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Kinetic Theory, Ensemble Simulations and Quantum Computing

Abstract. We discuss a functional kinetic theory approach to perform ensemble simulations on quantum computers. It is argued that the approach requires several hundreds of logical noiseless qubits, hence commanding major technological breakthroughs in noise correction and mitigation practices.

Keywords. Quantum computing, kinetic theory, fluid dynamics.

Mathematics Subject Classification: 68Q12, 82C40, 76205.

1 - Introduction

The extreme complexity of most problems in modern science and society raises a very steep challenge to our best theoretical and computational methods. As an example, even the most powerful supercomputers, reaching up to exascale operations (one billion billions floating point operations per second) pale in front of the task of predicting the weather on a planetary scale based on the direct simulation of the equations of fluid motion [**17**]. Besides, the aforementioned problems are typically subject to various sources of uncertainity on initial data and other parameters affecting the solution. As a result, each single case-study requires several realizations in order to accumulate sufficient statistical information (Ensemble Simulations), further magnifying the quest of computational power.

Given that electronic computers are facing very stringent energy constraints, alternative simulation strategies are constanly sought for. Among these, enormous efforts have been devoted in the last decade towards the development of quantum computers, namely hardware devices capable of exploiting the weirdest features of quantum mechanics, particularly the ability of quantum systems to occupy a multitude of states at the same time (quantum entanglement). The

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immediate perk is that a quantum system can *in principle* perform a multitude of parallel quantum computations, as opposed to classical computers which can only operate on binary states (bits). Lately, not a day goes by without hearing the last quantum computing breakthrough, but, leaving aside the huge commercial hype, the fact remains that turning the immense potential of quantum computing into a concrete tool for scientific purposes remains a very challenging goal [**3**]. The reasons are many, but, in a nutshell, the bottomline is that entanglement is very fragile and tends to crumble pretty quickly under the effects of environmental noise, which is extremely hard to avoid at any reasonable temperature, a problem know as "decoherence" and "noise". Notwithstanding these major barriers, it is worth exploring what quantum computers can possibly contribute to the prospect of Ensemble Simulations.

2 - Ensemble simulations

Ensemble simulations have gained popularity in the recent years, thanks to the availability of large supercomputers. The main idea is accumulate statistics over the many sources of uncertainities associated, for instance to weather forecast, by running series of simulations with different initial conditions and/or parametric realizations [**11**, **17**].

Let us illustrate the idea in some more detail.

We consider a set of nonlinear partial differential equations and discretize them on a grid with, say, G grid points. Let $u(t)$ the set of unknowns after discretization, for instance the velocity field of a three-dimensional fluid; they obey a set of $O(G)$ first-order ODE's in (generalized) Langevin form:

$$\frac{du}{dt} = f(u;\eta) \tag{1}$$

with initial condition $u(0) = u_0$ and where the noise η stands for the various sources of uncertainty. Ensemble simulations respond to the idea of generating a statistics of solutions upon changing initial conditions and/or perturbing the system parameters. Formally, this amounts to generating a probability distribution function (PDF) for the solutions $u = u(t; x_0)$, defined by:

$$p(u,t)d\mu(u) = \frac{dt}{T} \tag{2}$$

where dt is the time spent by the set of trajectories, spanning the time interval $[0 \leq t \leq T]$, in a volume of phase-space $d\mu(u)$.

Generating the trajectories is extremely demanding, since by construction each single simulation is going to stress the most advanced computer resources to their limit [**1**, **11**].

Quantum computing could help realizing an exponential speedup on each of these simulations. Besides all standard concerns affecting quantum computing, two additional issues stand on the way of this route: quantum mechanics is linear and energy-conserving, while the physics of fluids is neither [**15**].

Several ways around these problems are currently under exploration, based on various strategies [**2**, **4**, **5**, **7**, **10**, **12**]. All of these, however, focus on the solution of the actual equations of motion, without addressing ensemble statistics.

In this brief note, we sketch a potential strategy which offers two major assets at the outset. First, it captures all the sought statistical information on the system dynamics by construction (statistical dynamics). Second, it does not resort to any linearization of the dynamic equations, but starts directly from an inherently linear representation of the corresponding probability distribution function (PDF).

The passage from dynamics to statistical dynamics is a standard topic in statistical physics, where it is known as Liouville formulation of classical N-body mechanics.

The Liouville formalism is very elegant and conducive to very valuable approximations, mostly at the level of one-body effective kinetic equations, the most outstanding examples in point being the Boltzmann and Fooker-Planck equations.

Unfortunately, at least on classical computers, it is completely unviable since the N-body distribution function lives in a N-dimensional space, with N of the order of the number of grid points of the dynamic simulation, hence easily in the order of billions or more for current supercomputer simulations.

This looks like a medicine worse than the disease, and it is therefore of interest to explore what quantum computing could possibly contribute to ease the issue [**6**, **16**].

3 - Functional Liouville formulation

By virtue of the Liouville theorem (Fig. 1), the N-point PDF associated with the (nonlinear) Langevin equations obeys a linear Liouville Fokker-Planck kinetic equation (LFPE) of the form

$$\partial_t p_N + \partial_u [f(u) p_N - D \partial_u p_N] = 0 \tag{3}$$

Liouville equation

$$p(u,t)|\delta u(t)| = p(u,0)|\delta u(0)|$$

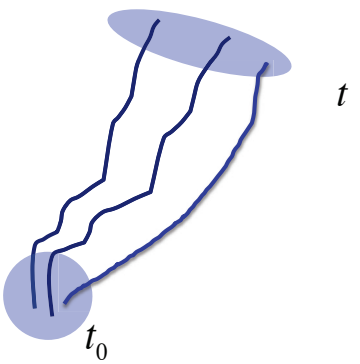

Fig. 1. Geometrical interpretation of the Liouville equation. The cloud of points representing various realizations of the system at $t = 0$ evolves each along its own trajectory dictated by the dynamic equation $\dot{u} = f(u)$, with initial conditions $u(0) = u_0$. As time unfolds, The cloud changes its shape but not its volume, and consequently the probability distribution $p(u,t)$ is invariant along the trajectory $dp/dt = 0$ leading to the Liouville equation.

where D is the diffusion coefficient associated with the noise in the (linear) Langevin equation (1).

Since the Liouville equation is linear by construction, it can operate under the same framework as quantum mechanics and it particular, it should benefit of quantum linear algebra solvers [**8**].

In particular, it is possible to map the Liouville equation onto a corresponding quantum many-body Schroedinger equation in imaginary time. The standard substitution $p(u,t) = g(u)\psi(u,t)$ is known to transform the above LFPE into a Schroedinger equation (SCE) in imaginary time, with the following Hamiltonian

$$\hat{H} = D\partial_{uu} + V[g] \tag{4}$$

where $V[g] = -D\partial_{uu}g/g$, where the guiding function g fulfills the constraint

$\partial_u g = f(u)g/2D$. The problem is now hermitian, hence fully within the realm of quantum computing. Yet, solving a SCE in billions of dimensions remains out of reach even for quantum computers, as it would require billions of qubits even in the most ideal scenario. However, some mitigating arguments can be brought up.

3.1 - *Marginalization*

These arguments relate to marginalization of the PDF, namely the fact that the N-point PDF $p_N(x,t)$ or the equivalent N-body wavefunction $\Psi_N(x,t)$ contain far more information than actually needed. Coming back to the case of the fluid flow, there is no need to know the simultaneous joint PDF of each fluid velocity at each given lattice site.

The count goes as follows. The N-body PDF associated to a discrete grid with $G = N$ lattice sites, each hosting F fields discretized over a set of n discrete values, takes up $(GF)^n$ discrete values. The number of qubits to represent the fully N-body discrete PDF is then

$$q = GFlog_2 n \tag{5}$$

which is clearly unfeasible even for any foreseeable ideal quantum computer, given that G is in the order of multi-billions for present-day supercomputer simulations.

Fortunately, marginalization presents a milder picture.

If each field on a discrete grid with G lattices sites is connected to $z << G$ neighbours, the lowest order irreducible marginal is of order $M = zF$ and the qubit count now reduces to

$$q = zFlog_2 n. \tag{6}$$

This is still very demanding but still enormously simpler than (5) since zF is of the order of tens.

4 - Practical examples

For the sake of concreteness let us spell out the Liouville formulation for the case of the Burgers equation, describing a one-dimensional pressureless fluid, as well as the three-dimensional Navier-Stokes equations.

4.1 - *Example 1: the Burgers equation*

The Burgers equation describing one-dimensional pressureless fluids, reads as follows

$$\partial_t u + u\partial_x u = \nu \partial_{xx} u \tag{7}$$

where ν is the kinematic viscosity.

A simple centered-finite difference scheme gives:

$$\dot{u}_j = -u_j(u_{j+1} - u_{j-1}) + \nu(u_{j+1} - 2u_j + u_{j-1}) \equiv \sum_{k=-1}^{1} B_{j,k}(u_j) u_{j+k} \equiv f_j(u) \tag{8}$$

where the space and time step are made unit for simplicity and B_{jk}, $j = 1, N$, $k = -1, 0, 1$ is the (nonlinear) "Burgers" matrix.

The N-point Burgers-LFPE takes the following form:

$$\partial_t p_N + \sum_{j=1}^{N} \partial_{u_j} [\sum_{k=-1}^{1} B_{j,k} u_{j+k}] p_N \tag{9}$$

where $p_N \equiv p[u_1 \dots u_N, t]$ is the N-body PDF associated to a spatial grid of $G = N$ gridpoints.

Next, let us consider a generic observable $A(u_1 \dots u_N)$, whose average value is given by

$$< A > (t) = \frac{1}{Z} \int_{-\infty}^{+\infty} p(u) A(u) du \tag{10}$$

where $Z = \int_{-\infty}^{+\infty} p(u) du$ is the partition function and u is a shortand for $u_1 \dots u_N$.

If the dependence on each of the $N = G$ independent variables u_j is irreducible, the average necessitates the full N-body PDF $p_N(u_1 \dots u_N)$. But this is rarely the case in classical physics. For instance if K is the total kinetic energy of the fluid, $K = \frac{1}{2} \sum_j u_j^2$, its average only depends on the one-point distribution

$$2 < K > (t) = \sum_{j=1}^{N} \int u_j^2 p_N(u) du = \sum_{i=1}^{N} \int u_i^2 p_1(u_i) du_i \tag{11}$$

where $p_1(u_i)$ results from integrating out all variables u_1 to u_N, but u_i. Likewise, if all we need is the value of the average velocity field at the space slice

x_i, the 1-point PDF will equally suffice

$$< u_i > (t) = \int u_i p_1(u_i) du_i. \tag{12}$$

By the same token, two-point observables require two-point PDFs and so on at all higher orders.

Since $\dot{u}_j$ depends on the triplet $[u_{j-1}, u_j, u_{j+1}]$ lowest order irreducible margibal is the three-point PDF p_3, which is defined by integrating out all independent variables but three, u_{j-1}, u_j, u_{j+1}, namely:

$$p_3[u_{j-1}, u_j, u_{j+1}] = \int_{\infty}^{+\infty} p[u_1 \dots u_N] du_1 \dots du_{j-2} du_{j+2} \dots du_N. \tag{13}$$

The corresponding three-point kinetic equation takes the form:

$$\partial_t p_3 + \partial_{u_{j-1}}[\sum_{k=-1}^{1} B_{j-1,k} U_{j-1+k}] p_3 + \partial_{u_j}[\sum_{k=-1}^{1} B_{j,k} U_{j+k}] p_3 + \partial_{u_{j+1}}[\sum_{k=-1}^{1} B_{j+1,k} U_{j+1+k}] p_3 = 0 \tag{14}$$

where by periodicity $j - 2 = j + 1$ and $j + 2 = j - 1$.

In the above we have defined:

$$U_j = \int u_j p(u) du_1 \dots du_{j-2} du_{j+1} du_N \tag{15}$$

which is a generally unknown function of u_{j-1}, u_j, u_{j+1}. Hence a suitable expression for U_j versus u_j needs to be worked out, which is the usual closure problem. A possible example of such closure can be found in [**16**].

With reference to the expression (6), we have $z = 3$ and $F = 1$, hence the corresponding qubit count gives

$$q = 3\, log_2 n. \tag{16}$$

Current quantum computers can offer up to $q \sim 500$ *nominal* qubits, implying that one can reach up to $n \sim 2^{500/3}$, far beyond any practical resolution need. For a reasonable resolution, say $n \sim 1000 \sim 2^{10}$, we obtain $q \sim 30$, which appears viable once noise and decoherence are tamed.

4.2 - *Example 2: the Navier-Stokes equations*

The Navier-Stokes governing the motion of compressible, dissipative fluids read as follows

$$\partial_t \rho + \partial_a(\rho u_a) = 0 \tag{17}$$

$$\partial_t(\rho u_a + \partial_b(\rho u_a u_b + P\delta_{ab} - \sigma_{ab}) = 0 \tag{18}$$

where ρ is the density, u_a, $(a = x, y, z)$ the flow velocity, $P = P(\rho)$ the fluid pressure and σ_{ab} the dissipative tensor.

With reference to the expression (6), we now have $F = 4$ (density and three velocity components) and $z = 7$ (each grid site connected to six nearest neighbors), hence the corresponding qubit count gives

$$q = 28\, log_2 n. \tag{19}$$

With $n = 10^3$, we have $q = 280$, much steeper than Burgers, but still within the nominal capabilities of current quantum hardware [**18**]. Different representations or different formulations altogether, such as as lattice Boltzmann [**13**, **14**], may lead to more favourable scalings, a topic of interest for further research.

The above considerations make abstraction of the many issues generally associated with quantum computing, particularly noise and decoherence. In the following, we briefly comment on a further issue which is peculiar to quantum simulations in real time: time marching.

5 - Quantum time-marching

On electronic computers time-marching proceeds quite seamlessy: update the present state to the future one and copy the future in the new-present, to start the next timestep. A pseudo-code for fist-order Euler forward time marching reads as follows:

```
Initialize u
For as many steps as needed:
 unew  = u+f(u)*dt
 u     = unew
End for
```

On a quantum computer such innocent-looking loop is basically unviable, the culprit being the no-cloning theorem (NCT), stating that you cannot make

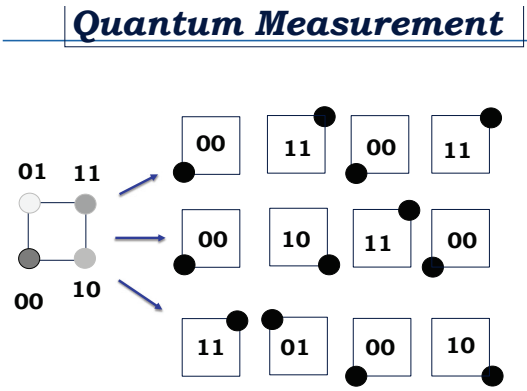

Fig. 2. The 2-qubit quantum systems consists of $2^2 = 4$ quantum states, $|00>$,$|10>$, $|11>$, $|11>$, each coming with its corresponding probability p_{ij},$i = 0, 1, j = 0, 1$ (color code). In the example in point, by keeping 12 replicas of the quantum state (left), one measures 5 occurrences of $|00>$, 4 of $|11>$, 2 of $|01>$ and 1 of $|10>$ (right). The corresponding probabilities $5/12, 4/12, 2/12, 1/12$, approximate the values p_{ij} within statistical accuracy.

a copy of a quantum state without destroying it. The no-cloning theorem is clearly rooted into the infamous "wavefunction collapse" paradox, whereby the very act of measuring a qubit turns it into a classical one, yielding zero or one as an answer, "tertium non datur". Hence the only way to perform the time-stepping without losing the "old" state is to keep at least 2^q replicas, q being the number of qubits encoding the quantum state. In fact, since there are 2^q states to be statistically reconstructed, the count exceeds 2^q (See Fig. 2) This basically spoils the purpose of the ordeal, and represents a very serious problem for the quantum solution of dynamical problems, including iterative methods.

To date, the most popular strategy to cope with this problem is to turn the dynamical equations into a corresponding eigenvalue problem, a standard procedure in quantum mechanics. Essentially this leads to hybrid algoritms whereby quantum computers are used to construct variational solutions based on a set of classical parameters λ. Since the parameters are classical, they can be changed at will to generate new variational quantum states without destroying the old ones, thus turning around the NCT. The optimal parameters are then found by minimizing a suitable cost function (energy for the case of quantum mechanics) using classical computers. This procedure is standard in quantum computing for quantum many-body problems and they may probably be extended to the case of fluids. Their application to the Liouville equation is just beginning to be explored [**9**].

6 - Summary

Summarizing, we have assessed the viability of the functional Liouville formulation for ensemble simulations on quantum computers. The present analysis refers to a blue-sky scenario whereby a quantum algorithm capable of logarithmic scaling with the number of dynamic degrees of freedom is available *and* up-and-running on *ideal* quantum computers, with no appreciable decoherence and noise problems. The former condition is contingent, among others, to the solution of the quantum time-marching problem. In actual practice, quantum computing ensemble simulations of the Navier-Stokes equations demand hundreds of noiseless *logical* qubits. Given that current quantum computing typically works only up to a few tens of logical qubits, the target appears many years away in the future. This is no invitation to surrender, but just a realistic appraisal to be contrasted with the current (mostly commercial) hype around quantum computing (for a highly informed assessment, see [**3**]).

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8 - Dedication

The matters discussed in this paper draw heavily on the author's background in kinetic theory, a subject that he first learned by Vincio Boffi, Vincenzo Molinari and Giampiero Spiga. This paper is dedicated to the memory of Giampiero, a magnificent mentor and master of kinetic theory and a dear friend.

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