Lattice Boltzmann Inspired Quantum Walk for Solving PDEs

Quantum Enhanced Verified Exascale Computing

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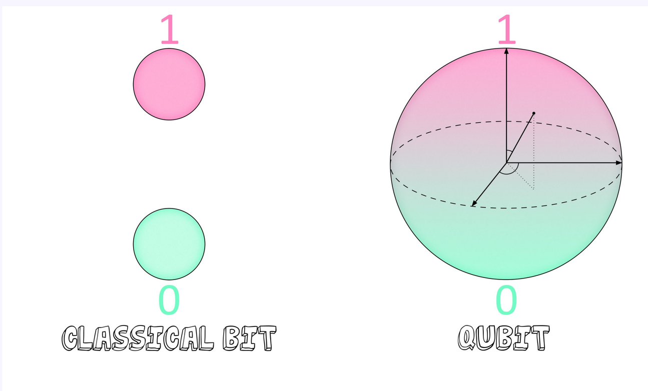
Problem

- Efficiently solving Partial Differential Equations (PDEs) holds potential for substantial scientific advancements across various disciplines.
- This work aims to create a quantum algorithm involving a quantum walk for solving PDEs in a fluid dynamics context. We seek an algorithm applicable on practical quantum computers.
- The algorithm being currently developed is inspired by Lattice Boltzmann methods, and aims to simulate families of PDE, enabling parameter tuning to match desired PDEs.

Quantum Computing

Quantum computing uses quantum bits (qubits) to process information, which can exist in superpositions of 0 and 1 and exhibit entanglement. Quantum gates manipulate qubits, enabling parallel processing and potential exponential speedup for certain problems [1].



Neutral Atom Arrays (Strathclyde)

Quantum SPH paper

The algorithm developed must be applicable on practical quantum devices, such as the SQuAre neutral atom array being developed at Strathclyde. Another quantum algorithm for fluid dynamics is being developed by the QEVEC team based on Smoothed Particle Hydrodynamics.

Lattice Boltzmann Methods

- We define the **Navier Stokes Equation**:

$$\rho\frac{d\vec{V}}{dt} = -\nabla p + \rho\vec{g} + \mu\nabla^2\vec{V}$$

- Lattice Boltzmann methods computationally simulate fluid dynamics and complex phenomena. Instead of solving Navier-Stokes equations directly, they discretize space and time into a lattice [2].
- Particles collide and propagate using simplified kinetic equations.
- **Both discrete time quantum walks and Lattice Boltzmann methods employ collision and streaming steps on a lattice.**

Discrete Time Quantum Walks (DTQW)

- DTQWs embody quantum evolution in discrete intervals, enabling superposition of states, unlike classical walks.
- The process involves a quantum particle carrying a multi-state quantum system for the coin. The coin toss is effected by a unitary operator [1].

We define the **evolution of a discrete time quantum walk** as [3]:

$$|\Psi_t\rangle = \mathbf{U}^t|\Psi_0\rangle \quad \text{where} \quad \mathbf{U} = \mathbf{S}(\mathbf{C}\otimes\mathbf{I})$$

The system evolves in discrete time steps. Each step involves a quantum coin operation (**C**) and a conditional shift (**S**) based on the coin's outcome. An example of the 1D DTQW shift and coin operators are:

$$\mathbf{C} = \frac{1}{\sqrt{2}}\begin{bmatrix} cos(\theta) & sin(\theta) \\ sin(\theta) & -cos(\theta)\end{bmatrix}$$

$$\mathbf{S}\,|\uparrow\rangle\langle\uparrow|\otimes\sum_i |i+1\rangle\langle i| + |\downarrow\rangle\langle\downarrow|\otimes\sum_i |i-1\rangle\langle i|$$

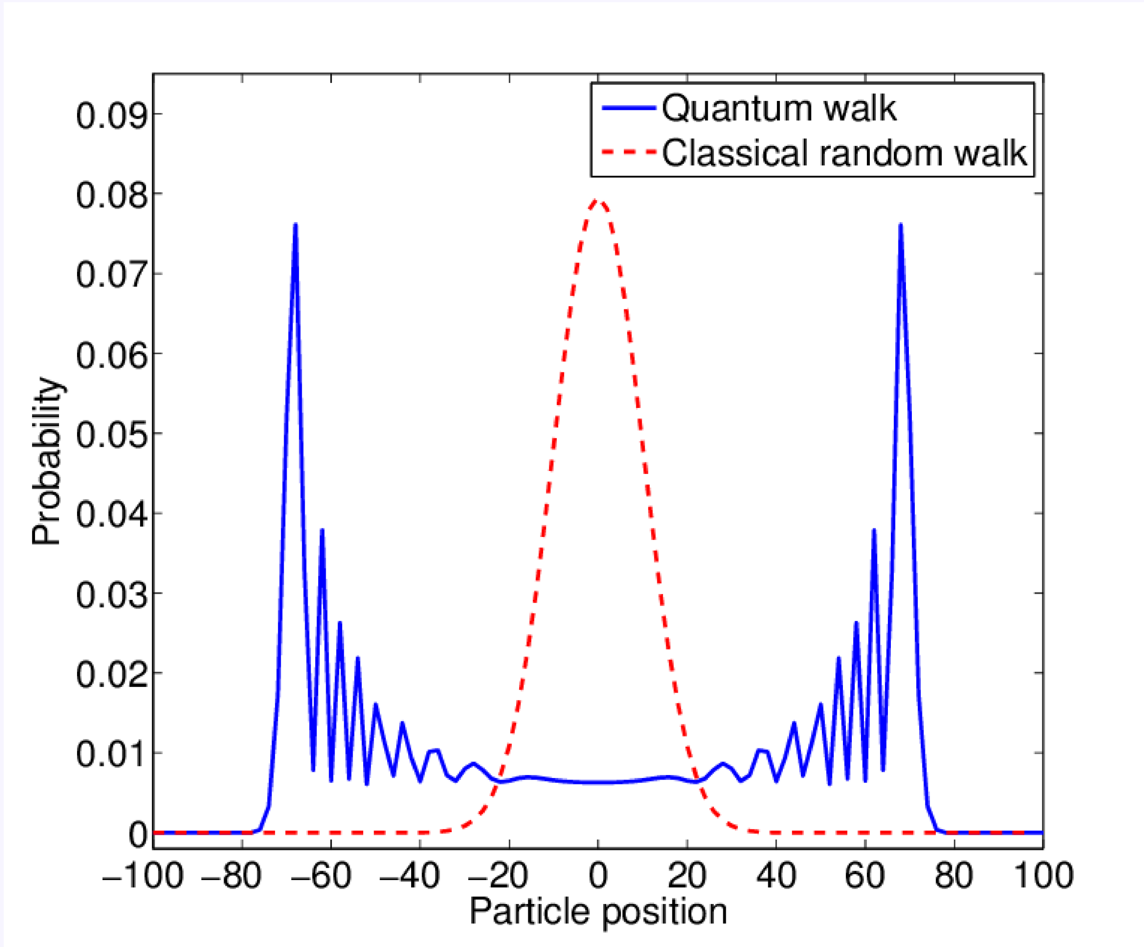


Figure 1: D2Q9 Lattice

- DTQWs discretely approximate continuum equations. E.g, the continuum limit of a simple 1D walk is the 1D Dirac equation.
- The coin operator's parameters determine the system's dynamics and the resulting family of differential equations in the continuum.
- Tunable coin parameters offer degrees of freedom to customise desired partial differential equations, and introducing nonlinearity is essential for simulating higher-order differential equations [3].

Lattice Boltzmann Inspired Quantum Walk

- A quantum walk may be performed on the same D2Q9 lattice used in Lattice Boltzmann, shown in Figure 2 [2].
- A D2Q9 walk involves a 9-dimensional coin operator.
- The quantum coin operator determines the family of simulated PDEs. Parameters in the coin facilitate user-adjustment for correct PDEs in the continuum limit.

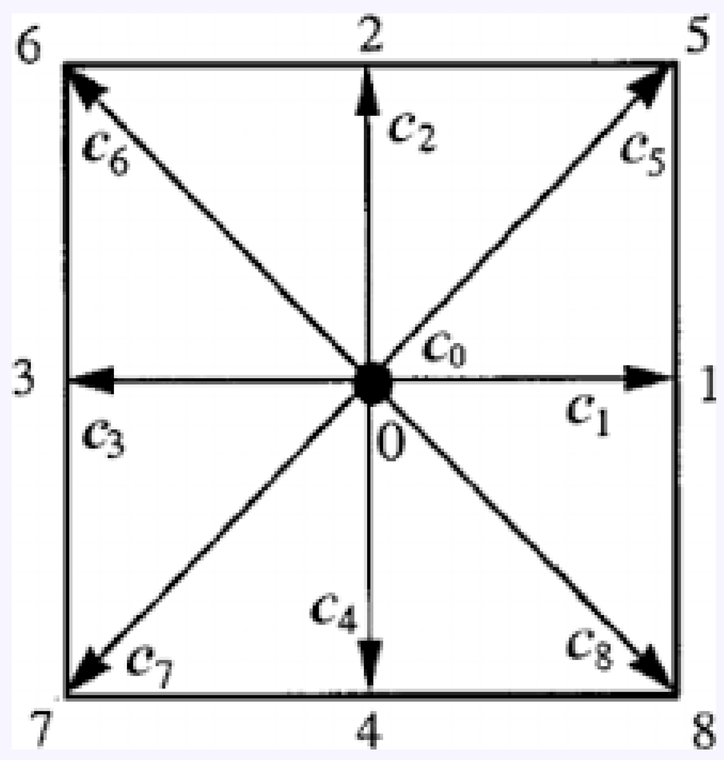


Figure 2: D2Q9 Lattice

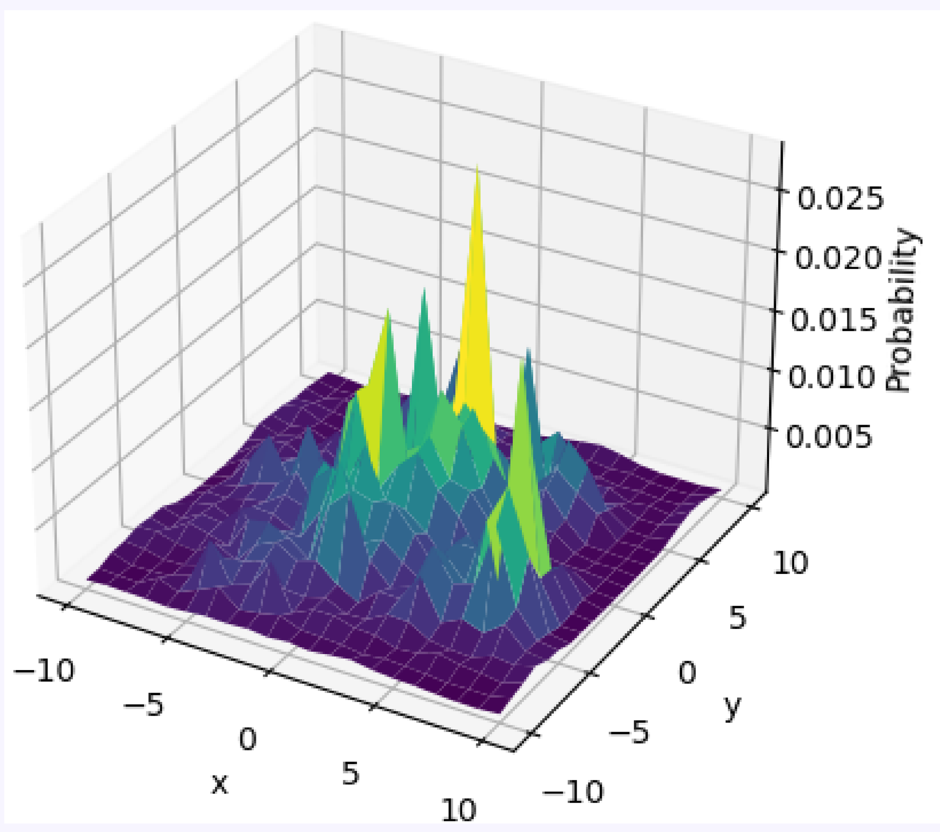


Figure 3: Simple D2Q9 walk with entangled coins

- We've successfully parameterised a 9-dimensional coin with Lattice Boltzmann dynamics. However, the non-linear relaxation term in Lattice Boltzmann must be integrated into the quantum walk.
- This non-linearity generates higher-order continuum equations, essential for a non-linear PDE solver. Efficiently incorporating this non-linearity while maintaining accurate dynamics is currently being explored.

References

[1] Lovett, N.B., Cooper, S., Everitt, M., Trevers, M. and Kendon, V., 2010. Universal quantum computation using the discrete-time quantum walk. Physical Review A, 81(4), p.042330.
[2] Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G. and Viggen, E.M., 2017. The lattice Boltzmann method. Springer International Publishing, 10(978-3), pp.4-15.
[3] Mlodinow, L. and Brun, T.A., 2018. Discrete spacetime, quantum walks, and relativistic wave equations. Physical Review A, 97(4), p.042131.