

Simulation of the Burgers equation by NMR quantum information processing

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We report on the implementation of Burgers equation as a type-II quantum computation on an NMR quantum information processor. Since the flow field evolving under the Burgers equation develops sharp features over time, this is a better test of liquid state NMR implementations of type-II quantum computers than the previous examples using the diffusion equation. In particular, we show that Fourier approximations used in the encoding step are not the dominant error. Small systematic errors in the collision operator accumulate and swamp all other errors. We propose, and demonstrate, that the accumulation of this error can be avoided to a large extent by replacing the single collision operator with a set of operators with random errors and similar fidelities. Experiments have been implemented on 16 two-qubit sites for eight successive time steps for the Burgers equation.

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It has been suggested that some classical computational problems can be solved by using a hybrid classical quantum device, a type II quantum computer [1, 2]. Such a device is essentially an array of small quantum information processors (QIP) sharing information through classical channels. NMR has proven to be a useful testbed for QIP, and in particular we have shown that a lattice of parallel QIPs can be mapped onto a spin system by creating a correspondence between the lattice sites and spatially distinct spin ensembles. A first proof-of-concept for numerically predicting the time-dependent solution of classical partial differential equation with dissipative terms using our NMR technique was demonstrated for the diffusion equation [3, 4].

One of the most important challenges to implementing a useful type-II quantum architecture is to avoid the accumulation of systematic errors. In the NMR implementations to date there are two important sources of systematic errors: (1) a linear approximation relating the excited magnetization to the Fourier components of the shaped RF pulse; and (2) errors from the repeated collision operators. Here we explore the impact of these errors on a simple computation and illustrate a simple means of reducing the accumulated error.

The ensemble nature of the spin system allows us to split the sample into a spatial array of lattice sites. Well developed methods from magnetic resonance imaging (MRI) allow us to selectively address the spins in each of these sites. Typically the addressing is carried out in a space reciprocal to the spatial mapping, called k -space, where k is the wave-number of the corresponding Fourier components. The k -space formalism [5] provides a recipe for writing a spatially varying spin rotation across an ensemble of spins that have been distinguished from each other by a magnetic field gradient. The k -space formalism is essentially the application of shaped radio frequency (RF) pulses in the presence of a linear magnetic gradient field as a means of exciting selective frequencies. For most studies the full k -space formalism is not employed and a linear approximation is invoked. If

the rotation angle of the shaped pulse is small, then the excited magnetization may be accurately calculated only to first order in that angle, and the excited magnetization is related to the RF waveform simply by a Fourier transform. As a result, the required RF waveform can also be determined by taking the inverse Fourier transform of the desired initial magnetization. This technique allows us to encode arbitrary magnetization profiles spanning the various spatial locations in our experiment and thereby approximating any desired initial conditions. In the previously implemented diffusion equation, higher order Fourier components of the number density are attenuated by the dynamics and the solution is stable even in the presence of substantial accumulated errors.

To push the development of type-II implementations we have chosen to explore the nonlinear Burgers equation to test the breakdown for the Fourier approximation. Over time, a shock front forms and high spatial frequencies in the magnetization profile become important and it is these high spatial frequencies that we expect to be most sensitive to errors. The numerical treatment of the QLG algorithm for the Burgers equation [6] therefore offers a stronger proof of our NMR quantum computing approach since the effect of the nonlinear convective term in the equation generates a sharp edge as a shock develops in time that is not mimicked by spin relaxation, random self-diffusion, nor RF inhomogeneities. In addition, we demonstrate shock-formation driven by a tunable viscosity parameter to show that the width of the shock front is not determined by implementation imperfections.

The first-order accurate Fourier approximation was expected to be the dominant error source in the NMR implementation. However, NMR simulations with controlled errors shows that the systematic error induced by the experimental implementation of the unitary collision operator associated with the quantum lattice gas (QLG) algorithm is the major challenge. Replacing the single collision operator with a set of operators to randomize errors allows us to improve the robustness of the implementation.

A quantum lattice gas is a system of quantum particles moving and colliding on a discrete spacetime lattice. This quantum particle system is isomorphic to a lattice-based qubit system. The mapping is as follows: the probability of a particle residing at a particular lattice node is equated to the moduli squared of the probability amplitude of a qubit at a unique location being in its excited quantum state. That is, each spatial location that a particle may occupy is mapped onto a qubit associated with a unique location.

The dynamics of evolution in the QLG algorithm can be described in three scales, the microscopic, mesoscopic, and macroscopic scales. At the microscopic scale, each particle has some probability of moving along the lattice. For example, the particle can move to the right or left lattice site in a one-dimensional construction. A simplified dynamics allows a particle to change its direction of motion (via a *collision* with another particle) or keep moving at constant speed in its original direction of motion (*streaming*). One can describe the dynamical behavior of particles at the mesoscopic scale by determining their occupation probabilities on the lattice points; in one-dimension, only left-moving and right-moving probabilities are needed. The mesoscopic dynamical behavior of the system is modeled by a finite-difference form of a quantum Boltzmann equation. Finally, to bridge to the macroscopic scale, the occupation probabilities of the particles residing at each lattice site are summed together to determine the number density. This number density quantity defined at each lattice node becomes a continuous field at the lattice resolution approaches infinity, which is called the *continuum limit*. Through a Chapman-Enskog perturbation procedure applied in the continuum limit, from the quantum Boltzmann equation emerges an effective field theory that is parabolic in time and space and nonlinear in the number density [7].

The QLG algorithm is initialized, in the NMR case, by encoding the particles' occupation probabilities as a spin-magnetization profile. To handle the one-dimensional Burgers equation, it is sufficient to use two qubits (two spin- $\frac{1}{2}$ nuclei) per lattice site, where each stores a single real valued occupation probability. A room-temperature solution of isotopically-labeled chloroform ($^{13}\text{CHCl}_3$) was chosen for implementing the experiments, where the hydrogen and the labeled carbon nucleus served as qubits 1 and 2, respectively. The difference of the gyro-magnetic ratio of two spins generates widely spaced resonant frequencies that allows us to address each spin independently. A lattice of QIPs are related to the ensemble sample by creating a correspondence between lattice sites and spatially dependent positions in the sample. A linear magnetic field gradient is used to generate distinct spatially-dependent resonant frequencies that we can distinguish and modulate by a shaped RF pulse. In this way, the magnetic field gradient allows the entire spin ensemble to be sliced into a lattice of smaller, and individually addressable, sub-ensembles.

The lattice initialization starts by transforming ther-

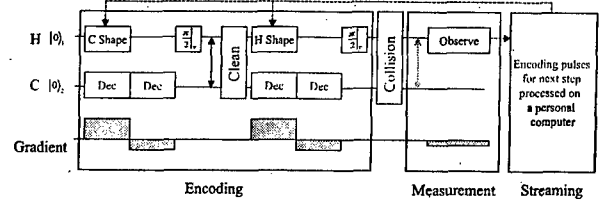


FIG. 1: QLG algorithm implemented in four steps. Three horizontal lines represent proton spin, carbon spin and fried gradients. Both starting magnetizations are encoded in proton channel first due to the high signal to noise ratio while decoupled in carbon channel to prevent interfering of scalar coupling. The collision operator is applied after the initialization. Measurements are also taken in two steps in the proton channel followed by data processing in a personal computer.

mal equilibrium states into pseudo-pure states [8]. The equilibrium state is highly mixed and the two nuclear spins have unequal magnetizations. Thus, equalization of the magnetizations is required prior to creating the pseudo-pure state. The dynamical evolution is caused by a collision operator (a quantum operation), and measurement and streaming (classical operations) according to the QLG algorithmic paradigm. The four main sections of the NMR implementation of QLG algorithm are graphically depicted in Figure 1.

First, each occupation probability is mapped onto a lattice site as the expectation value of a number operator at a spacetime site $n\Delta x$ at time $m\Delta t$. As a result, the initial state of the a^{th} qubit is $\sqrt{f_a(n\Delta x, m\Delta t)}|1\rangle + \sqrt{1-f_a(n\Delta x, m\Delta t)}|0\rangle$. The combined the wave function for a lattice site is a tensor product over the qubits,

$$|\psi(n\Delta x, m\Delta t)\rangle = \sqrt{f_1 f_2}|11\rangle + \sqrt{f_1(1-f_2)}|10\rangle + \sqrt{(1-f_1)f_2}|01\rangle + \sqrt{(1-f_1)(1-f_2)}|00\rangle \quad (1)$$

In the basis of a two-qubit system, the number operators for the occupancy of qubits are defined in terms of the singleton qubit number operation $\hat{n} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ as follows: $\hat{n}_1 = 1 \otimes \hat{n}$ and $\hat{n}_2 = \hat{n} \otimes 1$. Therefore, the occupation probability is represented as follows:

$$f_a(n\Delta x, m\Delta t) = \langle \psi(n\Delta x, m\Delta t) | \hat{n}_a | \psi(n\Delta x, m\Delta t) \rangle. \quad (2)$$

The macroscopic scale dynamical quantity of the quantum lattice gas is the number density, ρ , defined as the sum of the occupancy probability. The equilibrium occupation probabilities that we use are

$$f_a^{\text{eq}} = \frac{\rho}{2} + e_a \frac{5}{8} \left[1 - \sqrt{1 - \left(\frac{32\rho}{25} \right) \left(1 - \frac{\rho}{2} \right)} \right], \quad (3)$$

where e_a is ± 1 for different qubits.

The initial magnetization is specified by using a RF pulse shaped by the Fourier transform of the desired magnetization (transform of the initial number density profile). While applying the shaped pulse, a carbon decoupling sequence is performed to prevent the scalar coupling from interfering with the low power shaped pulses. In addition, the $\frac{\pi}{2}$ pulse, which rotates the information from the x-axis to the z-axis, is applied separately just after each initialization. This is done to keep the valuable information along the longitudinal direction where it will not be affected by the gradient and chemical shift. The encoding of initial states on both spins is accomplished in two steps: The initial carbon magnetization is recorded on the protons before being transferred to the carbons and followed by the initialization of proton magnetization. Furthermore, a short pulse sequence, called the *clean sequence*, is executed after the first swap gate to erase the phase distortion that may be caused by the decoupling sequence.

Second, the evolution of f_a is governed by the combined action of the collision operator, measurement and streaming. The collision operator is applied to all the lattice sites independently, resulting in $|\psi'(n\Delta x)\rangle = \hat{C}|\psi(n\Delta x)\rangle$, for all n . The choice of the particular components of the unitary collision operator determines the form of the macroscopic effective field theory (a parabolic partial differential equation) and the value of its transport coefficients (coefficients of the dissipative terms). A general representation of the collision operator for the Burgers equation is a block diagonal matrix. This single quantum operator is chosen to be

$$\hat{C} = \exp \left[-i \frac{\pi}{4.882} (\sigma_x^H \sigma_y^C - \sigma_y^H \sigma_x^C) \right], \quad (4)$$

which has the following matrix representation:

$$\hat{C} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.8 & 0.6 & 0 \\ 0 & -0.6 & 0.8 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (5)$$

The unitary operator $\hat{C}$ can be decomposed of a sequence of RF pulses and scalar coupling. The product operators in the exponent commute with each other, resulting in $\hat{C} = \exp \left[-i \frac{\pi}{4.882} \sigma_x^H \sigma_y^C \right] \exp \left[-i \frac{\pi}{4.882} \sigma_y^H \sigma_x^C \right]$. Both terms can be expanded as natural scalar Hamiltonian couplings sandwiched with the appropriate single rotations, resulting in

$$\hat{C} = e^{-i\frac{\pi}{4}(\sigma_y^H + \sigma_y^C)} e^{-i\frac{\pi}{4}\sigma_z^H \sigma_z^C} e^{-i\frac{\pi}{4.882}(\sigma_x^H - \sigma_x^C)} \times e^{i\frac{\pi}{4}(\sigma_y^H + \sigma_y^C)} e^{-i\frac{\pi}{4}(\sigma_x^H + \sigma_x^C)} e^{-i\frac{\pi}{4}\sigma_z^H \sigma_z^C} e^{i\frac{\pi}{4}(\sigma_x^H + \sigma_x^C)}. \quad (6)$$

The exponential terms of single spin rotations are implemented by $\pi/2$ and $\pi/4$ pulses. The exponents of terms with $\sigma_z^H \sigma_z^C$ represent the natural internal Hamiltonian evolutions with time period $1/2J$, where J is 214Hz . Here, the evolution of the internal Hamiltonian is ignored

while the RF pulse is applied. This approximation leads to a systematic error that will accumulate during the course of the computation. In general, these errors are easy to avoid, but since the purpose of the investigation was to explore the sensitivity to accumulated errors we did not correct it. The collision operator follows the encoding (Step 2), and it is implemented without magnetic field gradients to ensure that all of the sites in the sample undergo the same transformation.

Third, we measure the occupation probabilities. This process erases all the superpositions and quantum entanglement that was created by the unitary collision operator in the second step.

The occupation numbers of each spin are obtained following the collision step by measuring the z-magnetization according to the following equation

$$f_a(n, m) = \frac{1}{2} [1 + \langle \psi(n, m) | \sigma_z^a | \psi(n, m) \rangle]. \quad (7)$$

Since only σ_x and σ_y are observable in our NMR spectrometer, a $\pi/2$ pulse has been used to bring the z-magnetization into the transverse plane. The measurements are done in two separate experiments, where a SWAP gate is applied to bring the magnetization from carbon channel to the proton channel. This SWAP operation is done because the higher signal-to-noise ratio in the proton channel allows us to improve the accuracy of our implementation. During the "readout" process (Step 3), a weak magnetic field gradient is applied to distinguish different sites. The observed proton signals are digitized and Fourier transformed, allowing us to record the spatially-dependent spin magnetization profile.

Fourth, and last step of the QLG algorithm, we shift the f_a obtained in the previous step to its nearest neighbor using a short MATLAB program. This step requires only classical communication between neighboring sites. The time is incremented after this step. Then, we loop back to step 1 and update the field of occupation probabilities over the lattice sites. In this way, we can continue to iterate forward in time and make a time-history record of the occupation probabilities, which in turn gives us the temporal evolution of the number density field. In the implementation of the Burger equation, we observed deviations between the numerically predicted data points and analytically predicted solutions. These errors can be attributed to imperfections in the NMR implementation. The major error sources in the NMR implementation are known, so to explore the source and relative strength of these errors, we have simulated the NMR experiments. The major error source in this implementation is the collision operator, and it is introduced by ignoring the scalar coupling between proton and carbon during the RF pulses. When applying an RF pulse on the proton qubit, the Hamiltonian in the rotating form is $H = 2\pi J \sigma_z^H \sigma_z^C + \gamma_H B_1 \sigma_x^H$, where B_1 is the strength of the RF pulse. With the presence of the scalar coupling, a small portion of the proton magnetization has been transferred to the carbon qubit. Therefore, the applied propagator can be recast as $U = U_{\text{desired}} U_{\text{error}}$.

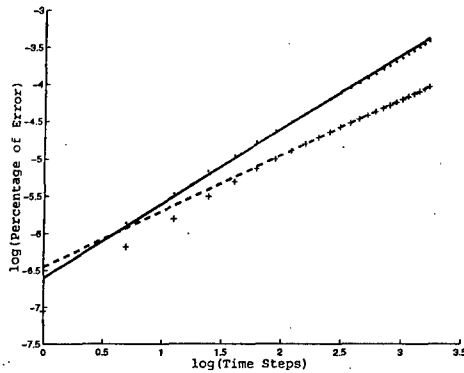


FIG. 2: The growth of the systematic errors due to the collision operator in two NMR implementation. The single collision operator data (dots) is fit (solid line) with a line of slope 1, which shows linear growth of the error. The collision operator data with modulated phases (pluses) is the fit with a line of slope 3/4 (dashed line). The buildup of the systematic errors has been slowed down by proposed method. However, the systematic errors have not been totally converted into random errors.

The error in the collision operator is a systematic error that builds up throughout the successive time steps. Although this is not the dominant error at the beginning of the implementation, it eventually dominates the first-order error due to the Fourier approximation and becomes the dominant issue after just several time step iterations. Notice that while the reduction of the initial magnetization from the Fourier transform is systematic, since the magnetization profile is changing the errors are not precisely repeated. In the collision operator, however, the errors are exactly the same from step to step. In addition we expect that the radio frequency inhomogeneity leads to strongly correlated errors in the lattice encoding. Hence, we have proposed replacing a single collision operator with a set of collision operators that have similar fidelity but randomized error terms.

Since the collision operator for the Burgers equation is a zero-order coherence term, the collision operator commutes with the rotation operator. Therefore, we apply a 90° rotation operator to the collision operator at each step to mitigate error growth. Consequently, a dramatic improvement is observed as shown in Figure 2. On a logarithmic plot, the simulation results fit a line with a slope of 3/4. If the error terms in the collision operators were totally randomized and hence followed a Gaussian distribution, the best-fit regression line should have had a slope of 1/2. The deviation between our simulation data and the ideal Gaussian case indicates residual systematic error in the collision operator. In a future study, we may use strongly modulated pulses to randomize the error terms. The experimental number densities are overplotted in Figure 3 with the exact analytical solutions. Eight successive time steps of the quantum algorithm

were implemented on 16 two-qubit sites. An improvement of our present experimental approach using collision

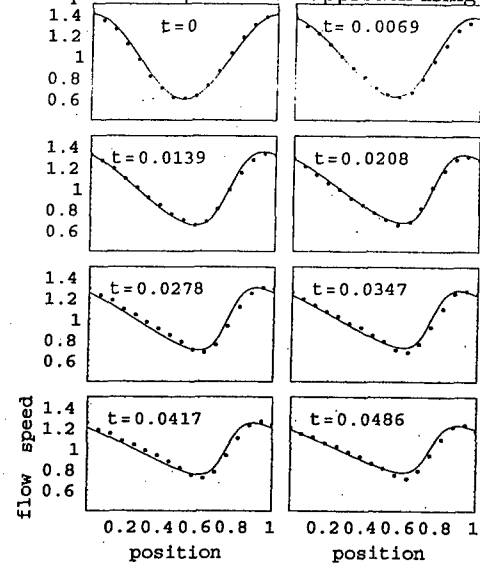


FIG. 3: The experimental data are plotted together with the analytical solutions for 8 time steps on a lattice of 16 parallel two-qubit QIPs. Viscosity: $\frac{1}{4} \frac{\Delta x^2}{\Delta t}$. Experimental NMR data (dots) versus analytical solution (curves). Randomizing the error terms in the collision operator has improved the experimental results dramatically.

operators with modulated phases is observed. The agreement of the data to the analytical solutions is encouraging and suggests that totally randomizing error terms in the collision operator may offer further improvement.

NMR quantum simulations has provided an alternative way to study the NMR spectroscopic implementations. From the simulation, we find the major error sources are due to imperfect control of the quantum spin system and the Fourier approximation associated with setting its magnetization profile. Our proposed method for converting the systematic errors into random errors is effective. The improvement we achieve relative to the previous experiment is encouraging, and it demonstrates the possibility of using the same technique in future studies. The closeness of the numerical data to the exact analytical results for the nonlinear Burgers equation further proves the practicality of implementing the QLG algorithm using a spatial NMR technique. In addition, although the limitation of the Fourier approximation is not dominant, the problem of precisely initializing a lattice of QIPs still remains an open issue.

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