



#### **PERSPECTIVE • OPEN ACCESS**

# Quantum computing for fluids: Where do we stand?

To cite this article: Sauro Succi et al 2023 EPL 144 10001

View the article online for updates and enhancements.

## You may also like

- A stock-flow consistent input—output model with applications to energy price shocks, interest rates, and heat emissions Matthew Berg, Brian Hartley and Oliver Richters
- <u>Contaminated land liability issues: legal</u> <u>perspective</u> Valerie M Fogleman
- Liquid Liabilities and Growth Finance Nexus: Implications for Nigeria's Energy Sector
- H T Bello, E S Osabuohien, F Ayadi et al.



EPL, **144** (2023) 10001 doi: **10.1209/0295-5075/acfdc7**  www.epljournal.org

### Perspective

# Quantum computing for fluids: Where do we stand?

SAURO SUCCI<sup>1(a)</sup>, W. ITANI<sup>2</sup>, K. SREENIVASAN<sup>2</sup> and R. STEIJL<sup>3</sup>

<sup>1</sup> Fondazione Istituto Italiano di Tecnologia, Center for Life Nano-Neuroscience at la Sapienza Viale Regina Elena 291, 00161 Roma, Italy

<sup>2</sup> Tandon School of Engineering, New York University - Brooklyn, New York, NY 11201, USA

<sup>3</sup> James Watt School of Engineering, University of Glasgow - Glasgow G12 8QQ, UK

received 6 July 2023; accepted in final form 27 September 2023 published online 16 October 2023

**Abstract** – We present a pedagogical introduction to the current state of quantum computing algorithms for the simulation of classical fluids. Different strategies, along with their potential merits and liabilities, are discussed and commented on.

open access

perspective Copyright © 2023 The author(s)

Published by the EPLA under the terms of the <u>Creative Commons Attribution 4.0 International License</u> (CC BY). Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

**Introduction.** – Quantum computing is one of the most uproaring topics of modern science, holding promises of spectacular applications far beyond the reach of classical electronic computers, at least for selected applications [1].

The manifesto of quantum computing can be traced back to Richard Feynman's epoch-making paper, in which he famously observed that physics "ain't classical", hence it ought to be simulated on quantum computers [2].

Following Feynman's observations, early theoretical work on quantum computing was performed in the 1980s, e.g., Deutsch's work on the link between quantum theory, universal quantum computers and the Church-Turing principle [3]. Then, with the publication of Shor's algorithm for integer factoring and Grover's search algorithm in the middle of the 1990s, the research area gathered significant momentum in terms of theoretical work and quantum computing hardware as well. The research area of quantum computing has continued to grow ever since [4–6]. In terms of applications for quantum computers, the simulation of quantum many-body systems has received the most attention, due to its scientific and industrial applications, as well as the relatively close link with quantum hardware, as per Feynman's original proposal. In this Perspective, however, we shall focus on a much less beaten track, namely the use of quantum computers for the simulation of classical fluids<sup>1</sup>. To this purpose, let us refer to a physics-computing plane defined by



Fig. 1: The four quadrants in the Physics-Computing plane. The CC and CQ quadrants are the mainstay of current simulation work. QQ is the quadrant invoked by Feynman, and QC is the quadrant addressed by the present Perspective.

the following four-quadrants:

CC: Classical computing for Classical physics;

CQ: Classical computing for Quantum physics;

QC: Quantum computing for Classical physics;

QQ: Quantum computing for Quantum physics.

as represented graphically in fig. 1.

Feynman was probably referring to the CQ sector shown in fig. 1, where one is often faced with exponential complexity barriers (in his Nobel speech, Walter Kohn defines

<sup>&</sup>lt;sup>(a)</sup>E-mail: sauro.succi@iit.it (corresponding author)

<sup>&</sup>lt;sup>1</sup>Despite their early appearance, we shall not discuss the so-called type-II quantum computers [7], since they do not appear to be universal.

the many-body Schrödinger wave function as "unphysical" precisely because of this reason [8]). The basic idea is that these barriers are unphysical because we are using the wrong formalism to ask the questions that lie behind them. Unlike Kohn, Feynman takes no issue at the *N*-body Schrödinger equation, but simply observes that it is unphysical only if we insist in solving it on the CQ quadrant instead of the QQ one. In line with this observation, the simulation of quantum many-body systems has received most of the quantum computing attention in the recent past [9,10].

In this Perspective, we shall focus on the much less explored off-diagonal QC quadrant, the natural question being whether the power of quantum computing can be brought to the benefit of classical physics as well, with specific focus on classical fluid dynamics.

Yet, there is another, subtler, motivation along the Kohn-Feynman discussion above: while it is undeniable that physics is quantum, it is no less true that physics has a very strong innate tendency to become classical at sufficiently large scales (high temperature). Such tendency, the major source of troubles for quantum computing, remains only partially understood and therefore the "foundational" question is whether at some point, classical computing takes over and cannot be beaten by any quantum algorithm. This is just the opposite of the standard notion of "Quantum Advantage", hence we may dub it "Classical Advantage". Speaking of Classical Advantage, the starting observation is that many classical problems feature two major elephants in the quantum computing room: non-linearity and non-Hermicity (dissipation). How does quantum computing deal with the two "elephants" above? This is the main question addressed by this Perspective, with specific focus on classical fluids [11].

Challenges facing quantum computational fluid dynamics (QCFD). – As mentioned in the introduction, realising the potential of quantum computing means leveraging distinctive features of quantum mechanics that, by definition, are not available on classical computers. However, it also follows that it is precisely these specific features that expose major challenges in realising simulations with a quantum advantage.

The main quantum mechanical concepts spawning the potential benefit of quantum algorithms are quantum superposition and quantum parallelism. The quantum state in a Q-qubit coherent register can be described by the Schrödinger wave function, defined by  $2^Q$  complex amplitudes for  $2^Q$  states in superposition. The square of each of these amplitudes defines the probability of finding the system in the corresponding state after quantum measurement. By encoding classical data in terms of these amplitudes an exponential saving in storage can be achieved when the number of qubits is compared to required number of classical bits.

Let us illustrate the idea for the specific case of turbulent flow simulation. Turbulence features a  $Re^3$ 

complexity, where the Reynolds number Re represents the relative strength of convection (nonlinearity) vs. dissipation. Most real life problems feature Reynolds numbers in the many-millions; for instance an airplane features  $Re \sim 10^8$ , implying  $O(10^{24})$  floating-point operations per simulation. This is basically the best one can afford on a nearly ideal exascale classical computer. The simulation of regional atmospheric circulation flows takes us at least another two decades above in the Reynolds number, hence totally out of reach for any foreseeable classical computer [12,13]. On the other hand, the minimum number of qubits Q required to represent  $Re^3$  complexity can be roughly estimated as  $2^Q = Re^3$ , namely,

$$Q \sim 3\log_2 Re.$$
 (1)

This simple estimate shows that about 80 qubits match the requirement of full-scale airplane design, while O(100)qubits would enable regional atmospheric models. However, several key challenges stand in the way of this task. First, quantum measurement needed to extract classical information collapses the quantum wave vector. Hence, to get classical values for each of the amplitudes, multiple realisations of the quantum state vector are needed with an associated set of measurements. Second, in the quantum circuit model, the "classical" information is not available to the quantum gate operations performed in the circuit. Specifically, gate operations can be conditional on the state of one or more control qubits, while specifying gate operations conditional on one or more of the complex amplitudes defining the wave function is impossible. Therefore, when classical data is encoded in terms of amplitudes, for example, a rotation angle in a quantum gate operation, this information is required at the time the circuit is compiled. During the execution of the circuit, this angle cannot be changed as a function of "classical" data encoded in quantum amplitudes. Third, in an algorithm involving multiple iterations or time-steps, the overhead associated with quantum measurements used to extract classical data and re-initialization of the quantum state for a next iteration, scale quadratically with the grid size [14] and consequently they severely tax the quantum CFD efficiency. Associated with these challenges, it should be observed that the well-known HHL [15] algorithm for linear system solution assumes that the input and output data are encoded in terms of quantum amplitudes without including the cost of setting up the quantum state and extracting the classical solution.

With the exception of quantum measurement operations, quantum mechanical operators are unitary, linear and reversible. These operators are implemented using a series of unitary quantum gates (quantum circuit model). If we further assume that the velocity field is represented in terms of *amplitude encoding* [16], *i.e.*, the components of velocity vector at all grid points are represented in terms of the amplitudes defining the wave function, then the *nocloning theorem* prevents the use of (temporary) copies of any of these amplitudes. So, evaluation of  $u^2$  or  $u\frac{\partial u}{\partial x}$  cannot be performed by storing a temporary copy temp = u, to perform the computation of the value of  $u^2$  as  $u \times temp$ . Also, for data encoded in terms of the complex amplitudes of the Schrödinger wave function, there is a need for this state vector to have a unit norm, since these amplitudes represent probabilities of states. This means that for an operator attempting to compute the squares of these complex amplitudes, the resulting state vector loses unitarity. So, even without the no-cloning theorem complicating such a step, this points to a further problem with computing nonlinear terms. A similar argument runs for orthogonality of the eigenstates, since a nonlinear propagator rotates the state by an angle which depends on the state itself. Dissipation is also a concern, since it breaks Hermicity of the quantum propagator. However, several ways out can be conceived, one of the most popular ones being to augment the system with its Hermitian conjugate, so that the doubled system is Hermitian by construction.

To summarize, dealing with nonlinear terms can be regarded as one of the main challenges for Quantum Computational Fluid Dynamics (QCFD).

**Hybrid quantum/classical approaches.** – The challenges sketched above relating to *nonlinearity*, *non-Hermicity*, in combination with quantum circuit depth limitations imposed by NISQ-era hardware, have resulted in most of the existing work in QCFD being based on a *hybrid quantum/classical approach*, with the quantum processor performing computations for which efficient quantum algorithms exist, while the output is then passed on to classical hardware to perform further computational tasks not (yet) amenable to quantum algorithms.

Figure 2 provides an illustration of the main concepts in this approach. As shown, quantum state  $\psi_0$  is advanced to the next quantum state  $\psi_1$  via a QQ algorithm. The quantum state  $\psi_1$  is then used to generate classical observables  $C_1$  which are advanced to  $C_2$  by a CC algorithm. The classical observables  $C_2$  are then used to reconstruct the quantum state  $\psi_2$ , ready for the next QQ step. The Q2C conversion shown in fig. 2 involves quantum measurements and requires averaging over a statistical sample of quantum states, since none of them can be reused. The C2Q reconstruction requires the preparation of all the quantum eigenstates, hence a full reset of the quantum circuits from scratch. Both operations impose a substantial computational burden on the hybrid algorithm. Specifically, the cost of initialization of an arbitrary quantum state with Q qubits scales exponentially with Q. Initialization techniques with smaller overhead have been developed but only for a limited set of specific quantum states.

Examples of previous works using the *hybrid quan*tum/classical approach include the works of Steijl [17], Gaitan [18] and Budinski [19]. The algorithm presented by Gaitan uses Kacewiz's quantum amplitude estimation ODE algorithm [20] as applied to the set of nonlinear ODE's resulting from standard discretization of the

#### Hybrid Quantum-Classical Algorithm



Fig. 2: Sketch of a hybrid quantum-classical algorithm. The illustration shows the steps involved in a single time step or single iteration, including preparation of the subsequent step/iteration.

Navier-Stokes equations. As shown, for certain "nonsmooth" problems (illustrated using the quasi-1D flow in converging-diverging duct with normal shock wave), the complexity analysis shows potential for exponential speedup, so that the challenges associated with hybrid quantum/classical computing can potentially be overcome. For the linear advection-diffusion equation, Budinski [21] presented a quantum algorithm based on the Lattice Boltzmann method [22]. The algorithm can perform multiple successive time steps with no need for quantum measurements and re-initialization of qubit register between the time steps if suitable re-scaling of solution vector is applied to deal with non-unitarity. In the quantum circuit model, the fact that velocity field is unchanged between successive timestep means that an operator implementing  $u\frac{\partial u}{\partial x}$  can be re-used in multiple time steps. Budinski [19] then extended the work to Navier-Stokes equations in streamfunction-vorticity formulation. Then, velocity-field updates during each time step mean that quantumcircuit implementation of convection terms cannot be re-used during multiple timestep and that the "classical" value of u (as well as other flow field data) is needed to define quantum circuit implementation of the next time step. This shows that the nonlinearity forces the use of a hybrid quantum/classical approach, similar to previous fluid simulations based on quantum-Poisson solvers [17].

In summary, key challenges for the *hybrid quantum/classical approach* are: i) cost and complexity of (repeated) measurements; ii) statistical noise due to sampling of the quantum solution; iii) cost and complexity of (repeated) re-initialization.

**Quantum fluid dynamics strategies.** – For the sake of concreteness, let us consider the Navier-Stokes equations for time-dependent incompressible flows. We write as follows:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{x}} = -\frac{\partial P}{\partial \mathbf{x}} + \nu \Delta \mathbf{u}, \qquad (2)$$

$$\nabla \cdot \mathbf{u} = 0, \tag{3}$$

where  $\mathbf{u}$  is the velocity vector, P pressure, defined for location  $\mathbf{x}$  as a function of time t. The kinematic viscosity (assumed independent of temperature) is defined by  $\nu$  and density has been conventionally set to a unit constant value. Equation (3) enforces mass conservation, while eq. (2) is based on momentum conservation in each coordinate direction. Equations (2) and (3) highlight that it is the convection term that represents the nonlinearity, *i.e.*, the second term on the left-hand side of eq. (2). Writing the Navier-Stokes equations in non-dimensional form, such that  $\mathbf{x}$  and  $\mathbf{u}$  are scaled by reference length  $L_{ref}$  and  $U_{ref}$ , respectively, it follows that in eq. (2) the term  $\nu$  is replaced by 1/Re, where Reynolds number  $Re = U_{ref}L_{ref}/\nu$ . For Stokes flow, *i.e.*, with Reynolds approaching 0, nonlinear terms are vanishingly small, but still not to be neglected since they are responsible for nontrivial long-range correlations especially important in biological flows [23]. For high Reynolds number (turbulent) flows, obviously the nonlinear terms play the leading role.

In the following we present a cursory view of various existing strategies to simulate fluid dynamics on quantum computers.

Nonlinear quantum ODE solvers. A straight approach to quantum simulation of fluids consists in tackling the nonlinearity head-on, without trying to establish any parallel to quantum mechanics. In this case, one would discretize the Navier-Stokes equations, turn them into a set of nonlinear ODEs, to be solved by appropriate quantum nonlinear ODE solvers, Symbolically,

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = f(\mathbf{u}),\tag{4}$$

where  $\mathbf{u}$  is a shorthand for the full set of unknowns hosted by the computational grid. A standard time marching scheme yields

$$\mathbf{u}(t + \Delta t) = \mathbf{u}(t) + \int_{t}^{t + \Delta t} f(\mathbf{u}(z)) dz$$
 (5)

and the quantum algorithm takes charge of performing the discrete summation implementing the time-integration at the right-hand side. This approach has been pioneered by Gaitan [18] for the case of a Laval nozzle with encouraging results on grids between 30 and 60 grid points over 1400 timesteps. The dangling issue, though, is identification of an appropriate quantum oracle for evaluating the right-hand side f(u), a task that as already mentioned, Gaitan leaves to classical computers.

Nonlinear variational quantum eigenvalue solvers. It has recently be proposed that variational quantum eigenvalue (VQE) solvers, a major tool of the QQ sector, might be exported to the fluid context as well [24]. The basic idea behind VQE is to use quantum computing to construct variational eigenfunctions and minimize the energy functional through a classical procedure. In [24], the authors propose to use a similar technique for the Navier-Stokes equations, *i.e.*, 1) construct variational trial functions and 2) minimize the associated (dissipative) functional via a classical procedure. Formally, step 1) consists in expressing the flow field in variational form,

$$\mathbf{u}(x,t;\lambda) = \sum_{n} \mathbf{u}_{n}(t)\phi_{n}(x;\lambda), \tag{6}$$

where  $\phi_n$  is a suitable set of basis functions parametrically dependent on the a set of variational parameters  $\lambda$ . Such variational parameters are then fixed by minimizing the energy dissipation functional  $D(\lambda) = \nu \int (\nabla u(x;\lambda))^2 dx$ where the integral runs over the entire volume occupied by the fluid. The appeal of this idea is twofold: first, it may borrow a lot of QQ know-how, second it bypasses the issue of quantum time marching. We are not aware of any practical implementation of the idea, but best guess is that they will become available soon.

Linearization: Carleman embedding. It has long been known that any nonlinear problem can be mapped into a linear one in a space of higher dimensions, a technique also known as Carleman embedding or Carleman linearization [25]. Spatial discretization of the non-dimensional form of eq. (2) using a spatial grid consisting of l = 1, Glattice sites, results in the following set of equations:

$$\frac{\mathrm{d}u_l}{\mathrm{d}t} = \mathcal{L}_{lm} u_{lm} + Re \ \mathcal{Q}_{lmn} u_m u_n \tag{7}$$

where  $\mathcal{L}_{lm}$  and  $\mathcal{Q}_{lmn}$  are the grid matrices associated with linear and nonlinear interactions, respectively. The pressure term was removed for simplicity, although it is all but a minor item, since pressure-flow-stress coupling heavily affects the structure of the Carleman matrix. It should be noted that in the discretization of the velocity derivatives at lattice point l, the values of the velocity at one or more neighboring lattice points are used. This means that when the Carleman linearization is used to introduce a new variable  $V_{lm} = u_l u_m$  to formally generate a linear system, marching the system of equations forward in time produces an ever growing hierarchy in which the Carleman variables at level k involve the Carleman variables at the next level k + 1. Note that at each level we are faced with a tensor of rank k, with  $O(G\kappa^{k-1})$  independent components,  $\kappa$  being the sparsity of the Q matrix. Furthermore the tensors occupy a neighborhood of the original field whose diameter grows linearly with the Carleman level. This shows that uplifting the nonlinearity of the fluid equations comes at a major cost in terms of increasing dimensionality and non-locality.

Nevertheless, in [26] the authors present an algorithm based on Carleman linearization along with the use of a quantum linear system solution approach for the solution of the one-dimensional Burgers equation. The presented algorithm shows a polylog scaling with the number of grid points, *i.e.*, an exponential improvement over classical approach. However, for a given time span T, the algorithm shows a complexity  $T^2 Poly(\log T)$ , *i.e.*, a significantly increased time-complexity compared to classical case. The authors simulate shock formation in a one-dimensional Burgers flow, with 16 grid points over 4000 time-steps, with a fourth-order Carleman truncation. They reach Reynolds numbers up to 40, an order of magnitude larger than predicted by the theoretical no-go analysis, a welcome discrepancy which begs for further analysis. Like for [18], exponential gain remains to be demonstrated in practice because of insufficient number of available qubits, as reflected by the very modest sizes of the grids employed.

The key question then is: how fast does the Carleman procedure converge as a function of the Reynolds number?

As we shall see, preliminary results offer room for optimism.

Carleman lattice Boltzmann method. The answer may depend on the chosen representation of the fluid equations, the Lattice Boltzmann (LB) method being a prominent candidate in this respect. In equations,

$$\partial_t f_i + \mathbf{v}_i \cdot \nabla f_i = -\frac{f_i - f_i^{eq}}{\tau},\tag{8}$$

where  $f(\mathbf{x}, \mathbf{v}, t) = \sum_{i} f_i(x, t) \delta(\mathbf{v} - \mathbf{v}_i)$  is the probability to find a representative particle with discrete velocity  $\mathbf{v}_i$ at position  $\mathbf{x}$  and time t,  $f_i^{eq}$  is the corresponding discrete local equilibrium and  $\tau$  is a local relaxation time, fixing the viscosity of the lattice fluid. Importantly, the local equilibrium is a quadratic function of the Mach number  $Ma = u/c_s, c_s$  being the speed of sound.

A key point of using the discrete-velocity Boltzmann formalism instead of Navier-Stokes is that, owing to the double dimensional phase-space, in the latter non-locality (streaming) is linear while nonlinearity (collision) is local, while in Navier-Stokes the two merge into a single  $\mathbf{u}\nabla\mathbf{u}$  convective term. On classical computers this disentanglement proves extremely beneficial and the idea is that similar benefits apply to the quantum case as well. Indeed, most importantly for the quantum case, in the Boltzmann formulation the nonlinearity is not measured by the Reynolds number, but by the Mach number instead, which is typically well below 1, thereby dramatically lowering the nonlinearity barrier.

Based on the Lattice Boltzmann method, Itani *et al.* [27] employ Carleman linearization to develop an approach termed *Carleman for second-quantized Lattice Boltzmann*. This terminology stems from the fact that the Boltzmann operator, defined by  $\mathcal{B}f_i = -\mathbf{v}_i \cdot \nabla f_i - \frac{f_i - f_i^{eq}}{\tau}$ , can be expressed in terms of the second-quantization annihilation and generation operators via the relation  $\nabla = (\hat{a} - \hat{a}^+)$ . As a result, the formal solution  $f_t = e^{\mathcal{B}t}f_0$  can be computed in close analogy with quantum mechanics.

The quantum computing algorithm for streaming is based on the approach used by Steijl and co-workers [28], while collisions follow the bosonic encoding first proposed by Mezzacapo *et al.*, whereby dissipative effects are represented as a weighted sum of two unitary operators [29]. The scheme is as "Feynmanesque" as it can possibly get, as it builds on a one-to-one analogy between LB and the Dirac equation, first proposed in [30]. However, it is subject to a number of additional questions: primarily truncation effects due to the finite number of bosonic excitations and the long-time behaviour of non-unitarity errors [31]. Recently, Cheung and coworkers performed a Taylor-Green vortex simulation based on a Carleman-LB scheme, showing excellent agreement at moderate Mach number, with just three Carleman iterations [32]. Although preliminary, these results invite some optimism on the use of Lattice-Boltzmann-Carleman quantum computing schemes.

Functional Liouville approach. The Carleman embedding provides a linearization of the actual equations of fluid motion. An alternative procedure is to take the statistical dynamics approach, whereby one seeks the probability distribution function (PDF) of the fluid velocity field [33]. This is formally straightforward since the PDF obeys a functional continuity equation, best know as Liouville equation:

$$\partial_t P[\mathbf{u}] + \frac{\delta}{\delta \mathbf{u}} (f(\mathbf{u}) P[\mathbf{u}]) = 0, \qquad (9)$$

where  $P = P[\mathbf{u}]$  is the functional PDF and  $\dot{\mathbf{u}} = f(\mathbf{u})$  is the nonlinear equation of motion (hence  $f(\mathbf{u})$  is an operator in function space). Note that regardless of the nonlinearity of the dynamics, reflected by  $f(\mathbf{u})$ , the functional equation is linear, by construction. Once the fluid equations are discretized on a grid with G lattice nodes, the Liouville distribution  $P_G$  becomes a G-variate PDF  $P_G(\mathbf{u}_1 \dots \mathbf{u}_G)$  which lives in a O(G)-dimensional space, where for large-scale turbulent flow applications, G can reach values of multibillions. However, it should be noted that for most practical purposes, the G-body Liouville PDF is an hotel with vastly more rooms than customers, meaning that (much) lower order marginals often suffice to deliver the essential physical information. Key to the success of the program is the ability to find an appropriate closure, namely an effective kinetic equation for the low order marginals. This is a classical topic in non-equilibrium statistical physics, which may draw significant benefits from modern developments in tensor networks theory [34,35]. In [36], the authors develop a general and elegant framework based on the Koopman-von Neumann and the level-set approach to classical nonlinear field theories [36]. The formalism is applied to hyperbolic PDEs and Hamilton-Jacobi equations, but its extension to the Navier-Stokes equations is addressed only marginally, making it difficult to draw firm conclusions.

Quantum-fluid duality: inverse Madelung transform. Formal analogies between quantum mechanics and fluid dynamics have been noted since the early days of quantum physics, most notably with the work of Madelung, who noted that upon writing the wave function in eikonal form  $\Psi = \rho^{1/2} e^{i\theta}$ , the imaginary part of the Schroedinger equation turns into the continuity equation, while the real



Fig. 3: Schematics of the quantum-fluid duality. The Schroedinger equation (SCE) maps one to one to the Madelung fluid (MAF), which is compressible, inviscid, irrotational and subject to quantum potential (pressure). The idea of the inverse Madelung transform is to generate a generalized Schroedinger equation (GSCE) equivalent to the compressible Navier-Stokes fluid. By solving the GSCE on a quantum computer one would then solve the Navier-Stokes physics.

one provides the following Madelung fluid equation:

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla (V_C + V_Q), \tag{10}$$

where  $\mathbf{u} = (\hbar/m) \nabla \theta$  is the fluid velocity,  $V_C$  the classical potential and  $V_Q = (\hbar^2/2m)\rho^{-1/2}\Delta\rho^{1/2}$  is the so-called quantum potential. The Madelung formulation shows that the Schroedinger equation behaves like an inviscid, irrotational fluid subject to the classical potential  $V_C$  plus a genuinely quantum potential  $V_Q$  (see fig. 3). This analogy has interesting interpretations for the hidden-variables theory of quantum mechanics, which are beyond the scope of this Perspective. Here we simply wish to highlight its operational value, *i.e.*, it permits to solve quantum problems using numerical methods for fluids. In the context of quantum computing, we are interested in taking the opposite path, namely using quantum computers to solve fluid problems in quantum mechanical vests. The major caveat is that the Madelung fluid is a far distant relative of classical Navier-Stokes fluids, the main points of departure being i) dissipation, ii) non-gradient flow, iii) absence of quantum potential. Very recent work has shown how to mend points ii) and iii) using quaternions, but still leaves item i) open [37]. Encouraging work to solve item i) as well has just appeared [38].

Quantum spectral methods. Given the major role played by spectral methods for the simulation of classical fluids (in simple geometries), it is natural to wonder about the viability of quantum computing analogues. Quantum spectral methods have been discussed recently in the literature [39], but only for linear differential equations. Spectral Chebishev representations have been used to define functions as expectation values of parametrized differential quantum circuits (DQCs) [40]. Such circuits have been utilized to solve a variety of non-trivial nonlinear equations, including the one-dimensional Navier-Stokes in a Laval nozzle, training the DQCs over a set of 20 to 40 grid points.

Low-Reynolds flows. – Last but definitely not least, the physics of fluids is rich in interesting problems at low-Reynolds flows, especially in microfluidics, soft matter and biology [41–43]. For instance, it would be of great interest to devise a *quantum multi-scale* application, coupling quantum algorithms for biomolecules swimming in a water solvent described by a quantum algorithm for low-Reynolds fluid flow. Given that low-Reynolds flows are non-local, perhaps the inherent non-locality of quantum mechanics could prove helpful in representing the classical non-locality of low-Reynolds flows.

Conclusions. – In summary, we have presented a survey of the main current approaches to the quantum simulation of classical fluids. Various obstacles stand in the way of the efficient simulation of fluid flows on quantum computers, especially at high Reynolds numbers. A few potential ways out have been illustrated, but their practical implementation commands major advances in quantum technology, particularly quantum error correction [44]. Assessing to what extent quantum computers can deal with nonlinearity and, more generally, withstand the tendency of quantum systems to become classical at macroscales/high temperatures, is not only of practical but also of major foundational interest. Quantum computers offer indeed a unique opportunity to ask questions that the founding fathers of quantum mechanics could only formulate as "Gedanken Experiments".

The authors have benefited from valuable discussions with S. S. BHARADWAJ, D. BUARIA, P. COVENEY, N. DE-FENU, G. GALLI, M. GROSSI, B. HUANG, A. MEZZACAPO, S. RUFFO, A. SOLFANELLI and T. WEAVING. SS wishes to acknowledge enlightening discussions with M. BERRY and S. DAS SARMA. He also acknowledges financial support form the Italian National Centre for HPC, Big Data and Quantum Computing (CN00000013).

\* \* \*

#### REFERENCES

- NIELSON M. A. and CHUANG I. L., Quantum Computation and Quantum Information-10th Anniversary Edition (Cambridge University Press) 2010.
- [2] FEYNMAN R., Int. J. Mod. Phys., 6 (1982) 467.
- [3] DEUTSCH D., Proc. R. Soc. London A., 400 (1985) 97.
- [4] Preskill J., Quantum, 2 (2018) 79.
- [5] https://www.ibm.com/quantum/roadmap.
- [6] BRAVYI S., DIAL O., GAMBETTA J. M., GIL D. and NAZARIO Z., J. Appl. Phys., 132 (2022) 160902.
- [7] YEPEZ J., *Phys. Rev. E*, **63** (2001) 046702.
- [8] KOHN W., Rev. Mod. Phys., **71** (1999) 1253.
- [9] O'MALLEY P. J. J. *et al.*, *Phys. Rev. X*, 6 (2016) 031007.
  [10] VORWERK C., SHENG N., GOVONI M., HUANG B. and
- GALLI G., Nat. Comput. Sci., 2 (2022) 424.

- [11] BHARADWAJ S. S. and SREENIVASAN K. R., Quantum computation of fluid dynamics, arXiv preprint, arXiv: 2007.09147 [quant-ph] (17 July 2020).
- [12] SPRAGUE M., BOLDYREV S., FISCHER P., GROUT R., GUSTAFSON W. I. and MOSER R., Turbulent Flow Simulations at the Exascale: Opportunities and Challenges Workshop, August 4–5, 2015, Washington D.C. (U.S. Department of Energy) 2017.
- [13] TENNIE F. and PALMER T. N., Quantum computers for weather and climate prediction: The good the bad and the noisy, arXiv:2210.17460v1 [quant-ph] (31 October 2022).
- [14] GRIFFIN K. P., JAIN S. S., FLINT T. J. and CHAN W. H. R., Investigation of quantum algorithms for direct numerical simulation of the Navier-Stokes equations, Center for Turbulence Research Annual Research Briefs (Center for Turbulence Research, Stanford University) 2019, pp. 347–363.
- [15] HARROW A. W., HASSIDIM A. and LLOYD S., Phys. Rev. Lett., 103 (2009) 150502.
- [16] BRASSARD G., HØYER P., MOSCA M. and TAPP A., AMS Contemp. Math., 305 (2002) 53.
- [17] STEIJL R., Quantum algorithms for fluid simulations, http://dx.doi.org/10.5772/intechopen.86685 (2019).
- [18] GAITAN F., npj Quantum Inf., 60 (2020).
- [19] BUDINSKI L., Int. J. Quantum Inf., 20 (2022) 2150039.
- [20] KACEWIZ B., Randomized and Quantum Algorithms Yield a Speed-Up for Initial Value Problems, arXiv:quantph/0311148 [quant-ph] (21 November 2003).
- [21] BUDINSKI L., Quantum Inf. Process., 20 (2021) 57.
- [22] SUCCI S., The Lattice Boltzmann Equation (For Fluids and Beyond) (Oxford University Press) 2001.
- [23] BERNASCHI M., MELCHIONNA S. and SUCCI S., Rev. Mod. Phys., 91 (2019) 025004.
- [24] LUBASCH M., JOO J., MOINIER P., KIFFNER M. and JAKSCH D., *Phys. Rev. A*, **101** (2021) 010301(R).
- [25] CARLEMAN T., Acta Math., **59** (1932) 63.
- [26] LIU J. P., KOLDEN H. O., KROVI H. K. et al., Proc. Natl. Acad. Sci. U.S.A., 118 (2021) e2026805118.
- $[27]\,$  Itani W. and Succi S., Fluids, 7 (2022) 24.
- [28] TODOROVA B. N. and STEIJL R., J. Comput. Phys., 409 (2020) 109347.
- [29] MEZZACAPO A., SANZ M., LAMATA L., EGUSQUIZA I. L., SUCCI S. and SOLANO E., *Sci. Rep.*, 5 (2015) 1.

- [30] SUCCI S. and BENZI R., Phys. D: Nonlinear Phenom., 69 (1993) 327.
- [31] ITANI W., SREENIVASAN K. and SUCCI S., Quantum Algorithm for Lattice Boltzmann (QALB) Simulation of Incompressible Fluids with a Nonlinear Collision Term, arXiv preprint, arXiv:2304.05915 [quant-ph] (12 April 2023).
- [32] LI X., YIN X., WIEBE N., CHUN J., SCHENTER G. K., CHEUNG M. and MUELMENSTADT J., Potential quantum advantage for simulation of fluid dynamics, arXiv: 2303.16550v2 [quant-ph] (8 April 2023).
- [33] SUCCI S., ITANI W., SREENVASAN K. and STEIJL R., Ensemble fluid dynamic simulations on quantum computers, arXiv preprint, arXiv:2304.05915 [quant-ph] (11 April 2023).
- [34] ORUS R., Nat. Rev. Phys., 1 (2019) 538.
- [35] GOURIANOV N., LUBASCH M., DOLGOV S. et al., Nat. Comput. Sci., 2 (2022) 30.
- [36] JIN S., LIU N. and YU Y., J. Comput. Phys., 487 (2023) 112149.
- [37] MENG Z. and YANG Y., Quantum computing of fluid dynamics using the hydrodynamic Schroedinger equation, arXiv:2302.09741.v1 [physics.flu-dyn] (20 February 2023).
- [38] SUCCI S. and TIRIBOCCHI A., Navier-Stokes-Schroedinger equation for dissipative fluids, arXiv preprint, arXiv: 2308.05879 [physics.flu.dyn] (10 August 2023).
- [39] CHILDS A. M. and LIU J.-P., Commun. Math. Phys. (2020) 1.
- [40] KYRIIENKO O., PAINE A. E. and ELFVING V. E., Phys. Rev. A, 103 (2021) 052416.
- [41] STONE H. A., STROOCK A. D. and AJDARI A., Annu. Rev. Fluid Mech., 36 (2004) 381.
- [42] DIOTALLEVI F., BIFERALE L., CHIBBARO S., LAMURA A., PONTRELLI G., SBRAGAGLIA M. and SUCCI S., *Eur. Phys. J. ST*, **166** (2009) 111.
- [43] SUCCI S., The Lattice Boltzmann Equation for Complex States of Flowing Matter (Oxford University Press) 2018.
- [44] DAS SARMA S., Quantum computing has a hype problem, MIT Technological Review, https://www.technologyre view.com/2022/03/28/1048355/quantum-computing-has -a-hype-problem/ (28 March 2022).