Qubit Lattice Algorithms

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Abstract

Qubit lattice algorithms consist of a sequence of interleaved unitary collision-stream operators which in the continuum limit recover the differential equations of interest. QLA can be viewed as a generalized quantum random walk process. Some QLA simulations are presented for scattering of an electromagnetic pulse from a localized dielectric object. Comments are made on how to generalize QLA to handle dispersive and dissipative media as well as its application to a magnetized plasma-Maxwell system.

1 Introduction

Qubit lattice algorithms (QLA) [1-23] can be viewed as a cousin of the more familiar lattice Boltzmann scheme (LB) [24] to solve classical physics problems computationally in a more efficient manner than standard computational (CFD) codes. In particular LB algorithms for nonlinear fluid systems achieved important status because of the simplicity of the code and their inherent parallelization on classical supercomputers. In LB, the fluid equations are modeled by a truncated kinetic description in which the permitted phase space velocity is minimized subject to recovering the required fluid equations and retaining appropriate symmetries to leading order by Chapman-Enskog expansions. An immediate advantage of the LB approach is that the notorious computational headaches of resolving the nonlinear convective derivative for turbulent flows in the momentum equation, $\mathbf{v} \cdot \nabla \mathbf{v}$, is now replaced by a simple linear kinetic advection (streaming) term $\mathbf{\xi_i} \cdot \nabla f_i(\mathbf{x}, \mathbf{\xi_i}, \mathbf{t})$. $\mathbf{\xi_i}$ define the chosen discrete phase space lattice velocities. The fluid nonlinearities are recovered by incorporating quadratic algebraic nonlinearities into the LB collision operator. The initial collision operator was of BGK form $(f_i - f_i^{eq})/\tau$. The relaxation distribution function f_i^{eq} is a function of the macroscopic variables, and τ is a relaxation time. The very early LB algorithms were restricted to low Mach number and low Reynolds number flows. However a literal explosion of research in LB has moved the field into mutlispeed-lattices, multiple relaxation times, entropic LB, supersonic flows using adaptive space-time reference frame based on the actual local fluid velocity and temperature [25-27]

The QLA employs a non-commuting sequence of unitary collide-stream operators acting on a chosen qubit basis set as a mesoscopic model that recovers the equations of interest in the continuum limit. In the beginning, QLA's were introduced for the solution of the Schrodinger equation [1-3]. For quantum entanglement one requires at least 2 qubits/lattice site. The four on-site basis kets are

$$|0\rangle \otimes |0\rangle = |1000\rangle, \quad |0\rangle \otimes |1\rangle = |0100\rangle, \quad |1\rangle \otimes |0\rangle = |0010\rangle, \quad |1\rangle \otimes |1\rangle = |0001\rangle. \tag{1}$$

The unitary collision operator required to recover the kinetic energy operator in the Schrodinger equation is just the square-root-of-swap gate

$$U_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-i)/2 & (1+i)/2 & 0 \\ 0 & (1+i)/2 & (1-i)/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{2}$$

It is convenient to work with the 2×2 sub-block, C, entangling the on-site qubits $\{q_1, q_2\}$. C^2 is just the standard swap gate on these 2 qubits,

$$C^2 \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} (1-i)/2 & (1+i)/2 \\ (1+i)/2 & (1-i)/2 \end{bmatrix}^2 \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} q_2 \\ q_1 \end{bmatrix} \tag{3}$$

while $C^4 = \mathcal{I}$, the identity operator.

The unitary streaming operator S_1 simply shifts the amplitude of qubit q_1 at lattice site x to site $x + \delta$, while the transpose S_1^T shifts q_1 to lattice site $x - \delta$. Similarly for the shift operator S_2 acting on the qubit q_2. The operators U and S do not commute.

If one considers the following sequence of non-commuting unitary interleaved collision-streaming operators for a time advancement of Δt for the qubits q_1, q_2:

$$\begin{bmatrix} q_1(t+\Delta t) \\ q_2(t+\Delta t) \end{bmatrix} = S_2^T.C.S_2.C.S_2^T.C.S_2.C \cdot S_1^T.C.S_1.C.S_1^T.C.S_1.C \begin{bmatrix} q_1(t) \\ q_2(t) \end{bmatrix} \tag{4}$$

one recovers the free Schrodinger equation for the x-dependent wave function ψ determined from the zero moment of our mesoscopic qubit representation $\psi(x,t) = q_1(x,t) + q_2(x,t)$. The error is $O(\delta^2)$, provided we have diffusion ordering, with $\Delta t = O(\delta^2)$. If one had performed just two collide-stream operators on each qubit then the scheme would become just $O(\delta)$. By using the alternate-direction implicit (ADI) scheme for the y-direction and z-direction independently, we recover the full 3D free Schrodinger equation.

It is very interesting to realize that if the collide-stream operators commuted, then Eq. (4) simply degenerates into the identity evolution:

$$\begin{bmatrix} q_1(t+\Delta t) \\ q_2(t+\Delta t) \end{bmatrix} = \begin{bmatrix} q_1(t) \\ q_2(t) \end{bmatrix} \tag{5}$$

The non-commutation of the collide-stream operators is essential in our QLA in order to recover the desired equations of interest.

The effect of the potential energy term in the Schrodinger equation is readily modeled in QLA by the introduction of an external collision operator. In this way one can consider the scattering of a wave packet from an external potential well, or the 1D Nonlinear Schrodinger equation (NLS), or the 1D Korteweg-de Vries (KdV) equation. These last 2 problems are examples of nonlinear physics - and this poses a stumbling block for immediate application onto a quantum computer which is based on linear operator theory alone. However, both 1D NLS and 1D KdV are exactly soluble nonlinear equations – with solitons as solutions. In particular exact soliton-soliton collision solution provided excellent benchmarking for our QLA on classical computers, on which there are no problems handling the nonlinear terms.

We have extended QLA to both 2D and 3D NLS - now non-integrable equations that can give a mean-field theory for the evolution of a ground-state Bose-Einstein condensate (BEC) wave function. Very high precision QLA simulations were performed on quantum turbulence in these systems and their further generalization to spinor BECs. We achieved these results because QLA is ideally parallelized on classical supercomputers, with no degradation in parallel performance as the number of cores are increased. In particular, on the *IGM* BlueGene *Mira* supercomputer at Argonne, using OpenMP on a grid of 5120^3 we attained strong scaling of 94.1% as the number of cores were increased from a base of 65, 536 to 524, 288 and achieving 1.17 PetaFlops (runs performed in 2016).

In some sense, QLA can be viewed as an example of a quantum random walk process.

2 QLA for Plasma Physics

Recently we have turned our attention to QLA for electromagnetic wave propagation in plasmas. Our approach has been to consider Maxwell equations and progressively include plasma effects into the constitutive equations. Eventually this will move into including the plasma evolution equations for mass, momentum and energy along with the evolution equations for the Maxwell electromagnetic fields $\mathbf{E}, \mathbf{H}$. With constitutive equations (in a coordinate representation in which the Hermitian tensor dielectric $\boldsymbol{\epsilon}$ is diagonal) for an inhomogeneous non-magnetic medium

$$\mathbf{D} = \boldsymbol{\epsilon} \cdot \mathbf{E}, \quad \mathbf{B} = \mu_0 \mathbf{H}. \tag{6}$$

the Maxwell equations can be written in a unitary representation on discerning the required Dyson map [28] on a 6-qubit representation of the electromagnetic field,

$$\mathbf{U} = \left(n_x E_x, n_y E_y, n_z E_z, \mu_0^{1/2} \mathbf{H} \right)^T = \mathbf{Q} \tag{7}$$

where the refractive indices $\{n_x, n_y, n_z\} = \{\epsilon_x^{1/2}, \epsilon_y^{1/2}, \epsilon_z^{1/2}\}$.

For 2D x-y spatially dependent fields and media, the unitary Maxwell equations take the form

$$\begin{gathered}
\frac{\partial q_0}{\partial t} = \frac{1}{n_x} \frac{\partial q_5}{\partial y}, \qquad \frac{\partial q_1}{\partial t} = -\frac{1}{n_y} \frac{\partial q_5}{\partial x}, \qquad \frac{\partial q_2}{\partial t} = \frac{1}{n_z} \left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y} \right] \\
\frac{\partial q_3}{\partial t} = -\frac{\partial (q_2/n_z)}{\partial y}, \qquad \frac{\partial q_4}{\partial t} = \frac{\partial (q_2/n_z)}{\partial x}, \qquad \frac{\partial q_5}{\partial t} = -\frac{\partial (q_1/n_y)}{\partial x} + \frac{\partial (q_0/n_x)}{\partial y}
\end{gathered} \tag{8}$$

where $\mathbf{Q} = \{q_0, q_1, q_2, q_3, q_4, q_5\}^T$. In Fig. 1 we present QLA simulations of scattering of a 1D electromagnetic wave packet from a 2D elliptic dielectric cylinder.There are considerable number of internal reflections/transmissions into the vacuum region since there is a sharp (but continuous) spatial gradient in the refractive index near the boundary of the vacuum-dielectric region. In Fig 1a, we see the wave packet propagating in a diagonal direction and interacting with the dielectric whose major axis is parallel to the wavefront. We are looking from above, so that the dielectric region is shown in the middle of the figure. Since the refractive index within the dielectric, $n_2 = 2$, is greater than that in the vacuum, the phase velocity of the wave packet within the dielectric is less than in the vacuum and so is retarded within the dielectric. One also sees the reflected wave packet from the first interaction of the wave packet with the dielectric. At a later time, Fig. 1b, one sees a reflected wave packet back into the vacuum, a focusing of the wave packet within the dielectric as it approached the dielectric-vacuum boundary as well as portions of the wave packet in the vacuum affected by transmitted parts of the wave packet leaving the dielectric region into the vacuum. In Fig 2a and 2b show the pronounced internal reflections/transmissions

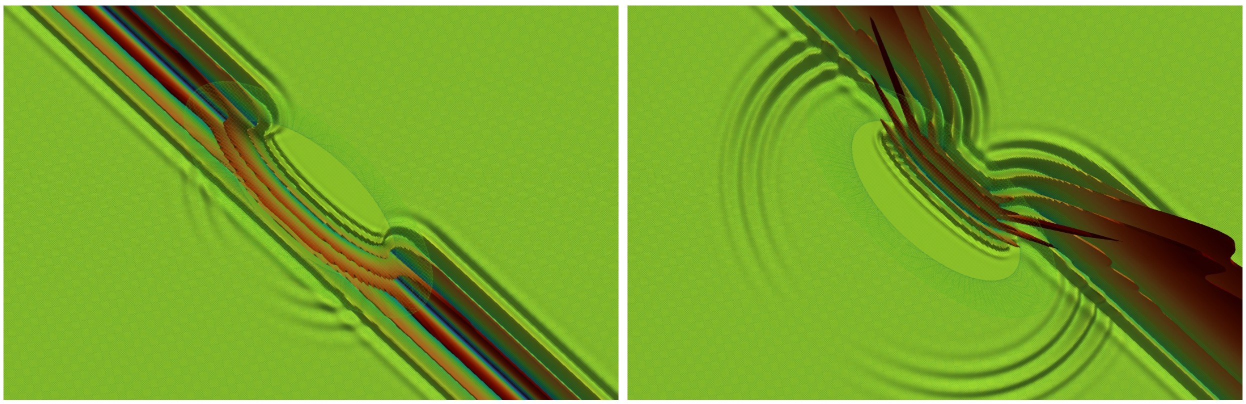

Figure 1: Top down view of a wave packet interacting with an elliptic dielectric cylinder. (a) The early stages of the reflected wave packet back into the vacuum as well as the penetration into the dielectric; (b) A slightly later time showing a focussing of the packet towards the front of the dielectric, and a well developed reflected pulse.

within the dielectric at even later times. It should be noted that QLA is an initial value algorithm. There are no internal boundary conditions imposed at the vacuum-dielectric interface. There are no Fresnel-like boundary conditions imposed, but the reflection and transmission wave fronts are self-consistently generated in QLA.

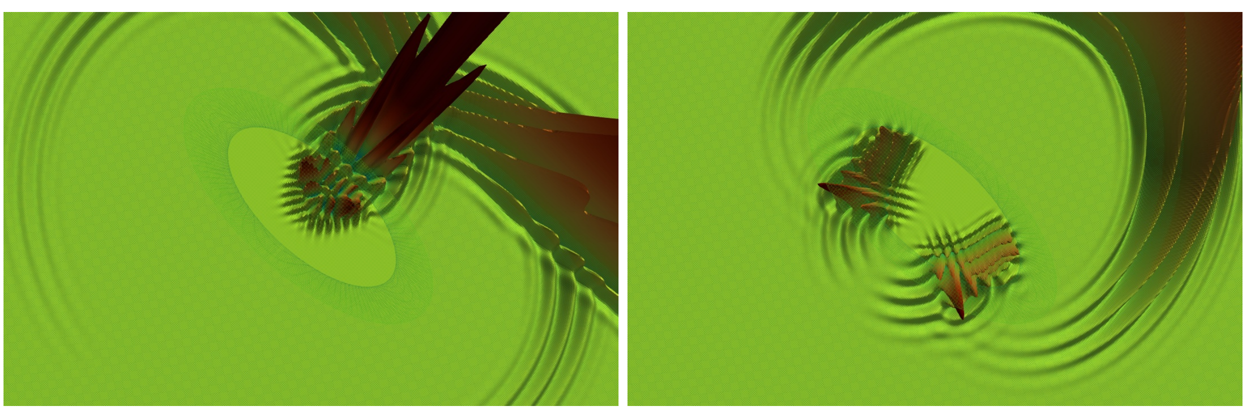

Figure 2: Top down view (a) Significant first reflected pulse back into the vacuum with the first reflected pulse within the dielectric and its transmission and constructive interference at the front of the dielectric ; (b) more complex wave front structures of the electric field.

2.1 QLA for Dispersive Media

The results presented here assumed the instantaneous (so-called "optical") response of the medium to the given electromagnetic field $\mathbf{u} = \{\mathbf{E}, \mathbf{H}\}^T$. Dispersion can be included in the constitutive equations by introducing the susceptibility kernel $\hat{G}$ [29]

$$\mathbf{d}(\mathbf{r}, t) = \hat{W}(\mathbf{r})\mathbf{u}(\mathbf{r}, t) + \int_0^t \hat{G}(\mathbf{r}, t - \tau)\mathbf{u}(\mathbf{r}, \tau). \tag{9}$$

Here $\mathbf{d} = \{\mathbf{D}, \mathbf{B}\}^T$, and $\hat{W} = diag(\boldsymbol{\epsilon}(\mathbf{r}), \mu_0)$. It is convenient to move to the high frequency limit in which the diagonal optical response reduces to that in a vacuum $\hat{W}_{vac} = diag(\boldsymbol{\epsilon}_0, \mu_0)$. The polarization of the medium is now incorporated into the integral kernel $\hat{G}$. The QLA will be unitary, but would now need to introduce extra qubits at each lattice site for the dynamics of the polarization and the handling of integrals of the form

$$\int_0^t \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-\tau)}}{\omega_e^2 - \omega^2} \mathbf{E}(\mathbf{r}, \tau) d\omega d\tau \tag{10}$$

where ω_e is a characteristic frequency of the medium.

2.2 QLA for Dissipative Media

The inclusion of dissipation into the plasma equations requires a fundamental change in the QLA representation. One method is to employ the techniques of quantum information science (QIS) when dealing with quantum system that interact with the environment. Such quantum systems are termed "open" systems since there is an energy exchange between it and the environment. However by considering the extended system of the dissipative quantum system and its environment one again recovers a closed system with energy conservation. This will then permit a unitary representation for the extended system.

The non-unitary time evolution of the open system takes the form [29]

$$i\frac{\partial \boldsymbol{\psi}}{\partial t} = [\hat{D}_0 - i\hat{D}_{diss}]\boldsymbol{\psi} \tag{11}$$

where $\hat{D}_0$ and $\hat{D}_{diss}$ are Hermitian. $i\hat{D}_{diss}$ is anti-Hermitian and represents the dissipation in the system. Thus

$$\boldsymbol{\psi}(\Delta t) = \hat{\mathcal{U}}(\Delta t)\boldsymbol{\psi}(0) = \exp\Big\{-i\Delta t[\hat{D}_0 - i\hat{D}_{diss}]\Big\}\boldsymbol{\psi}(0). \tag{12}$$

A first crude approximation is to apply the zeroth order-Suzuki-Trotter decomposition to Eq. (12)

$$\exp\Big\{-i\Delta t[\hat{D}_0 - i\hat{D}_{diss}]\Big\} = e^{-i\Delta t\hat{D}_0} e^{-\Delta t\hat{D}_{diss}} + O(\Delta t^2), \tag{13}$$

which neglects the effect of the non-commutation of $\hat{D}_0$ and $\hat{D}_{diss}$. This approximation, extremely common in QIS, permits the treatment of the non-unitary operator $exp[-\Delta t\hat{D}_{diss}]$ separately from the unitary operator $exp[-i\Delta t\hat{D}_0]$.

In QIS, one technique to handle the non-unitary operators is the introduction of Kraus operators $\hat{K}_\mu$ for the evolution of the open system density matrix ρ_S

$$\rho_S(t) = \sum_\mu \hat{K}_\mu \, \rho_S(0)\hat{K}_\mu^\dagger. \tag{14}$$

The individual Kraus operators are arbitrary, but subject to the sum constraint be unitary:

$$\sum_{\mu} \hat{K}_{\mu}^{\dagger}\hat{K}_{\mu} = \mathcal{I}. \tag{15}$$

By defining the Kraus operator $\hat{K}_0$

$$\hat{K}_0 = exp\{-\Delta t \hat{D}_{diss}\} \tag{16}$$

and introducing a second Kraus operator $\hat{K}_1$ such that $\hat{K}_1^{\dagger}\hat{K}_1 = \mathcal{I} - \hat{K}_0^{\dagger}\hat{K}_0$ one can extend to a higher dimensional Hilbert space (which in QIS is called a dilation) in which the dilation operator $\hat{\mathcal{U}}_{diss}$ is unitary

$$\hat{\mathcal{U}}_{diss} = \begin{bmatrix} \hat{K}_0 & -\hat{K}_1^{\dagger} \\ \hat{K}_1 & \hat{\mathcal{X}}\hat{K}_0\hat{\mathcal{X}} \end{bmatrix}. \tag{17}$$

The operator $\hat{\mathcal{X}}$, is an appropriate extension of the Pauli $\hat{X}$ operator to the appropriate dimensionality.

2.3 QLA for Plasma-Maxwell System

To develop a QLA to simulate directly the nonlinear two fluid plasma equations for mass, momentum and energy is not at all straightforward. Extending the work of Meng & Yang [30], one may utilize the Madelung transformation on the 3D NLS BEC equation (known in condensed matter at the Gross-Pitaevskii equation) for the scalar wavefunction ψ:

$$\psi = \sqrt{\rho}\, e^{i\phi}. \tag{18}$$

One can immediately identify $\rho = \sqrt{\psi^{*}\psi}$ as the fluid density, and $\mathbf{v} = -\nabla\phi$ as the fluid velocity. The scalar BEC equation for ψ can be rewritten in the form of fluid conservation equation of mass, momentum and energy, not unlike the compressible Navier-Stokes system. The major difference between the quantum NLS equation and the classical Navier-Stokes system is the addition of an extra quantum pressure term in the momentum equation and the fact that for scalar NLS quantum vorticies are singular, with $\rho \to 0$ at the vortex core. A classical vortex, on the other hand is non-singular. To remove these quantum irregularities, Meng & Yang achieve extra degrees of freedom by moving to a quaternion representation of the qubit fields whose zeroth moment yields the wave function, and thereby remove the quantum pressure term and singular vortices.

It seems very worthwhile to extend this approach to spinor BECs, with the Hamiltonian augmented to incorporate the electromagnetic field. We already have very well benchmarked and parallelized QLA's for spinor BECs and separate QLA's for Maxwell equations.

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