heat equation: $\frac{\partial T}{\partial t} = \alpha\nabla^2 T - \varphi$
- Simulates the fluid density with streaming and collision processes
- In the streaming step, fluid flows in each direction to adjacent nodes
- In the collision step, arriving fluid from each direction is averaged towards the equilibrium distribution
- This method is localized and therefore highly parallelizable
- $f_\alpha(\boldsymbol{r} + \boldsymbol{c}_\alpha \Delta t, t + \Delta t) = f_\alpha(\boldsymbol{r}, t) + \Omega_\alpha[f_\alpha(r,t)]$





Quantum Algorithm

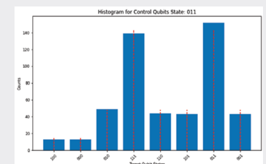


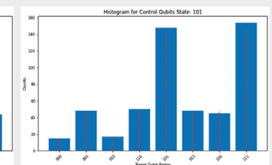


- 1 qubit per direction per node
- Initialization by Ry(θ_α) gate
  - $\theta_\alpha = 2\arccos\sqrt{1 - f_\alpha(x_i, t)}$
- Collision applied by entangling the qubits at each lattice point
- $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{i\varphi}e^{i\xi}\cos\theta & e^{i\varphi}e^{i\zeta}\sin\theta & 0 \\ 0 & -e^{i\varphi}e^{-i\zeta}\sin\theta & e^{i\varphi}e^{-i\xi}\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
- Φ, ξ, ζ, θ, determined by LBM collision operator
- Example is 1D heat transfer with fixed T_w on left + phase change
- Benchmarked against classical LBM and analytic solutions

Quantum Monte Carlo

- Monte Carlo (MC) methods use randomness to estimate complicated systems using repeated sampling
- Can improve runtime quadratically using amplitude estimation
  - Generalization of Grover's algorithm
- Nature of quantum computing allows for easy incorporation of these methods





$P(x1, x2, x3) = 0.5 * x1 + 0.25 * x2 + 0.25 * x3$

- Unitary operation $W|x\rangle|0\rangle = |x\rangle\left(\sqrt{1-\phi(x)}|0\rangle + \sqrt{\phi(x)}|1\rangle\right)$ to assign target qubits
- Repeated for successive target qubits
- Use amplitude estimation to increase accuracy
- Qubits are fully integrated into the larger circuit and are initialized and measured at the same time