Potential Applications of Quantum Computing in Pore Scale Modeling

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Executive Summary

Pore scale modeling can be seen as a tool to implement governing physics of fluid flow and particle transport on a microscopic level as the basis of understanding macroscopic systems.

Due to the vast number of thermodynamic, physio-chemical, and mechanical variables, pore scale modeling approaches are either too abstract to be representative or too computationally expensive.

Quantum Computing in conjunction with pore scale modeling is a fast developing and very promising route with a few examples of how to revolutionize computational efficiency.

Leveraging quantum mechanical effects, natural fluid flow and particle transport might be suitable candidates for quantum simulations.

Current quantum computers are too error prone and impractical to use in every day's simulation efforts, but the field is fast growing.

Problem Statement

Three major challenges of today's society are ensuring energy sustainability, security, and affordability for a growing population.

To overcome these challenges, models need to incorporate governing physics from the smallest scale to be representative in upscaling efforts to larger, more distinct scales.

Continuum scale reservoir modeling does not capture microscopic fluid flow behavior, simplifies flow assumptions, and averages key rock properties over grid cells.

Current techniques in pore scale modeling with conventional computing such as Pore Network Modeling (PNM), Direct Numerical Simulation (DNS) with Stokes equations, or DNS with the Lattice Boltzmann Method (LBM) are either too abstract or too computationally expensive.

Solids Precipitation Modeling

The formation and precipitation of solids in porous media alters key rock property parameters and their relationships such as permeability and porosity by creating barriers to fluid flow.

This reduces the injectivity of reservoirs in the near-wellbore zone, and is responsible for bypasses throughout the reservoir.

Quantum computing could help in modeling and understanding quantum interaction of fluid-solid interfaces and aid in testing underlying hypotheses of solids precipitation on the pore scale.

Potential applications of solids precipitation modeling include:

- Gas Hydrate formation
- Geothermal applications with insitu mineral precipitation
- Carbon Capture and Storage (CCS) modeling with mineralization over large time scales requiring huge computational power (tens of thousands of years)

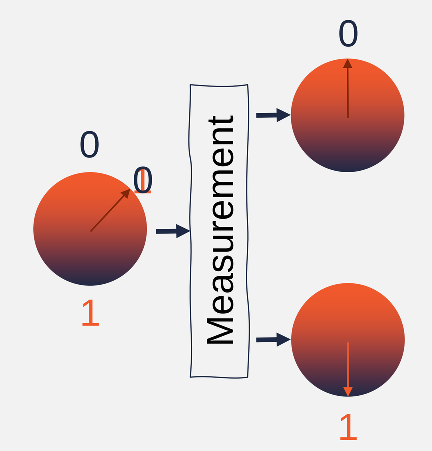
Introduction to Basic Concepts of Quantum Computing

Spinning Coin

What does a spinning coin show while spinning: Heads or tails?

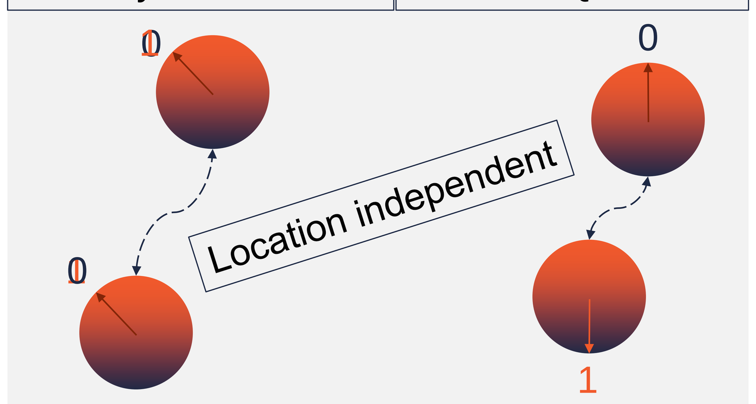
Principle of Superposition

Classic Bits	Quantum Bits
Either 0 / Or 1	(diagram below)



Principle of Entanglement

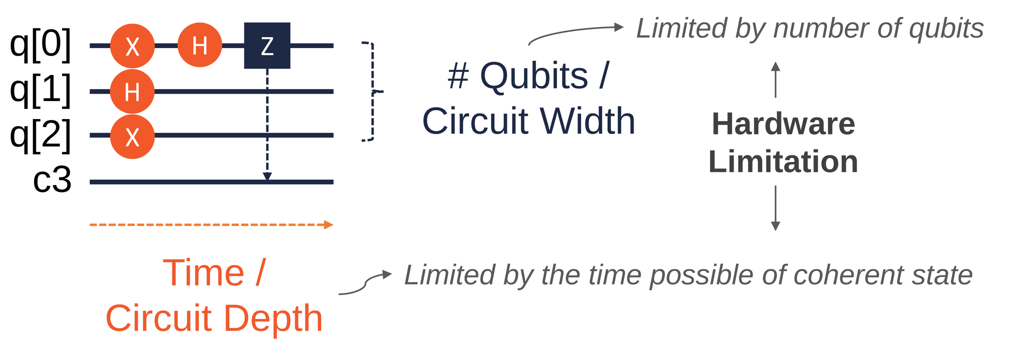
Both in indeterminate state separated by any distance	Measuring Qubit 1 gives information about Qubit 2



Example on 2-Bit System

Classic Bits	Quantum Bits
Possible States	Possible States
0 0, 0 1, 1 0, 1 1 (I, II)	I → a *00; II → b *(01+10); III → c *(01-10); IV → d *11
Need 2 classic bits of information; 2*n classic bits **linear** increase	Need 4 classic bits of information; 2^n qubits **exponential** increase

Quantum Circuit



- Quantum algorithms are called Quantum Circuits
- The number of qubits represent the circuit width (vertically)
- The time progression is the circuit depth (horizontally)
- Qubits are modified by gates acting on one or more qubits

Basic Quantum Notation / Quantum Gates

Ground state (Value 0): $|0\rangle = \binom{1}{0}$

Value 1: $|1\rangle = \binom{0}{1}$

- Gates manipulate quantum state similar to classical computing
  - For example: Pauli-X Gate is similar to NOT Gate and swaps Value 0 to Value 1, or vice versa

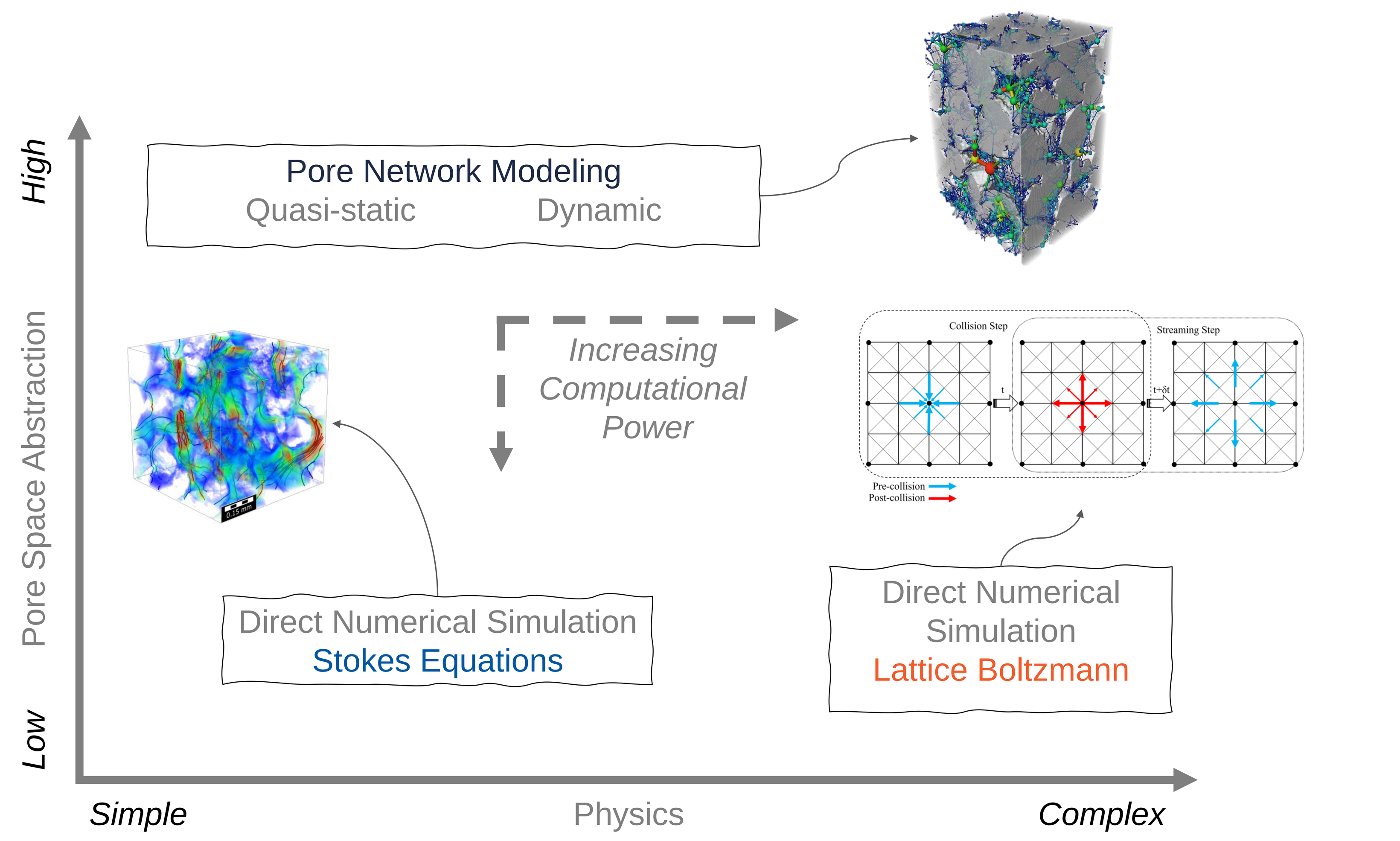
Operating Conditions of QCs

- To achieve the ground state, system conditions are ~15 mK and almost zero atmospheric pressure
- Quantum computers are insulated from external influences (including Earth's magnetic field) to minimize errors, and operated with conventional computers
- QC's operate at very short intervals of time (coherent state)
- Current best QC: IBM Osprey (433 qubits); Qiskit Runtime Kernel

Quantum Computing in the Framework of Pore Scale Modeling

Pore Scale Modeling as the study of fluid flow and transport phenomena in porous *materials* such as reservoir rocks at the microscopic scale (µm) needs to compromise with computational power and the desired complexity of physics simulated.

The **more complex** the physics get, the **greater** the computational power
The **less abstract** the pore space gets, the **greater** the computational power



Quantum Computing shows potential applications in:

- Optimization problems
  - Optimal design of porous materials (e.g., filters)
- Reconstruction of porous media
  - Segmentation improvement
- Advanced sensing and imaging enhancements
- Quantum-enhanced machine learning algorithms for predictions
- Simulating particle and fluid transport
  - Quantum transport in nanoscale pores (below resolution)
- Simulating quantum effects in multiphase, reactive flow
  - Quantum interactions of fluid-fluid and fluid-solid interface

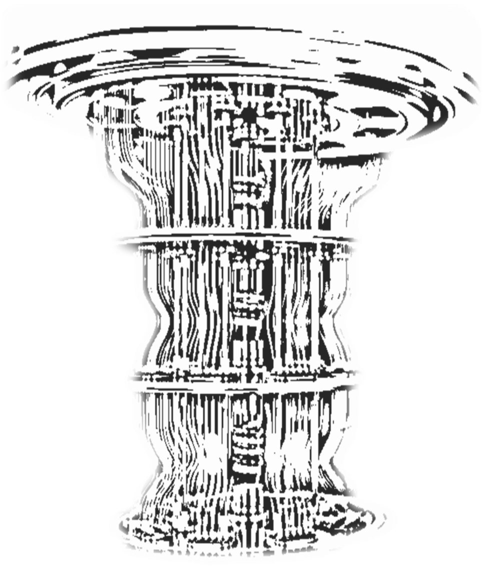
Probably in every step of the Digital Rock Physics workflow including imaging, processing, segmentation, and simulation, Quantum Computing can aid either by increasing the computational speed, applying quantum effects, or enhancing existing pore scale modeling techniques.

Simulating natural phenomena including the behavior of fluids and particles in porous systems can be described with quantum physics and quantum mechanics – Quantum Computers have the unique ability to harness these effects and, therefore, show the potential of revolutionizing pore scale modeling.

This gives fundamental physics insights in pore scale phenomena, fluid flow, transport of particles, and reactions.

Challenges and Future Directions

- Develop practical and scalable quantum computers
- Development of error correction techniques and quantum stability
- Development of quantum algorithms and integration with "traditional" pore scale modeling techniques
- Energy concerns for creating QC working conditions such as cooling to almost absolute zero (15mK)



Concluding Remarks

Quantum Computing shows immense potential in advanced pore scale modeling by leveraging quantum mechanical effects and, thereby, mimicking nature.

The potential applications are numerous; from advanced fluid flow and particle transport simulation, to porous media characterization and manipulation, to quantum machine learning and optimization.

Leading into a new era of computational efficiency, quantum computing in pore scale modeling might be able to account for the vast number of variables required and bridge the gap of simulating multiphase fluid flow and reactive transport.

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