A quantum-inspired approach to exploit turbulence structures

Nikita Gourianov1✉, Michael Lubasch2, Sergey Dolgov3, Quincy Y. van den Berg1, Hessam Babaee4, Peyman Givi4, Martin Kiffner1,5 and Dieter Jaksch1,5,6✉

Understanding turbulence is key to our comprehension of many natural and technological flow processes. At the heart of this phenomenon lies its intricate multiscale nature, describing the coupling between different-sized eddies in space and time. Here we analyze the structure of turbulent flows by quantifying correlations between different length scales using methods inspired from quantum many-body physics. We present the results for interscale correlations of two paradigmatic flow examples, and use these insights along with tensor network theory to design a structure-resolving algorithm for simulating turbulent flows. With this algorithm, we find that the incompressible Navier–Stokes equations can be accurately solved even when reducing the number of parameters required to represent the velocity field by more than one order of magnitude compared to direct numerical simulation. Our quantum-inspired approach provides a pathway towards conducting computational fluid dynamics on quantum computers.

Turbulence can phenomenologically be described by mutually interacting eddies stretching across an extremely broad range of length and time scales. These spatial scales range from the largest size of the energy-containing eddies (known as the integral scale, $L$) to the smallest ones, known as the Kolmogorov microscale (1). The separation between these scales is $L/\eta \approx Re^{1/4}$ where $Re$ is the Reynolds number. A salient feature of turbulent flows is the scale-locality of the turbulent energy cascade, in the sense that eddies at a given length scale predominantly interact with other eddies of similar scale.

Since the pioneering work of Orszag and Patterson, direct numerical simulation (DNS) of the Navier–Stokes equations has been widely regarded as the computational method with the highest fidelity in capturing the dynamics of turbulent flows. Virtually all classical DNS methods (for example, spectral polynomial/Fourier, finite volume and finite element) are scale-resolving, and increasing the number of variables (for example, grid points $M$) resolves increasingly finer scales. However, the wide separation of turbulent flow scales limits the range of Reynolds numbers that can be computationally considered. Straightforward estimates indicate that simulation of an incompressible flow inside a three-dimensional (3D) volume of $(10^5)^3$ with $Re \approx 1 \times 10^5$ would require decades of central processing unit time on a 1 teraflop computer.

To mitigate this huge numerical complexity, the importance of exploiting so-called coherent structures of turbulence has long been recognized. This eventually led to the rise of structure-resolving methodologies (for example, proper orthogonal decomposition) that extract and exploit coherent structures of the solution. They represent the flow field down to the Kolmogorov microscale through a superposition of modes, but with their number being much smaller than the total number of grid points in DNS. Up to now, the majority of the developed techniques have been used for diagnostic purposes. Using reduced-order models for predictive purposes is hampered by difficulties in identifying suitable modes and remains an active area of research.

A similar challenge has been successfully tackled in a completely different area of physics. Quantum many-body systems are described by elements of a vector space whose dimension grows exponentially with the number of particles. This makes direct simulations quickly impossible with increasing system size. Tensor network methods made a revolutionary advance in simulating quantum systems with local interactions by removing unrealized long-distance correlations, thus enabling the simulation of physical systems that are otherwise intractable. The correlations of interest for quantum systems are known as quantum entanglement, and weakly entangled systems or those where quantum correlations are concentrated at the boundaries between different parts of the system (that is, they are structured to follow a so-called area law) can be efficiently simulated with tensor network methods.

In this Article we adapt these successful strategies for treating quantum many-body systems to exploit the scale-locality of turbulence. This quantum-inspired approach allows us to develop structure-resolving methods for both diagnostic and predictive purposes.

We first introduce tools from tensor network theory to analyze different length scales of flow in a manner different from both the traditional wavenumber approach and more recent investigations in real space. We then apply these diagnostic tools to study DNS solutions of two paradigmatic flow configurations: a 2D temporally developing jet (TDJ) and the 3D Taylor–Green vortex (TGV). Our study reveals that the scale-locality of turbulence restricts the amount of correlation present between different length scales. This motivates us to encode turbulence in a simple tensor network called matrix product state (MPS). The connectivity of the MPS network is well adapted to describing scale-local flows and hence exploiting the structures of turbulence. We design an algorithm for simulating the incompressible Navier–Stokes equations (INSE) in the compressed MPS format. This algorithm remains accurate even when reducing...
the number of variables parametrizing the solution (NVPS) by more than one order of magnitude. The conceptual similarity between the tensor network algorithm presented here and those used in quantum physics opens the possibility of conducting computational fluid dynamics on a quantum computer.

**Results**

**Quantifying interscale correlations.** Throughout this work we follow the standard approach in computational fluid dynamics and discretize the computational domain. Each spatial dimension is discretized by $2^N$ grid points, where $N$ is a positive integer. In this way, the velocity field

$$V(t, r_q) = \sum_{i=1}^{K} u_i(t, r_q) \chi_i$$

and its Cartesian components $u_i$ are discrete functions of the grid points $r_q$ where $K$ is the spatial dimension and $\chi_i$ are Cartesian unit vectors. We measure the interscale correlations by using the Schmidt (singular value) decomposition to systematically divide the computational grid into sub-grids, as illustrated in Fig. 1a for $K=2$.

We decompose (for details, see the Schmidt decomposition section in the Methods) each component $u_i$ on this $2^N \times 2^N$ grid into functions $R$ and $f$ on a coarse and a fine subgrid, respectively:

$$u_i(t, r_q) = \sum_{\alpha=1}^{d(n)} \lambda_{\alpha} R_{\alpha}(t, X_\alpha) f_{\alpha}(t, x_\alpha), \quad r_q = X_\alpha + x_\alpha.$$ (2)

Positions $X_\alpha$ correspond to a quadratic grid with $2^N \times 2^N$ points (coarse grid), and $x_\alpha$ correspond to a fine sub-grid with $2^{N-n} \times 2^{N-n}$ grid points. The functions $R_{\alpha}$ and $f_{\alpha}$ obey the orthonormality condition

$$\sum_{\beta} R_{\alpha}(t, X_\beta) R_{\beta}(t, X_\alpha) = \sum_{\beta} f_{\alpha}(t, x_\beta) f_{\beta}(t, x_\alpha) = \delta_{\alpha\beta},$$ (3)

where $\delta_{\alpha\beta}$ is the Kronecker delta. The parameter $n=1, \ldots, N-1$ labels the possible bipartitions of the square lattice in coarse and fine grids (in Fig. 1a $N=10$ and $n=2$). The Schmidt number $d(n)$ denotes the number of retained terms in the summation in equation (2), and each product $R_{\alpha} f_{\alpha}$ is weighted by a Schmidt coefficient $\lambda_{\alpha} \geq 0$. These coefficients appear in descending order $\lambda_1 \geq \lambda_2 \geq \lambda_{d(n)}$, so varying $d(n)$ will only add or remove the least important of the orthonormal basis functions. Here we take $d(n)$ as a quantitative measure for the interscale correlations of turbulent flows at a given bipartition $n$ of the lattice: $d(n)=1$ corresponds to an uncorrelated product state, and with increasing $d(n)$ the flow becomes more strongly correlated between the coarse and the fine grid. Note that although the $d(n)=1$ product state exhibits no interscale
correlations, it is still highly correlated in space because the fine grid dependence is repeated.

Truncating the Schmidt decomposition in equation (2) approximates \( u_1 \) in an orthonormal time-dependent basis that evolves with the fluid flow to optimally capture spatially correlated structures. This is in contrast to classical scientific computing techniques (implemented through, for example, finite-difference or spectral methods) where the bases are structure-agnostic; that is, they are chosen a priori and disregard any structure in the solution.

We first apply the decomposition in equation (2) to DNS solutions of the INSE (equation (7)) for the TDJ shown in the top row of Fig. 2a. The TDJ comprises a central jet flow along the \( x \) direction, and Kelvin–Helmholtz instabilities in the boundary layer of the jet eventually cause it to collapse (see equations (9)–(15) for the initial flow conditions). We decompose each velocity component according to equation (2), which is an exact representation if \( d(n) = \Gamma^{2D}(n) \) with (for details, see Supplementary Section 2)

\[
\Gamma^{2D}(n) = \min(4^n, 4^{N-n}).
\]  

(4)

The Schmidt numbers \( d_{00}(n, t) \) resulting in a 99% accurate representation of the DNS solutions are shown in Fig. 1c. We find \( \chi_{00} = 207 \),

\[
\Gamma^{3D}(n) = \min(8^n, 8^{N-n}).
\]  

(5)

**Fig. 2 | 2D temporally developing jet.** Dynamical simulation of the INSE in 2D for a planar jet streaming along \( x \) with \( Re = 1,000 \), as defined in the Set-up of numerical experiments section in the Methods. a. Snapshots of the vorticity and velocity fields taken at \( t/T_0 = 0.25, 0.75, 1.25, 1.75 \) (left to right). Red corresponds to positive vorticity (counter-clockwise flow) and blue to negative vorticity (clockwise). The top row corresponds to DNS results on a quadratic \( 2^n \times 2^n \) grid (cf. Fig. 1a). Rows 2–4 are MPS results with different maximal bond dimensions \( \chi \). The bottom three rows are for URDNS on quadratic grids, as indicated. b. Reynolds stress \( \tau_{yz} \) (equation (14)) between the streamwise and cross-stream directions as a function of time and \( y \) coordinate. Red (blue) corresponds to positive (negative) stress.
such that all values of $d_w$ in Fig. 1c are contained within the blue-shaded area $\mathcal{M}$ corresponding to $d(n) = \min \left( f^{3D}(n), 207 \right)$ in equation (2). Because $\chi_w$ is much smaller than the upper vertex of the area $\mathcal{T}$ at $f^{3D}(4) = 2^{12}$, the interscale correlations of DNS solutions are far from being saturated (more details on the Schmidt coefficients are provided in Supplementary Section 1).

Next we investigate how the maximal Schmidt number $\chi_w$ scales with the Reynolds number Re (Fig. 1d). We find that $\chi_w$ saturates in the 2D case for Re $\gtrsim 200$. This suggests that interscale correlations of 2D flows are bounded, in analogy to quantum correlations in gapped 1D quantum systems with local interactions. In the 3D case, $\chi_w$ increases according to a power law. The NVPS for $d(n) = \min \left( f^{3D}(n), \chi_w \right)$ scales as $\sim \chi_w^2 \log M$ (Supplementary Section 2). Kolmogorov’s theory\(^3\) states that the number of grid points $M = 8^d$ must scale with the Reynolds number according to $M \sim (\ell/\eta)^3 \sim Re^{9/4}$ to resolve all spatial scales. This implies that the NVPS of $\mathcal{M}$ only scales as $\sim Re^{9/4} \log Re$, which is a substantially slower increase with Re compared to the NVPS of DNS, $\sim Re^{9/4}$.

**Tensor network algorithm.** The previous results demonstrate that it is beneficial to find a representation of flow fields where limiting the amount of interscale correlations directly translates into a reduction of the NVPS. This can be achieved by expressing each velocity component in a compressed tensor network format known as a matrix product state (MPS) or tensor train decomposition.\(^{13,14,25,26}\) Our MPS encoding of function values is chosen such that it is consistent with the decomposition in equation (2) (Supplementary Section 2). It comprises products of $N$ matrices $A^{n_1}$ with dimension $d(n-1) \times d(n)$, where $2^n$ is the number of grid points in each spatial direction, $n=1, \ldots, N$ and $d(0) = d(N) = 1$ (refs. \(^{27,28}\)). The matrix $A^{n_1}$ is associated with a length scale $L_{n_1}/2^n$, and its dimension $d(n)$ controls the maximum amount of correlations allowed between neighboring scales. The nearest-neighbor correlations are mediated directly by each matrix product, while correlations between further distant length scales can only be captured indirectly by traversing several matrix products. These properties make MPS well suited for the description of scale-local turbulent flows where correlations between vastly different length scales are expected to be small.

Here we consider MPSs of bond dimension $\chi$ where we set $d(n) = \min \left( f^{3D}(n), \chi \right)$ in 2D and $d(n) = \min \left( f^{3D}(n), \chi \right)$ in 3D. The bond dimension $\chi$ controls the level of compression in the MPS format. For example, the interscale correlations captured by an MPS with bond dimension $\chi = 25$ ($\chi = 207$) are represented by the blue-shaded area in Fig. 1b (Fig. 1c). If $\chi$ is kept constant as $N$ increases, the number of MPS parameters scales logarithmically with the total number of grid points, resulting in an exponential reduction of the NVPS compared to DNS. However, we emphasize that this reduction does not truncate the range of length scales covered by the MPS ansatz—it only limits the amount of interscale correlations.

To fully utilize this dimensionality reduction for numerical simulations on large grids, we devise an algorithm for solving the INSE without leaving the compressed MPS manifold $\mathcal{M}$ (Matrix product state algorithm section in the Methods). We use a second-order Runge–Kutta time-stepping scheme and discretize spatial derivatives in the same way as the DNS solver, which utilizes an eighth-order finite-difference stencil.

**Validation of the tensor network algorithm.** We now investigate how well the dynamics of turbulent flow are captured inside the MPS manifold $\mathcal{M}$ by comparing our algorithm against DNS for different compressions $\chi$. Reducing the bond dimension $\chi$ reduces the NVPS. The analog of reducing the bond dimension in traditional DNS is to perform under-resolved DNS (URDNS), where the simulation is carried out on a coarse grid not covering all relevant length scales. URDNS can be considered as the most basic form of large eddy simulations,\(^{29,31}\) where no explicit models are employed to account for the disregarded subgrid scales (Direct numerical simulation algorithm section in the Methods). For a fair comparison...
between MPS and URDNS, we choose for every bond dimension $\chi$ a corresponding URDNS grid such that the NVPS is approximately equal for both methods.

The results for the TJF and for the different solvers are shown in Fig. 2. The top row in Fig. 2a corresponds to DNS and illustrates how the background perturbations in the shear layer are amplified ($t/T_s = 0.25$) until the layer rolls up into vortices that in turn pair up and merge into progressively larger vortices ($t/T_s = 0.75, 1.25$) until $t/T_s = 1.75$, when pairing is terminated. The stress exerted upon the mean flow by turbulent fluctuations is given by the Reynolds stress tensor, one of whose components is plotted in Fig. 2b. These results are in accord with the Boussinesq approximation, which indicates that the Reynolds stresses are of the opposite sign of the mean streamwise velocity gradients along the cross-stream direction. The exception is when the vortex pairing is terminated, and the growth of the shear layer is temporarily paused. Correctly resolving $r_{12}$ is important for the physical validity of the simulation.

We now evaluate the accuracy of the MPS and URDNS simulations. Rows 2–4 in Fig. 2 show MPS results for $\chi=118, 74$ and 33, corresponding to compression ratios of approximately $1:8, 1:16$ and $1:64$ compared to DNS, respectively. These results show that the large-scale dynamics of the jet are correctly captured by all the MPS simulations, with $\chi=74$ and 118 practically indistinguishable from DNS. The bottom three rows in Fig. 2 show the URDNS results for different grid sizes. We find that the $362^2$ grid (corresponding to $\chi=118$) is only accurate until $t/T_s \approx 1.2$, while the lower-resolution URDNS already fails at $t/T_s \approx 0.75$. This is observed in both the instantaneous vorticity dynamics results and the Reynolds stresses. The MPS algorithm achieves a much higher accuracy than URDNS for the same NVPS (Table 1 provides quantitative results). This result can also be understood in terms of the interscale correlations shown in Fig. 1b, where the domain corresponding to URDNS on the $256^2$ grid is shown by the gray-shaded area $\mathcal{W}$. A substantial amount of correlations present in the DNS solutions are outside of $\mathcal{W}$, which is consistent with our finding that URDNS cannot accurately represent the DNS solutions.

Next we discuss the corresponding results for the dynamics of the TGV. The top row in Fig. 3a corresponds to DNS and illustrates how the original vortex collapses ($t/T_s = 0.2$) into turbulent worm-like structures ($t/T_s = 0.8$) that become progressively more turbulent ($t/T_s = 1.4$) until viscosity eventually dissipates these vortical structures ($t/T_s = 2$). Rows 2–4 and 5–7 in Fig. 3a correspond to the results of our MPS algorithm and to URDNS, respectively. The bond dimensions and grid sizes have been chosen such that the compression ratios compared to DNS are approximately $1:25$ (rows 2 and 5), $1:49$ (rows 3 and 6) and $1:78$ (rows 4 and 7). Although MPS produces a solution comparable to DNS for a compression ratio of $1:49$ ($\chi=128$), the corresponding URDNS results clearly deviate from DNS. Discrepancies between URDNS and DNS are even visible for the largest URDNS grid (compression 1:25).

A more quantitative analysis of the performance of MPS versus URDNS is shown in Fig. 3b. In the non-DNS simulations, a portion of the energy is erroneously lost to numerical diffusion. The amount of numerical diffusion can be measured by comparing the physical global dissipation (enstrophy) to the global kinetic energy dissipation (equations (17) and (18)). The MPS predictions at $\chi \geq 128$ are consistent with both the DNS results here and in previous work\cite{24}. We find that the MPS simulations with $\chi = 128$ and 192 dissipate the energy more accurately than any of the URDNS results, especially for $t/T_s \geq 1.4$ (Table 1). As in the 2D case, this outcome is in line with the interscale correlations shown in Fig. 1c, where the domain corresponding to URDNS on the $64^2$ grid is shown by the gray-shaded area $\mathcal{W}$. The bipartitions at $n = 5$, 6 and 7 are associated with comparatively large Schmidt numbers for $t/T_s \geq 0.8$, and hence these interscale correlations cannot be captured by URDNS.

**Table 1 | Quantitative comparison between MPS and URDNS simulations for the TDJ and TGV flow cases.**

| Case | Compression | Scheme | Inaccuracy |
|------|-------------|--------|------------|
| TDJ  | 1:1         | DNS    | 0          |
| TDJ  | 1:8         | MPS    | 0.0119     |
| TDJ  | 1:8         | URDNS  | 0.2612     |
| TDJ  | 1:16        | MPS    | 0.0485     |
| TDJ  | 1:16        | URDNS  | 0.3333     |
| TDJ  | 1:64        | MPS    | 0.2404     |
| TDJ  | 1:64        | URDNS  | 0.3201     |
| TGV  | 1:1         | DNS    | 0.002      |
| TGV  | 1:25        | MPS    | 0.0385     |
| TGV  | 1:25        | URDNS  | 0.1599     |
| TGV  | 1:49        | MPS    | 0.0844     |
| TGV  | 1:49        | URDNS  | 0.2133     |
| TGV  | 1:78        | MPS    | 0.2618     |
| TGV  | 1:78        | URDNS  | 0.4563     |

The rows corresponding to the TDJ flow tabulate $e(s,c)$, as defined in equation (19). $e(s,c)$ measures the discrepancy between the URDNS and MPS Reynolds stresses and those of DNS in Fig. 2b. The TGV flow case rows tabulate $e(s,c)$, which is defined in equation (20) and represents the total numerical diffusion in Fig. 2b. The nearer $e(s,c)$ or $e(s,c)$ is to 0, the closer the simulation in question is to DNS.

**Discussion**

The structure-resolving properties of MPSs can lead to a reduced computational cost. The computational complexity of our MPS algorithm is $\sim \chi^4 \log M$, as explained in Supplementary Section 4. Resolving down to the Kolmogorov microscale $\eta$ requires $M \sim (1/\eta)^K \sim \text{Re}^{K/4}$ grid points. Assuming $r \approx \text{Re}^{1/4}$, the overall scaling of the MPS algorithm becomes $\sim \text{Re}^{9/4} \log \text{Re}$. Comparing this to the scaling of DNS, which is $\sim M \log M \sim \text{Re}^{3/4} \log \text{Re}$ (Direct numerical simulation algorithm section in the Methods), we see that the MPS algorithm outperforms DNS when $r < 3K/16$. For our 2D example, Fig. 1d suggests $r = 0$, which leads to an exponential speed-up of the MPS algorithm over DNS for sufficiently large Re. It would be interesting to investigate whether this saturation of the Schmidt number with Re is a unique case for just the TJF flow, or if it is a more general property of 2D turbulence. If this is indeed general, it would have important practical consequences, for example, for the simulation of atmospheric flows. For the TGV flow $r \approx 0.71$, which is larger than $3K/16$. However, we note that numerical methods for manipulating high-dimensional tensors are an active field of research\cite{32}, potentially enabling an improved scaling of MPS algorithms with $r$ in the future. We also remark that MPS can be exponentially faster than DNS at simulating shock waves, as illustrated in Supplementary Section 3 through analytical studies of the 1D Burgers’ equation.

Our initial choice of MPS networks was motivated by the scale-locality of turbulent flows. However, MPS might be numerically inefficient when correlations between distant scales are relevant. One then needs a very large bond dimension $\chi$ to maintain an accurate description of the flow. Other tensor network geometries like tree tensor networks (TTNs) or multiscale entanglement renormalization ansatz (MERA) and its derivatives$^{33,34}$ might then be worthwhile considering. These network geometries (Supplementary Section 6) have direct bonds between further distant length scales and might require smaller bond dimensions. However, TTNs maintain numerical efficiency by abandoning direct bonds between neighboring length scales, which are important for exploiting scale-locality. MERA is numerically challenging because of loops in the network.
The utility of tensor networks in fluid dynamics goes beyond the INSE. Future avenues of investigation for MPS include compressible flows, in which the Mach number is an important parameter, and transport of scalar quantities under both passive and chemically reactive conditions where the effects of Prandtl, Peclet and Damkohler numbers should be taken into account. It would be interesting to examine how these parameters affect the fidelity of low-r MPS simulations. Moreover, as tensor network methods are naturally suited to tackle high-dimensional problems, their applicability to the transported probability density function (PDF) of turbulent reactive flows should be considered. In these flows, in addition to temporal and spatial variations, the PDF is a function of the 3D velocity field and all of the pertinent scalar variables (energy, pressure and species mass fractions). With just ten species (a very simple chemical kinetics model), the unsteady PDF must be resolved in a 17D space. High-fidelity modeling and simulation of such complex flows can potentially be enabled through a well-chosen tensor network ansatz.

The close connection of our tensor network-based approach to quantum physics points towards the prospect of solving the Navier–Stokes equations on a quantum computer. Recently, several algorithms for solving nonlinear partial differential equations on quantum computers have been proposed. In particular, the work in ref. introduces tensor networks as a programming paradigm for quantum computers, which makes our approach especially well suited for quantum hardware implementations (see Supplementary Section 5 for details). Replacing classical floating point operations by quantum gates reduces the scaling with bond dimension to $\sim r^3$ (Supplementary Section 5). In addition, potentially exponential speed-ups are possible by choosing an optimized quantum network that goes beyond the MPS ansatz for encoding the solution. In this way, our work holds the promise of enabling large-scale computational fluid dynamics calculations that are well beyond the scope of current approaches.

Methods

Schmidt decomposition. We consider a 1D system and scale all lengths with its spatial dimension $L_{\text{box}}$. We discretize the spatial domain $[0,1]$ of the velocity $u$ with $N$ bits into $2^n$ grid points $r_j=q/2^n$ with $q=0,1,\ldots,2^n-1$. Next, we introduce $n=1,\ldots,N-1$ bipartitions of this grid into coarse and fine subgrids. For a given $n$, the coarse subgrid comprises the points $x_j=k/2^n$ with $k=0,\ldots,2^n-1$. The spacing between neighboring points is thus $2^n$ and this defines the coarse length scale. To each coarse grid point $x_j$ is attached a fine subgrid with points $x_{j,q}=(j+q)/2^n$ with $q=0,1,\ldots,2^{n-1}$, and adjacent points are separated by the fine length scale $2^{-n}$. In this way, any point $r_j$ of the 1D grid can be written as $r_j=r_{j,n}+x_{j,n}$. Finally, we arrange the function values $u(r_j)=u(x_j)+y_j$ into a $2^n \times 2^n$ matrix where the rows and columns correspond to increments along the coarse and fine grids, respectively. Performing a singular value decomposition (SVD) on this matrix gives the desired Schmidt decomposition of $u(r_j)$ at bipartition $n$:

$$u(r_j) = \sum_{n=1}^{D} \alpha_n \mathbf{R}_n(X_j) f_\alpha(x_j).$$

This is the 1D result corresponding to equation (2). For a full SVD the Schmidt number takes its maximal value $\delta(n)=\|F^0(n)\|$, where $F^0(n)=\min(2^n,2^{2n})$. If, instead, a truncated SVD is performed by keeping only the $n$ largest singular values, the error in the L2 norm due to this approximation is $\|F^0(n)\|^{-1} \delta^2(n)$. This procedure can be straightforwardly generalized by replacing bits with quaternaries (2D) or octals (3D), that is, by replacing 1D line segments with squares (2D) or cubes (3D). The maximal Schmidt numbers are then given by equation (4) in 2D and equation (5) in 3D.

Matrix product state algorithm. The INSE comprises a coupled set of partial differential equations for the velocity field $V$ and pressure $p$:

$$\nabla \cdot V = 0$$

$$\nabla \cdot (V \cdot \nabla V) = -\nabla p + \kappa \nabla^2 V,$$

where $\kappa$ is the kinematic viscosity and $V$ is the nabla operator. After discretizing the computational domain as described at the beginning of this Article, we solve equation (7) in time via a second-order Runge–Kutta method by a variational scheme. Furthermore, we use the penalty method to satisfy the incompressibility condition $\nabla \cdot V=0$.

We illustrate the principle of our method by considering a simple Euler time step. To advance $V$ from time $t$ to $t+\Delta t$, we minimize the cost function

$$\Theta(V) = \mu \| \nabla \cdot V \|^2 + \| \nabla^2 V + (V \cdot \nabla) V - \kappa \nabla^2 V \|^2,$$

where $\| \cdot \|$ is the L2 norm, $\nabla$ is the nabla operator in finite-difference form, $V^*$ is the trial solution at time $t$, $\Delta t$, and $V$ denotes the solution at the previous time step $t$. The term $\| \nabla \cdot V \|^2$ in equation (8) enforces $\nabla \cdot V=0$ for sufficiently large values of the penalty coefficient $\mu$. Note that the penalty method for enforcing the incompressibility condition preserves the pressure $p$ from equation (8). It can be calculated from the velocity fields via its Poisson equation.

We represent the flow field $V$ in terms of the MPS ansatz at all time steps $t_j$ and all operations on $V$, such as differentiation, are realized via standard matrix product operators acting on the MPS (ref. 12, p. 391 and ref. 13, p. 22). In this way, the entire computation is carried out in the MPS manifold. A derivation of our minimization scheme is provided in Supplementary Section 4.

Direct numerical simulation algorithm. Our DNS scheme is based on a second-order Runge–Kutta temporal discretization combined with an eighth-order central finite-difference discretization of the spatial derivatives on a Cartesian grid. The incompressibility condition is enforced through the projection method of Chorin at every substep of each full Runge–Kutta time step.

The computational complexity of the DNS scheme is $M^2 \log M$. This is because it is dominated by the projection step, which is performed through repeated fast Fourier transforms and inverse fast Fourier transforms that scale as $M \log M$. If there are just enough gridpoints to resolve all scales from $\ell$ to $\eta$, the scheme is DNS and solves the Navier–Stokes equations exactly within the sufficiently large $D$ of Fig. 1b,c. However, if the finest scales are removed (without invoking any subgrid scale model) such that the smallest remaining resolved scale is considerably larger than $\eta$, then the scheme becomes an URDNS operating within the scale-restricted $\mathbb{W} \subset \mathcal{D}$. The Navier–Stokes equations cannot be solved exactly within $W$ due to the finest scales being subject to unphysical numerical dissipation. In comparison, the MPS algorithm operates within the MPS manifold of $M$ where the interscale correlations are limited while all the scales between $\ell$ and $\eta$ are still present.

Set-up of numerical experiments. For the TDJ simulations, we consider a square with edge length $L_{\text{box}}$ with periodic boundary conditions and the initial conditions

$$V(x,y,t=0) = f(y) + D(x,y),$$

where $f(y)$ is the initial jet profile

$$f(y) = \frac{h}{\eta} \left( \tanh \left( \frac{y-y_{\text{max}}}{h} \right) - \tanh \left( \frac{y-y_{\text{min}}}{h} \right) \right).$$

with the streamwise direction along $\hat{e}_x$, $v_0$ is the magnitude of the velocity difference between the jet and its surroundings, $y_{\text{max}}$ and $y_{\text{min}}$ describe the extent of the jet and $h$ is the initial thickness of the vortex sheet. These parameters define the Reynolds number $Re = u_0 h / v$ and the timescale $T_2 = L_{\text{box}} / u_0$. The function

$$D = \delta(\hat{e}_x d_1 + \hat{e}_y d_2)$$
where \( u'_i = u_i - \bar{u}_i \) is the fluctuating part of the velocity component. The overbar denotes the ensemble average across the statistically homogeneous streamwise direction

\[
\bar{u}_i = \frac{1}{L_{box}} \int_0^{L_{box}} u_i(x, y, t) \, dx.
\]

(15)

Scaling all lengths with \( L_{box} \) velocities with \( u_i \) and time with \( T_{box} \), we set \( \nu = 0.4 \), \( y_{max} = 0.6 \) and \( h = 1/200 \), and the penalty coefficient is \( \mu = 2.5 \times 10^3 \) in all MPS simulations.

The TGV simulations in 3D are conducted on a cube with edge length \( L_{box} \) with periodic boundary conditions. We consider the initial flow field

\[
u (r, 0) = -u_0 \sin (k_x x) \cos (k_y y) \cos (k_z z),
\]

\[
u (r, 0) = u_0 \cos (k_x x) \sin (k_y y) \cos (k_z z),
\]

\[
u (r, 0) = 0,
\]

(16)

where \( u_0 \) is the velocity amplitude of the initial vortex and its wavenumber is \( k_r = 2 \pi / L_{box} \). The corresponding energy at \( t = 0 \) is \( E_0 = u_0^2 / 2 \), and the Reynolds number is defined using the integral scale as \( R_e = u_0 / (k_0) \).

In Fig. 3b we show the total kinetic energy dissipation

\[\varepsilon (t) = \frac{1}{2} \frac{d}{dt} \int_0^t \| V(r, t) \|^2 \, d \tau,\]

and entropy

\[\xi (t) = \nu \int_0^t \| \nabla \times V(r, t) \|^2 \, d \tau,\]

(17)

(18)

where we integrate over the whole space \( V, \xi \) is related to the viscous dissipation of kinetic energy. For incompressible flows with periodic boundary conditions, the INSE imply \( \varepsilon (t) + \xi (t) \). However, restricting the NVPS results in numerical diffusion violating this equality. In all TGV simulations, we set \( T_{box} = L_{box} / u_0 \) and scale lengths and velocities with \( L_{box} \) and \( u_0 \), respectively. In these units, the dimensionless penalty coefficient for MPS simulations is \( \mu = 6.25 \times 10^6 \).

Quantitative comparison between simulations. The accuracies of the MPS and URDNS gauges are gauged by comparing the ensemble-aggregated quantities of Figs. 2b and 3b against DNS. Statistical quantities such as those must always be used when comparing different simulations due to the chaotic nature of turbulence. To aid the reader, we here provide a quantitative measure of the accuracies of MPS and URDNS by integrating the discrepancy DNS has with respect to MPS and URDNS in Figs. 2b and 3b. We numerically calculate the visual difference between the Fig. 2b Reynolds stress of DNS (row 1) and that of MPS (rows 2–4) and URDNS (rows 5–7) as

\[\sigma (s, c) = \frac{\int_0^{T_{box}} \int_{\Omega_{box}} \sigma \left[ \frac{\rho u_i}{T} \frac{\partial T}{\partial y} + \frac{\partial T}{\partial y} \right] \frac{\partial T}{\partial y} }{\int_0^{T_{box}} \int_{\Omega_{box}} \sigma \left[ \frac{\rho u_i}{T} \frac{\partial T}{\partial y} \right] \frac{\partial T}{\partial y} } \, d \tau \]

(19)

with \( s \) being the scheme in question and \( c \) the compression ratio of said scheme relative to DNS (as defined in the Results). \( \sigma (s, c) \) quantities the root-mean-square of the visual difference between the subplots in Fig. 2b, and the closer \( \sigma (s, c) \) is to 0, the nearer the Reynolds stress in question is to that of DNS, \( \sigma (s, c) \) is tabulated in Table 1.

We also quantify the accuracy of URDNS and MPS against DNS for the TGV flow by integrating the numerical diffusion \( \xi (t) \) of Eq. 10 of Fig. 3b. This is equivalent to

\[\varepsilon (s, c) = \frac{1}{E_0} \int_0^{T_{box}} \left| \xi (s, c) - \varepsilon (s) \right| \, dt,\]

(20)

when normalized by the initial total kinetic energy \( E_0 \). The lower \( \varepsilon (s, c) \) is, the better is the accuracy of the relevant simulation. \( \varepsilon (s, c) \) is tabulated in Table 1. For comparison, we note that the corresponding (miniscule) error of DNS is \( \varepsilon (DNS) = 0.002 \).

Data availability

Our Code Ocean capsule\(^49\) contains the raw output data from our MPS simulations. These data were generated using the C functions tntMpsBoxTurbulence2DTimeEvolutionRK2(...) and tntMpsBoxTurbulence3DTimeEvolutionRK2(...), using the initial conditions and parameters defined in the Set-up of numerical experiments section in the Methods. Source data for Figs. 1, 2 and 3 are available via Code Ocean\(^5\).
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Author contributions
D.J. conceived the research project and N.G., M.L., P.G. and D.J. jointly planned it. N.G., M.L., S.D., H.B. and P.G. developed the quantum-inspired measure for interscale correlations based on Schmidt decompositions and hierarchical lattices. N.G., M.L. and S.D. formulated the matrix product state algorithm and carried out the analytical calculations. N.G., Q.Y.v.d.B. and M.K. wrote the software. N.G., H.B. and P.G. designed the numerical experiments for comparing MPS, URDNS and DNS. N.G. performed the numerical experiments. N.G., M.L., S.D., H.B., P.G., M.K. and D.J. analyzed and interpreted the numerical results. N.G., M.K. and D.J. wrote the manuscript with contributions from M.L., S.D., H.B. and P.G., and Q.Y.v.d.B. helped revise the manuscript. The Supplementary Information was written by N.G., M.L., S.D. and M.K. The project was supervised by D.J.

Competing interests
The authors declare no competing interests.

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Correspondence and requests for materials should be addressed to Nikita Gourianov or Dieter Jaksch.

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