Lattice-Gas Quantum Computing*
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1 Objectives

It is well known that the exponential growth in computing power over the last fifty years has accurately followed Moore's Law (i.e. memory doubling every 18 months). Hence, by the about year 2020, the industry's standard should be atomic-scale computation (erasing a bit 1 nanometer in size should dissipate only 1 $k_B T$). Manipulating information at this small scale requires a new computing paradigm based on quantum mechanics: *quantum computing* [1, 2, 3, 4, 5, 6, 7]. In existing prototype quantum computers (NMR machines), information is stored on spin-$\frac{1}{2}$ atomic nuclei [8, 9, 10, 11]. The machine architecture uses no wires, no conventional processors, and no heat sinks (when running reversible algorithms). The "computational substrate" is a liquid and each "computational engine" is contained within a single molecule.

Several fundamental questions are raised: (1) What type of physical exploration, achieved by simulation and modeling, is possible using quantum computers? (2) Are there really vast computational resources arising from quantum superposition? (3) And, what are the quantum generalizations of

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the areas of classical universal logic, communications, factoring and search algorithms, error correction, and control theory? Many theoretical physicists, over the past several years, have focused on aspects of question No.3 [12, 5, 13, 14]. Many experimental physicists have more recently considered No.2, building prototype single-gate quantum computers as a first step [8, 9, 10, 11]. The primary objective of my lattice-gas research (task 2304CP initiated in 1992) has been to answer No.1 [15, 16, 17]. In addition, the objective of my quantum computing research (task 2304TD) is to address the second question given that we now have certain answers to the first [18].

Specifically, we have a quantum algorithm to simulate the many-body Schrödinger equation [19, 20, 21, 22] and, more practically, a quantum algorithm to simulate a Navier-Stokes fluid on a network of small quantum computers [15]. I stress the importance of the latter not only because CFD is very relevant to the USAF modeling and simulation community, but because of the present day feasibility of constructing a network of small quantum computers. In collaboration with D. Cory and R. Nelson at the MIT Francis Bitter Magnetic Lab, our objective is to build the first quantum computer network (presently, we have designed an NMR quantum computer array and expect to test a 1D prototype) [18].

2 Status of Effort

Traditional approaches to complex fluid simulation include "low-level" molecular dynamics (MD) and "high-level" partial differential equation (PDE) schemes. MD suffers from insufficient spatial and temporal scales to model hydrodynamic scale behavior adequately. PDE schemes suffer from numerical instabilities, coarseness in the physical description and in most cases a lack of knowledge of the correct effective field theory to describe a complex fluid. We have focused on lattice-gas schemes, a "mid-level" approach achieving greater scales than MD while possessing unconditional numerical stability. Due to its underlying physics-like microscopic dynamics, lattice gases capture all relevant physics at the macroscopic scale without specifying an effective field theory a priori. Our fluid models not only obey the conservation laws (conserving mass, momentum, and energy) but they also obey the Second Law of Thermodynamics (which drives the system towards thermal equilibrium by increasing entropy). Most high level PDE descriptions of fluids obey the conservation laws but not the Second Law, and failing to do so gives rise

to their numerical instabilities. Reversible lattice-gas algorithms are specially suited to quantum computers and provide a way of "discretizing PDEs" and modeling complex physical behaviors on quantum computers. The most well understood lattice-gas algorithms apply to the simulation of Navier-Stokes fluids [23, 24, 25, 26, **?**, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41] and complex fluids (immiscible binary liquids and microemulsions) [42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55]. Lattice-gas algorithms are also known for electromagnetic waves and magnetohydrodynamics. The only data operations used in quantum lattice-gas algorithms are reversible *permutations* and *superpositions* [16] (the latter is based on the principle of quantum mechanics known as the superposition of states). These operations can be realized with a NMR quantum computer network.

3 Large Array of Small Quantum Computers

In the NMR machine, an ensemble of molecules ($\sim 10^{18}$) embodies a single "n-qubit quantum gate," which is mathematically represented by a unitary matrix in the group SU(n) (where n is a small number presently limited to be ≤ 12) that acts on n-qubits in a 2^n submanifold of the full Hilbert space. Since a laboratory liquid sample comprises an Avagodro number of molecules ($\sim 6 \times 10^{23}$) there are millions of quantum gates per mole (the sample can be partitioned into a "Bravais lattice" with a gate at each node of the lattice). In a large liquid sample (placed in the largest NMR machine at the MagLab), a 512^3 array of 12-qubit quantum gates can be accommodated (massive classical parallelism).

There are many benefits to using such NMR arrays. The computational medium is at room temperature (although surrounded by a supercooled superconducting magnetic) and the experimental apparatus is nearly "off-the-shelf" (costing about $150K in FY99 dollars). The large number of "identical" molecules per quantum gate gives a high signal-to-noise ratio when "reading" the quantum state of a gate (affecting about one in a trillion molecules of the gate). Since the atomic nuclei resonate at a unique Bloch frequency fixed by an externally applied magnetic field (like a top processing in a uniform gravity field), a uniform gradient in the field allows for spatial localization within the network. Individual qubits are differentiated by energy level splitting arising from magnetic dipole-dipole coupling within the molecule. This provides a means of "addressing" data within an individual

gate. Since each node (with a ~ 1 millimeter gate-size clocked at ~ 1 kHz) is effectively isolated from every other node (thermal diffusion of molecules in the liquid causes them to move about a micron every millisecond), quantum computation can be done independently and simultaneously across the entire network. This allows for homogeneous parallel computation of the particle collisions occurring at the nodes in the lattice. Furthermore, because of superposition of classical electromagnetic fields, multiple quantum computer nodes within the network can be simultaneously addressed. This allows for parallel computation of the particles' motion between the node-pairs (via transmission of classical information).

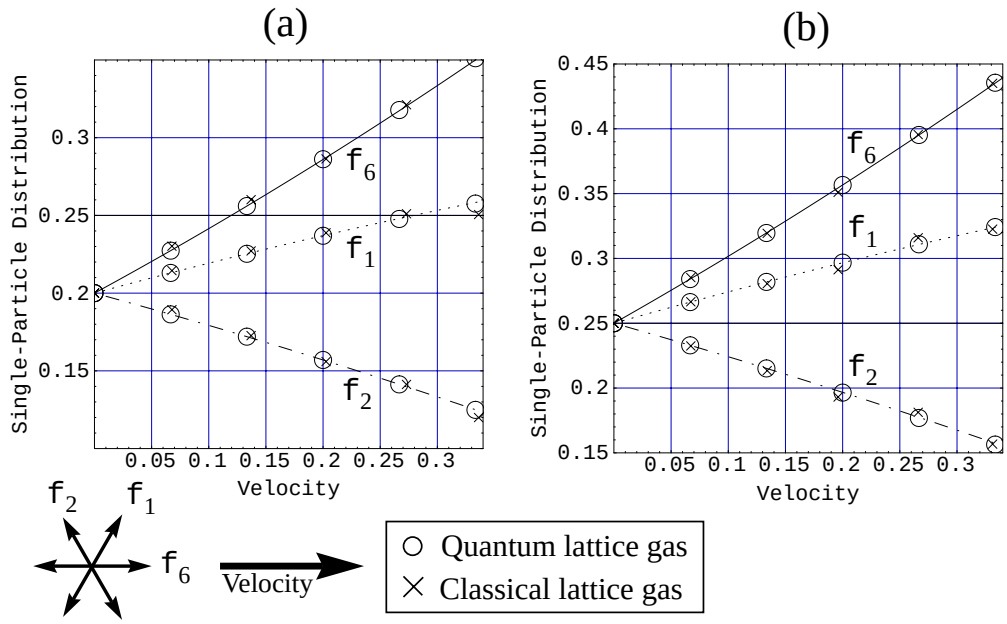

Figure 1: Theory vs. simulation comparison of the velocity dependence of the single-particle distribution function in the non-Galilean parameterization: $f_a = \langle\psi|\hat{n}_a|\psi\rangle = d + dD\hat{e}_a \cdot \vec{v} + gdD(D/2+1)\hat{Q}_a : \vec{v}\vec{v}$ (see ref. [16]). FHP simulation data is overplotted on this predicted mesoscopic distribution function. Plots (a) and (b) are for background densities of $d = 0.20$ and $d = 0.25$, respectively. A velocity shift is imparted along the x-axis; that is, along the f_1 direction indicated in the figure. Data was collected from a 128×128 classical FHP simulation (crosses) and coarse-grained averaged over 1600 time steps from time step $t = 400$ to $t = 2000$ and collected from a smaller 32×32 quantum FHP simulation (circles) measured at a single time step at $t = 200$.

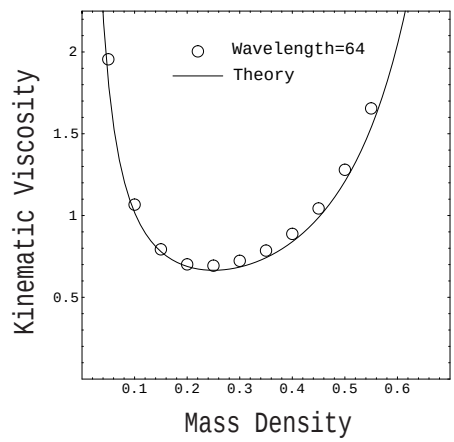

Figure 2: Kinematic shear viscosity of a quantum FHP lattice-gas simulation. "Calibration" test done on a 64×64 grid. The qubits are initially unentangled. The simulation is initialized with a "long-wavelength" sinusoidal perturbation on the momentum density field, equaling the system's grid size. The peak amplitude of an exponentially decaying shear wave is sampled every 4 out of 100 time steps. Simulation runs were carried out for a range of reduced background densities, form $d = 0.05$ up to $d = 0.55$. The particle-particle correlations are *not* neglected.

4 Quantum Lattice-Boltzmann Equation

My primary accomplishment has been to sort out the details for doing fluid dynamics simulation on a quantum computer (a special test case application of a general-purpose quantum-computing scheme). The algorithm requires only short-range and short-term quantum entanglement, which has already been demonstrated to work. (To be competitive with conventional computers, the other known quantum algorithms require millions of fully coherent entangled qubits, not likely to be experimentally realized in the near future). The crucial step is to reformulate the quantum wave equation (governing the evolution of the quantum computer's wavefunction, $|\Psi\rangle$) as a lattice-Boltzmann equation. In the Heisenberg picture, the network's evolution can be expressed using a unitary *streaming matrix*, $\hat{S}$, and a unitary *collision matrix*, $\hat{C}$, as follows

$$|\Psi(t+\tau)\rangle = e^{i\hat{H}\tau/\hbar}|\Psi(t)\rangle = \hat{S}\hat{C}|\Psi(t)\rangle. \tag{1}$$

Writing the Hamiltonian, $\hat{H}$, in (1) is done as a formality because only $\hat{S}$ and $\hat{C}$ are known. An essential idea is to define the probability of finding a

lattice-gas particle at position $\vec{x}$ moving in lattice direction a at time t by the following matrix element: $f_a(\vec{x},t) \equiv \langle\Psi(t)|\hat{n}_\alpha|\Psi(t)\rangle$, where $\hat{n}_\alpha$ is the number operator for the αth-qubit associated with the lattice vector $\hat{e}_a$ at the lattice node at position $\vec{x}$. If $\hat{S}$ is a permutation matrix (a unitary matrix with component values of 0 or 1), causing particles to hop between neighboring sites of the Bravais lattice (say from $\vec{x}$ to $\vec{x}+\ell\hat{e}_a$), then (1) can be rewritten exactly as the following lattice-Boltzmann equation [**?**]

$$f_a(\vec{x}+\ell\hat{e}_a, t+\tau) = f_a(\vec{x},t) + \langle\Psi(t)|\hat{C}^\dagger\hat{n}_\alpha\hat{C} - \hat{n}_\alpha|\Psi(t)\rangle. \tag{2}$$

The collision matrix $\hat{C}$, in separable tensor product form since it acts on each lattice node independently, causes local quantum entanglement of outgoing collisional configurations of the particles at each node.

On conventional workstations, I numerically simulated the lattice-Boltzmann equation (2) using various approximations (quantum Monte Carlo, a symbolic math solution using second-quantization formalism, and a scheme using wave-function collapse) [17]. I verified that detailed balance holds (see Figure 1) and that there is a damped shear mode in the long-wavelength hydrodynamic limit (see Figure 2) in the quantum lattice-gas system. The numerical results agree with the analytical predictions.

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