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# Potential Applications of Quantum Computing in Pore Scale Modeling

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The three major concerns of today's society that relates to the energy sector are sustainability, security, and affordability for a growing population. Tackling the challenges that come along with that, requires a multiscale approach where modeling results incorporating the governing physics from the smallest scale can be translated into larger, more distinct scales to understand macroscopic systems. The tool of choice to predict the underlying microscopic behavior of multiphase fluid flow in porous media is pore-scale modeling. The vast number of variables that describe chemical, thermodynamic, and mechanical effects between fluids as well as the fluids-solids interactions require computationally very expensive simulations that may take months even with cutting-edge high-performance computing. This problem raises the question if classical computers are suitable for these kinds of simulations or if other, faster computing systems might be applicable. In the last two decades, theoretical concepts describing the use of quantum computing to simulate natural phenomena have been developed and the first quantum computers have been created. In contrast to classical computers that rely on a binary system for computation and data transfer, i.e., classical bits that can either be zero or one, quantum computers make use of quantum mechanical effects such as superposition and entanglement that potentially increase the computational efficiency exponentially. Superposition means that rather than zeros and ones, bits in quantum computers, so-called qubits, can have a linear combination of both different states at the same time based on a probability-related concept of amplitudes. The second important concept is entanglement, which describes the close correlation of two quantum particles to each other independent of their location which makes it possible to mathematically compute the value of one entangled qubit by knowing the value of the respective other one. This becomes important in describing the working principle of quantum computers and how we can translate the computation results into our classical understanding for interpretation. These quantum mechanical effects are primarily responsible for the exponential increase in computational power with respect to classical computers by two to the power of n qubits (2^n). For example, to describe one of the four distinct states of a two-bit system such as 00, 01, 10, and 11, we would need the values of two classical bits, the first one to the left and the second one to the right. In order to describe the same states quantum mechanically with two qubits, we would need four values instead of two because of the principles of superposition and entanglement: a*00, b*(01+10), c*(01-10), d*11, where a, b, c, and d are coefficients. Therefore, two qubits contain four classical bits of information. This presentation introduces quantum computers and their potential applications and pitfalls concerning pore-scale modeling. It highlights methods of solving complex partial differential equations such as the Navier Stokes equation as well as discrete modeling with the Lattice Boltzmann Method quantum mechanically. Particular emphasis is made to the applicability of quantum algorithms to study solids precipitation during fluid flow in porous media with carbon sequestration applications.

## Participation

In-Person

## References

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