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# FLUID DYNAMICISTS NEED TO ADD QUANTUM MECHANICS INTO THEIR TOOLBOX

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## ABSTRACT

The Navier-Stokes equations describing fluid dynamics predate the thorough development of thermodynamics, let alone quantum mechanics. This is disconcerting given the utility of the hydrodynamic interpretation in the latter field. In this piece, we motivate the modernization of the fluid dynamics field through the progress that has been made in quantum mechanics and quantum computing.

Quantum computing is set to transform fluid dynamics, just as quantum and molecular mechanic methods transformed material science. It would provide a more rigorous framework with transferrable representation<sup>1</sup>, beyond scaling fluid dynamics' scaling analysis, on which innovative multiscale systems would be designed. However, 2020, and November in particular, saw a spree of algorithms for generic nonlinear systems of equations citing fluid flow amongst their applications<sup>2-4</sup>. This is in stark contrast to the earlier more physically involved developments, such as the quantum lattice gas algorithms<sup>5</sup> and the simulation of lattice Boltzmann equation by its analogy to Dirac's<sup>6</sup>. Despite the genericity of the former approach of utilizing quantum algorithms as a generic numerical solver<sup>7</sup>, it demonstrates a practical interest of quantum computing for fluid flows. A course-correction is due, based on placing fluid dynamics in context within quantum theory.

Apart from the exponential increase of computational space with system size, and possible quantum speed up expected, quantum mechanics offer the added advantage of fundamental representation empowering the computationally-expensive concurrent coupling<sup>8</sup> for multiphysics simulations. The unifying framework would allow such simulations to benefit from consistent deductive analysis<sup>9</sup> to reduce the problem size. Such reduced problems could be solved variationally<sup>10</sup>, with variational methods proving to be a universal model of quantum computing<sup>11</sup>.

Soon after Schrodinger put his equation in place, Madelung reformulated it to give a hydrodynamic interpretation. More recently, the quantized theory of fluid mechanics was reviewed and formulated as a quantum field theory<sup>12</sup>, and the effective field theory has been demonstrated as a tool for simulating and coupling different physical systems including fluid flows and gravity<sup>13,14</sup>. The hydrodynamic interpretation of quantum field theory arises from the applicability of the Madelung transform. We note that effective field theory could give a more rigorous framework for computation on a graph and the fully-discrete cellular automata as a fluid flow simulation tool. The approach, introduced in the 80s<sup>15</sup>, has been revived by efforts to reduce fluid flow problems into finite connected weighted graphs<sup>16,17</sup>, and, more recently, to simulate complex systems with physics-informed and neural and graph networks leveraging particle representation<sup>18,19</sup>. Afterall, universal physical theories and predictive modelling in other disciplines share the same parameter space hierarchy, whereby space compression gives rise to emergent theories<sup>20</sup>. It is, thus, unsurprising to see symbolic regression arising from graph modularity<sup>21</sup>.

Nobel laureate Hooft suggests that we consider quantum mechanics as a tool, not a theory<sup>22</sup>. Recent insights on Hooft's ontological quantum mechanics show that our physical reality could possibly be modeled by classical dynamics on a Hilbert space<sup>23</sup>. This further explains that the indeterministic nature of quantum mechanics is due to it being an incomplete, but not necessarily incorrect theory. Accordingly, the "Standard Model, together with gravitational interactions, might be viewed as a quantum mechanical approach" to analyze a classical system, and the existence of the "Arrow of Time" is better explained<sup>22</sup>. Similarly, fluid dynamics could be understood as a tool to arrive at breakthrough scientific insight. The fluid-gravity correspondence has long been established, and extended to matter fields and non-relativistic systems<sup>24</sup>. The quantum fluid dynamics formalism has been pioneered by Madelung with his transformation of the Schrodinger equation, detailed on by de Broglie, and further expanded by Bohm and others<sup>25</sup>. The hydrodynamical description has become as a popular tool for describing quantum mechanical systems<sup>26</sup>, as it allows a more intuitive interpretation of the dynamics<sup>25</sup>. This allows for leveraging the wealth of computational tools available for fluid dynamics<sup>25</sup>. Most recently, the de Broglie-Bohm theory has been repostulated so that it is no longer at odds with the Schrodinger equation, within a unified field theory of wave and particle quantum mechanics<sup>27</sup>. The quantum fluid dynamics formulation has also been coupled with the path integral approach<sup>28</sup>. With the de Broglie-Bohm quantum mechanical formulation rewritten into Navier-Stokes' over half a century ago<sup>29</sup>, bridging the fields of fluids and quantum mechanics, beyond the confines of quantum fluids, still has the potential to offer potential insights into both, and beyond.

Turbulence remains one of the "greatest unresolved" problems of physics because it is not a problem, it is an emergent phenomenon. Quantum mechanics eludes to its origins and its onset<sup>30</sup>. While there are claims that no mechanistic framework that captures how the interactions of vortices drive the turbulence cascade<sup>31</sup>, the cascade is observed in quantum fluids<sup>32</sup> with similarities to its classical analog despite distinct velocity statistics<sup>33</sup>. The differences observed in the two turbulent states owe to the long-range quantum order, and being to lose their significance as with the number of interacting quanta. This allows for the investigation of quantum and classical effects concurrently, helping us fundamentally understand turbulence. Geometric quantum hydrodynamics shows that vortex lines seek to decompose localized regions of curvature into helical configurations<sup>34</sup>. Moreover, quantum effects at sub-atomic levels deal with a compressible fluid susceptible to wave propagation, rather than a particle<sup>35</sup>. In addition, self-gravity contributes to the decoherence of a quantum state<sup>36</sup>.

The interchange between quantum mechanics and fluid dynamics as tools is readily available. The Navier-Stokes equations could be recovered from the Navier-Stokes-Poisson equation describing the motions of the electrons in a plasma<sup>37</sup>. The quantum Navier-Stokes equations have been derived from the Wigner-Fokker-Planck equation<sup>38</sup>. The full Navier-Stokes equations can be transformed into an extended Schrodinger equation<sup>35</sup>. We see that stochastic variation methods could derive the Schrodinger equation in a Lagrangian of particles, the Navier-Stokes and Gross-Pitaevski equations in a Lagrangian of continuum<sup>39</sup>. Information-loss mechanism gives rise to a probabilistic theory like that of a particle governed by Schrodinger's equation, from a deterministic one as that of a fluid described by Navier-Stokes<sup>40</sup>. The coarse-graining stance from quantum mechanics is that of the Einstein-Podolsky-Rosen paper which argued that the framework is a practical approach to circumvent working with the more complex underlying reality. Apart from randomness as a resource<sup>41</sup>, and quantum uncertainty, or locally consistent indeterminism at most quantum phenomena<sup>42</sup>, quite a bit of uncertainty still underlies the current-adopted quantum mechanical framework<sup>43</sup>. The de Broglie-Bohm pilot-wave theory offers a deterministic non-local alternative to standard quantum mechanics<sup>43,44</sup>. The transformed Schrodinger equation shows trace of de Broglie-Bohm formulation with the coefficient of the quantum potential being the only place where Planck's constant appears.

Said interchange could help us further expand our computational abilities. Shor pointed out that the Church-Turing statement is in fact about the physical world. Dirac noted that despite the laws underlying the mathematical theory of physics being largely known, the difficulty remains in applying them such they are soluble. It might be that the future of computing is indeed analogue<sup>45</sup>. In the spirit of cellular automata and von Neumann's self-building machines, we see that quantum computing platforms help understand, design and simulate quantum systems, which in turn feedback into the development of the former<sup>46</sup>. The study of fluid dynamics within the quantum framework, say for nanofluidics could set the stage for novel computation platforms, similar to microfluidic transistors<sup>47</sup>. Quantum fluids have already been shown to promote relatively stronger phonon-mediated optical coupling, key for configurable optical switches, circuits, and quantum interfaces, as well as further exploration of quantum fluid dynamics<sup>48</sup>. Perhaps fluid-based platforms would be more suitable for reaching the full capabilities of a quantum computer, with the ability to interconvert stationary and flying qubits, to faithfully transmit flying qubits between specified locations<sup>49</sup>.

While noisy intermediate-scale quantum (NISQ) computers are currently considered of limited use in the field<sup>50</sup>, the situation is expected to improve. The current qubit count at the order 70 already presents a computational space  $2^{70}$  larger than that of cutting edge direct numerical simulations (DNS)<sup>51</sup>. In addition, we already see the number of qubits doubling nearly every six months. Moreover, noise on NISQ devices is being tackled at a fast pace. It has now been shown that digital quantum simulation could retain controlled errors with relatively large steps in time evolution<sup>52</sup>, and hybrid classical-quantum algorithms have been put in use to mitigate errors. Both reduce the overall gate complexity of algorithms<sup>53</sup>. Most recently, the optimality of various query schedules in the noisy regime has been reported<sup>54</sup>. Overall, as of 2020, we are well on our way for practical interest in quantum computing for CFD by 2030, as per NASA'S CFD Vision 2030<sup>55</sup>.

Quantum computing, as it is, doesn't only help us poke holes in the quantum mechanic framework, putting us on the verge of a new theory, but also is of practical interest as applied to fluid flow problems. The drawback of not being able to access the full state vector might be irrelevant to engineering applications, where key performance metrics are in use such as stochastic moments for turbulent flow, heat transfer rate or drag coefficient. Stimulated by recent progress in computational frameworks for chemistry and material science<sup>56,57</sup>, we motivate that quantum algorithms for fluid flow simulation would find themselves in amicable company of quantum chemistry<sup>58-60</sup>, and light-matter interaction algorithms. This is set to accelerate the design and simulation of innovative multiphysics nanosystems<sup>61</sup> solving some of the world's most pressing challenges. From globe-saving photoelectrochemical reactors for carbon reduction<sup>62</sup> and water splitting, through tumor growth simulations for cancer treatment<sup>63-65</sup>, to fusion power<sup>66,67</sup>, the application are bountiful.

We see that thermodynamically consistent Navier-Stokes equations have already been developed<sup>68</sup>, and a quantum probability fluid model has been proposed mapping quantum mechanics to thermodynamics<sup>69</sup>. The latter map hints at the holographic principle of quantum gravity whilst the holographic duality relating fluids and horizons has thoroughly developed<sup>70</sup>. We are reminded that digital computers, and more generally computer science as a discipline were born after the their corresponding mathematical theory<sup>71</sup>.

Navier-Stokes predate the rigorous formulation of thermodynamics<sup>68</sup>, and the first quantum revolution<sup>72</sup>. It is now time to update it, along with its derivatives and application to leverage nearly two centuries of scientific breakthroughs. This could only be done by a change of perspective, and the combined efforts of the broad fluid dynamics community.

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