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A Quantum-Inspired Algorithm for Solving Differential Equations

A Quantum Inspired Approach to Exploit Turbulence Structures
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The Navier-Stokes equations, which describe Newtonian fluids, play a central role in fields like climate modeling, aerospace engineering, and astrophysics. Computational solutions to Navier-Stokes are crucial for theoretical investigations and practical applications.

Recently, a team of condensed matter quantum physicists and applied mathematicians simulated the incompressible Navier-Stokes equations in a surprising way, using techniques originally developed for quantum wavefunctions [1]. Not only does this idea work, but leads to highly accurate solutions that achieve high parameter compression ratios. It is also superior to certain previous approximations used in the field. As a bonus, the method can be straightforwardly ported to a quantum computer. The quantum-inspired approach they used takes advantage of developments from condensed-matter physics for representing wavefunctions with limited quantum entanglement, repurposed to describe the velocity field of a classical fluid. This approach was pioneered in the applied mathematics community where it is known as "quantics tensor train" (QTT) [2, 3, 4].

To understand how a classical function can be mapped to a quantum state, consider a one-dimensional function $f(x)$ with $0 \leq x < 1$. The variable x can be expressed to high precision as a *binary fraction*

$$x = 0.b_1 b_2 \cdots b_n = b_1/2 + b_2/2^2 + \ldots + b_n/2^n \ . \tag{1}$$

described by bits $b_i = 0, 1$. (For example, $1/3 \approx 0.010101$.) This way of writing numbers is similar to the to the binary representation of integers, but with the numbers stepping through a finely-spaced grid of spacing $1/2^n$ instead of steps of size 1. Next we can write the values the function $f(x)$ takes on this grid as $f(x) = f(0.b_1 b_2 \cdots b_n) = F^{b_1 b_2 \cdots b_n}$ so that the values of $f(x)$ have been repackaged into an n-index tensor F. The last move is to think of F as labeling the amplitudes of a many-body wavefunction of n qubits:

$$|f\rangle = \sum_{b_1, b_2, \ldots, b_n} F^{b_1 b_2 \cdots b_n} |b_1 b_2 \cdots b_n\rangle \ . \tag{2}$$

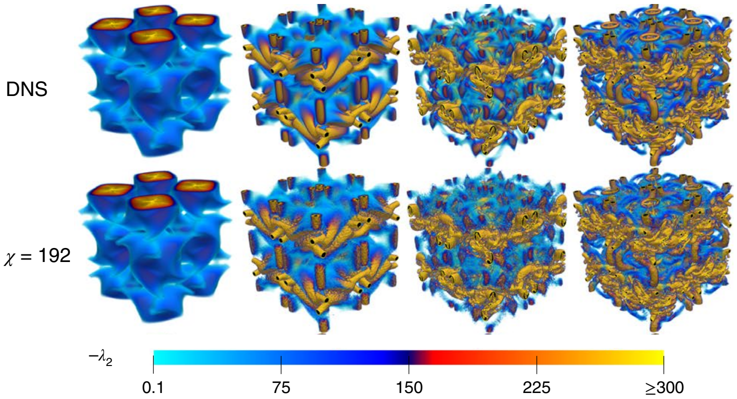

Figure 1: Solutions to the 3D Navier-Stokes equations for the Taylor-Green vortex configuration. Shown from left to right are results for times $t/T_0 = 0.2, 0.8, 1.4, 2.0$ where T_0 is a characteristic time scale. The upper row shows results obtained via precise direct numerical simulation (DNS) while the lower row shows results obtained using quantum-inspired techniques based on matrix product states (MPS) of maximum bond dimension or rank $\chi = 192$. (Taken from the highlighted paper; Copyright Springer Nature Ltd. (2022).)

States of this type turn out to have low entanglement for a wide class of functions $f(x)$ [2]. For example, both the functions $f(x) = e^{ikx}$ and $f(x) = \delta(x - k)$ give states $|f\rangle$ with precisely zero entanglement, while many other smooth functions have entanglement rather less than a typical ground state of a many-body Hamiltonian. Some functions require more entanglement though, such as momentum-space Green's functions for systems with large Fermi surfaces [5] and 3D Navier-Stokes flows with high Reynolds numbers [1]—see more below.

States with low entanglement can be represented compactly using tensor networks such as matrix product states (MPS), originally developed for solving quantum condensed-matter physics problems, as well as tasks like simulating quantum computers. An MPS representation of an n-qubit quantum state approximately factorizes the state into n tensors, contracted together with "virtual" or bond indices that run over χ values. The size of χ determines how entangled a state the MPS can represent and how costly they are to store and perform computations with. Differential operators such as $\partial^2/\partial x^2$ can also be easily represented (as "MPO" tensor networks). Powerful algorithms for time evolving (such as "TDVP") or solving eigenvalue problems (such as "DMRG") turn out to be essentially the same in the continuum setting. The generalization to multiple variables is straightforward, and is just an MPS with two physical indices on each tensor for a 2D function $f(x, y)$ or three physical indices for a 3D function $f(x, y, z)$ and so on.

Let us pause to note how remarkable this is: for decades, tensor networks have been used primarily for representing quantum many-body states which are high-dimensional functions of *discrete* variables $\Psi(s_1, s_2, s_3, \ldots, s_n)$ where the $s_j = 1, 2, ..., d$ could be spins or particle occupations. It turns out they are just as good, if not better, at representing low-dimensional, continuous functions $f(x)$ too. For continuous functions, the meaning of entanglement turns out to be rather different, and captures *correlations between scales* rather than correlations between the left and right halves of a quantum system.

The authors of the highlighted paper emphasize the connection between low entanglement and approximate scale-separability throughout their work. In the theory of fluids, the ratio of the largest to smallest scales is related to the *Reynolds number Re* describing the flow. Because the efficiency of the MPS ansatz for the velocity field relies on scale separability, the authors find that the MPS bond dimension χ needed to get accurate results grows with the Reynolds number. For two-dimensional fluids it grows for small *Re* then plateaus, while for three-dimensional fluids the bond dimension grows as a power law in *Re*.

Looking into the future, what other ideas from the quantum physics toolbox can be applied to classical differential equation solving? One can certainly envision the connection between Reynolds number and entanglement being made more rigorous and being generalized to other differential equations. In fact, a vision of quantum-inspired classical methods based on tensor networks is beginning to emerge for a wide variety of mathematical problems [6], including other differential equations such as the Fokker-Planck [7] and Vlasov-Poisson [8] equations, and is already coming full circle back into quantum many-body physics for applications such as such as solving the Dyson equation [5].

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