Quantum Computation as a New Paradigm for Simulating Physics

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Summary

Quantum computers are being developed in order to provide exponentially greater computational and storage capability. In light of this, the development of quantum algorithms to run on future quantum computers is necessary both for the optimal design of these quantum computers and to provide algorithms for use on the quatnum computers. In the course of developing these algorithms we have developed new programs which can run on classical computers and provide a new paradigm for computations necessary to solve important physics problems and those of other disciplines.

Introduction

Quantum computers are being developed in order to provide exponentially greater computational and storage capability. In light of this, the development of quantum algorithms to run on future quantum computers is necessary both for the optimal design of these quantum computers and to provide algorithms for use on the quantum computers. In the course of developing quantum computer algorithms we have developed new programs which can run on classical computers and provide a new paradigm for computations necessary to solve important physics problems and those of other disciplines. Among the most useful and most challenging of all computer applications are the Navier Stokes Equations (NSE) applied to turbulent flows interacting with complex bodies. We summarize new results of simulations of quantum computers solving Navier Stokes Equations flow dynamics over complex objects. Our approach is to simulate few qubit per node but many node quantum computers with classical communications between the nodes. Such quantum computers are termed Type II Quantum computers. Quantum computers that can compute classical physics systems using the operations of few qubit quantum computers at each node of the system and using inter node classical communications are discussed in [1] and [2]. In this paper the Navier Stokes equations were simulated by computation on a classical computer corresponding to that which could be calculated by Type II quantum computers. The theory is outlined and extended to turbulent flows about complex objects.

In addition we have developed new programs which simulate sound signals and perform mathematical quantum transforms on the signals resulting in lossy compression of the signals.

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Quantum Computation of Three Dimensional Navier Stokes Equations

In this section the 3-D quantum computation of the Navier Stokes Equation is developed. The compressible Navier Stokes Equations (NSE)

$$\rho(\frac{\partial u}{\partial t}+u\cdot\nabla u)=\mu\nabla^2 u-\nabla p+F \tag{1}$$

$$\frac{\partial\rho}{\partial t}+\nabla(\rho u)=0, \tag{2}$$

can be approximately represented by quantum field equations. The approach is to use quantum lattice gas formulations of one dimension [2], [3] and extend them to three dimensions with complex geometry and implement our novel method of boundary conditions. The quantum lattice gas computations can be written as the lattice Boltzmann collision expansion of the occupation probability function

$$P_a(\mathbf{x}+\Delta\mathbf{x},t+\tau)=P_a(\mathbf{x},t)+\Omega_a(\mathbf{x},t) \tag{3}$$

where the collision term is given by

$$\Omega_a(\mathbf{x},t)=\langle\psi(\mathbf{x},t)|\,(\widehat{U}\widehat{n}_a\widehat{U})-\widehat{n}_a\,|\psi(\mathbf{x},t)\rangle\,. \tag{4}$$

The Navier Stokes equations are recovered from the expansion of the quantum lattice Boltzmann equation and then by forming quantum moment equations from it. In general $\widehat{U}$ can be viewed as a block diagonal unitary matrix. The quantum wave function ket evolution operator for each site is given by

$$\left|\psi'(\mathbf{x},t)\right\rangle=\widehat{U}\,|\psi(\mathbf{x},t)\rangle \tag{5}$$

where the implementation we use below must satisfy constraints for each $i=1,2,3$ component as

$$\left|(a^i)^2\right|+\left|(b^i)^2\right|+\left|(c^i)^2\right|+\left|(d^i)^2\right|=1 \tag{6}$$

and

$$a^i c^{i*}+b^i d^{i*}=a^{i*}c^i+b^{i*}d^i=0. \tag{7}$$

Fluid dynamics can be constructed from creating nodes with on-site qubits where quantum computation using unitary operations take place and connecting them with classical communications. It is possible to model one dimensional fluid flow with as few as two or three qubits per node. Two qubits can model the Burgers equation and three qubits can model the one dimensional Navier Stoke Equation because it can include a pressure gradient[3]. In three space dimensions the i^{th} component three qubit unitary matrix operator is

$$\widehat{U}^i = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a^i & b^i & 0 & 0 & 0 \\ 0 & 0 & 0 & c^i & d^i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{8}$$

A key advantage of a quantum computer is that it is based on qubits (as opposed to bits) and exhibits 2^n computational complexity for n qubits and thus uses quantum superposition. The quantum superposition of states for each qubit ket is represented as

$$\left|q_a^i\right\rangle = \alpha_a^i \left|0\right\rangle + \beta_a^i \left|1\right\rangle . \tag{9}$$

This type of quantum computer implements quantum superposition by using on-site kets each of which are the direct product of the qubit kets. For a three qubit node $a = 0, 1, 2.$ The three qubit ket is

$$\left|\psi^i(\mathbf{x}, t)\right\rangle = \left|q_0^i\right\rangle \otimes \left|q_1^i\right\rangle \otimes \left|q_2^i\right\rangle . \tag{10}$$

Expanding, explicitly the three qubit ket becomes

$$\begin{aligned} \left|\psi^i(\mathbf{x}, t)\right\rangle = & \\ & \beta_0^i\beta_1^i\beta_2^i \left|111\right\rangle + \beta_0^i\beta_1^i\alpha_2^i \left|110\right\rangle + \beta_0^i\alpha_1^i\beta_2^i \left|101\right\rangle + \beta_0^i\alpha_1^i\alpha_2^i \left|100\right\rangle + \\ & \alpha_0^i\beta_1^i\beta_2^i \left|011\right\rangle + \alpha_0^i\beta_1^i\alpha_2^i \left|010\right\rangle + \alpha_0^i\alpha_1^i\beta_2^i \left|001\right\rangle + \alpha_0^i\alpha_1^i\alpha_2^i \left|000\right\rangle . \end{aligned} \tag{11}$$

The fine grained representation requires masses having different velocities to move between sites and interact by quantum unitary evolution in collisions. The m_0 mass does not move. The m_2^1 and m_1^1 masses move in the negative and positive x directions with velocity negative and positive one at each step. The m_2^2 and m_1^2 masses move on the negative and positive y directions with velocity negative and positive one. The m_2^3 and m_1^3 masses move on the negative and positive z directions with velocity negative and positive one.

In three dimensions the wave function ket governing the quantum properties is

$$\left|\psi(\mathbf{x}, t)\right\rangle = \left|\psi^1(\mathbf{x}, t)\right\rangle \otimes \left|\psi^2(\mathbf{x}, t)\right\rangle \otimes \left|\psi^3(\mathbf{x}, t)\right\rangle , \tag{12}$$

where

$$\left|\psi^i(\mathbf{x},t)\right\rangle = \left|q_0^i\right\rangle \otimes \left|q_1^i\right\rangle \otimes \left|q_2^i\right\rangle . \tag{13}$$

is the three dimensional wavefunction component ket. The three qubit ket evolution becomes

$$\left|\psi^{i\prime}(\mathbf{x},t)\right\rangle = \widehat{U}^i \left|\psi^i(\mathbf{x},t)\right\rangle = \tag{14}$$

$$\begin{pmatrix} \beta_0^i\beta_1^i\beta_2^i \\ \beta_0^i\beta_1^i\alpha_2^i \\ \beta_0^i\alpha_1^i\beta_2^i \\ a^i\beta_0^i\alpha_1^i\alpha_2^i + b^i\alpha_0^i\beta_1^i\beta_2^i \\ c^i\beta_0^i\alpha_1^i\alpha_2^i + d^i\alpha_0^i\beta_1^i\beta_2^i \\ \alpha_0^i\beta_1^i\alpha_2^i \\ \alpha_0^i\alpha_1^i\beta_2^i \\ \alpha_0^i\alpha_1^i\alpha_2^i \end{pmatrix} = \begin{pmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&a^i&b^i&0&0&0 \\ 0&0&0&c^i&d^i&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&1 \end{pmatrix} \begin{pmatrix} \beta_0^i\beta_1^i\beta_2^i \\ \beta_0^i\beta_1^i\alpha_2^i \\ \beta_0^i\alpha_1^i\beta_2^i \\ \beta_0^i\alpha_1^i\alpha_2^i \\ \alpha_0^i\beta_1^i\beta_2^i \\ \alpha_0^i\beta_1^i\alpha_2^i \\ \alpha_0^i\alpha_1^i\beta_2^i \\ \alpha_0^i\alpha_1^i\alpha_2^i \end{pmatrix} .$$

Fluid Properties

For the fluid evolution we define the density and the fluxes based on the geometry of the quantum gas lattice. Various schemes are possible and we have implemented several. The simulations generating the figures have been implemented using the following density and flux schemes. The density ρ is constructed from operations of the qubits and number operator, $\widehat{n}$,

$$\rho = \rho(q_0, \widehat{n}, q_i^1, \widehat{n}_i^{1j}) \tag{15}$$

The flux is determined from functions of

$$\rho v_x = -cf(q_i^1, \widehat{n}_i^1) \tag{16}$$

$$\rho v_y = -cf(q_i^2, \widehat{n}_i^2) \tag{17}$$

and

$$\rho v_z = -cf\left(q_i^3, \widehat{n}_i^3\right) . \tag{18}$$

Turbulence Solutions

The Navier Stokes solutions evolve from quantum lattice gas dynamics. Fig. 1 displays velocity streamlines and density shading in a rectangular box. Initial conditions were of some test particles static and some with momentum to upper right. Boundary conditions were reflective. After time evolution the display shows typical turbulent structures such as expansion and compression front and vortex dynamics. Other Navier Stokes calculations were of two and three dimensional flow over aircraft, and urban buildings.

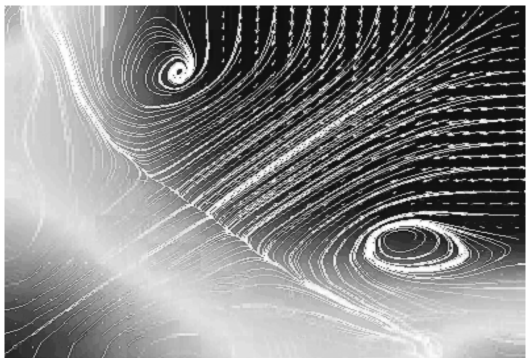

Figure 1: Simulation of Type II Quantum Computer Solving 2 Dimensional Compressible Navier Stokes Equation Flow as a function of time in a Box. Computed on a grid of 32 by 32 quantum nodes.

Quantum Sound Simulation

One can also use superpositions of Qubits to store and process signals such as sound [4]. The amplitude of the "signal" can be stored as the amplitudes of the of a superposed quantum state

$$\Psi = \sum \alpha_i \, |k\rangle_i \tag{19}$$

Where $|k\rangle$ is the eigenstate of Ψ. Ψ can be decomposed as a direct product of qubits $|q\rangle_1 \otimes |q\rangle_2 \otimes ... \otimes |q\rangle_N$ which compacts storage requirements by a factor of $\log_2$ a signal of size 2^N can be stored and operated on in N quantum bits. Mathematical transforms can also be performed on the quantum stored signal with the associated computational savings Fig. 2

Discussion

Computations simulating the solutions of the Navier Stokes Equations (NSE) on a Type II quantum computer were carried out on classical computers. Two and three dimensional NSE solutions to compressible flow with a variety of initial and boundary conditions were computed, e.g. Fig.1. It is important to note that the Quantum computer simulations produce turbulent fluid dynamics flow which is always numerically stable and therefore the simulations are important for use on classical computers as well as on quantum computers. The evolution by unitary operators prevents the numerical solutions from going unstable. It was shown that quantum Navier Stokes calculations can be made over arbitrary complex geometry and can produce turbulence. In additional problems the boundary conditions on complex geometries were calculated using a novel method that we will report elsewhere.

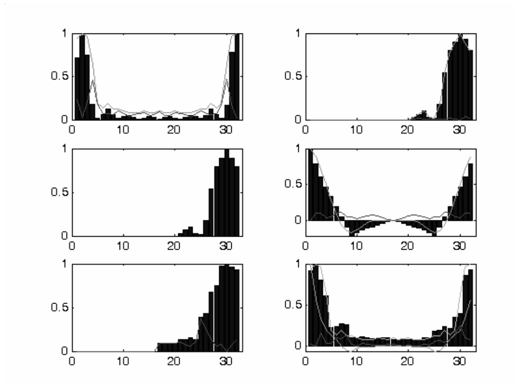

Figure 2: Section of 32 sound samples. Top Left Spectrum of single evaulations, Top Right Single evaluation of the signal. Middle Left input signal. Middle Right reconstructed signal quantum and classical. Bottom Left alternate evaulation of signal. Bottom Right alternate spectrum and reconstructed signal

It is shown that such quantum simulations can be made in the near term on quantum computers that can solve the Navier Stokes equations for flow over arbitrary geometry in three dimensions quadratically faster than can classical computers. The quantum computer processing of signals such as sound signals can be expected to be exponentially faster. The classical simulation of quantum algorithms also provides a stimulating and tantalizing picture into the future. It is perhaps surprising that algorithms designed to work on quantum computers can provide powerful paradigms for solving both new and unsolved classical problems better on classical computers.

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