Quantum inspired approaches for simulations of differential equations

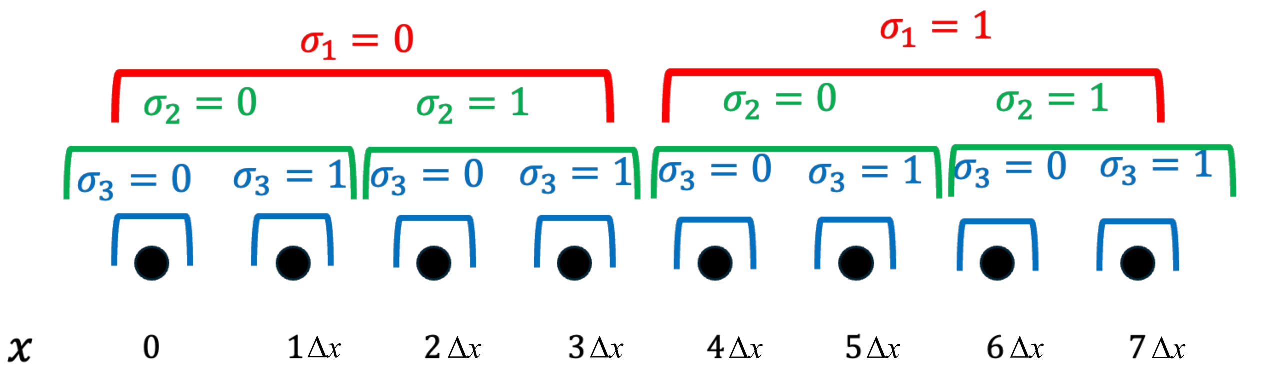
Ryan J. J. Connor [1,*] and Andrew J. Daley [1]
[1] Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, UK.
* ryan.connor@physics.ox.ac.uk

Abstract: Non-linear partial differential equations are ubiquitous across physics and engineering. For some applications, numerically accessible grid spacing can become a limiting factor leading to large computational resources. In recent years, quantum-inspired methods based on **tensor networks (TN)** have emerged as a promising route to address these issues on classical hardware. Tensor networks achieve physically motivated data compression without sacrificing length scales, which makes simulations possible on large spatial grids.

1. Encoding spatial grid into Tensor Network

Function $f(x)$ defined on a uniform spatial grid given by $x \in [0,1]$ and $\Delta x = 1/2^N$. Can express interms of a binary register,

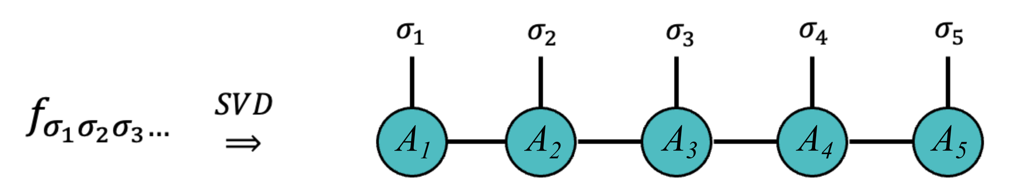
$$x = \frac{\sigma_1}{2^1} + \frac{\sigma_2}{2^2} + \frac{\sigma_3}{2^3} + \cdots + \frac{\sigma_N}{2^N}\,.$$



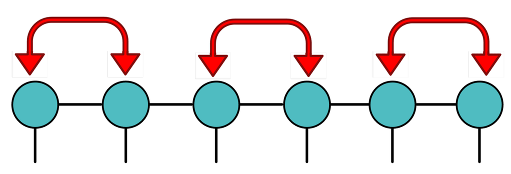
Perform singular value decompositions to obtain a Matrix Product State (MPS) [1],

$$f(x) = f_{\sigma_1,\sigma_2,\cdots} = A_1^{\sigma_1} A_2^{\sigma_2} A_3^{\sigma_3} \cdots A_N^{\sigma_N}\,.$$

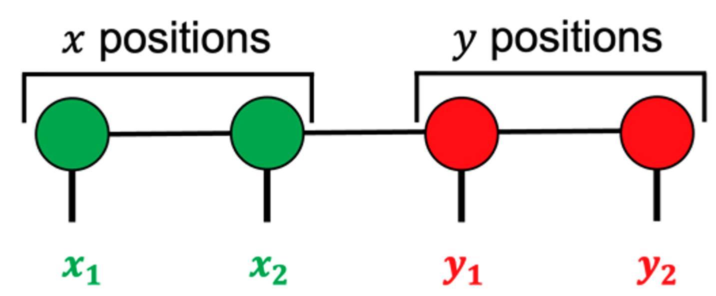
Define χ **as number of rows/cols of each tensor** A^{σ_n}**, known as bond dimension**. Each tensor represented as circle with lines emerging. Connecting bonds carry correlations.



Desire tensors correlated locally with neighbours as allows to **restrict** χ **without loss of accuracy**. Limiting χ to be small provides data compression



Can extend the MPS representation to 2D and beyond. How data is encoded into MPS is important but non-unique. Often choose to encode each dimension sequentially.



2. Finite Differences

Given a function in MPS form, can construct Matrix Product Operators (MPOs) to perform differentiation. Express the function f in a quantum register $|f\rangle$ with N qubits $|\sigma_1\sigma_2\cdots\sigma_N\rangle$,

$$|f\rangle = \sum_{\sigma_1,\sigma_2,\cdots} f_{\sigma_1,\sigma_2,\cdots,\sigma_N} |\sigma_1,\sigma_2,\cdots,\sigma_N\rangle\,.$$

The differential operator can be approximated using raising/lowering operators, which can then be written as an MPO with $\chi = 3$ [2],

$$\hat{\partial}_x \approx \frac{\hat{S}^+ - \hat{S}^-}{2\Delta x} = \frac{1}{2\Delta x}\begin{pmatrix} s_1^+ & s_1^- & I_1\end{pmatrix}\begin{pmatrix} s_n^- & & \\ & s_n^+ & \\ s_n^+ & s_n^- & I_n\end{pmatrix}^{\otimes N-2}\begin{pmatrix} s_N^- \\ -s_N^+ \\ s_N^+ - s_N^-\end{pmatrix}\,.$$

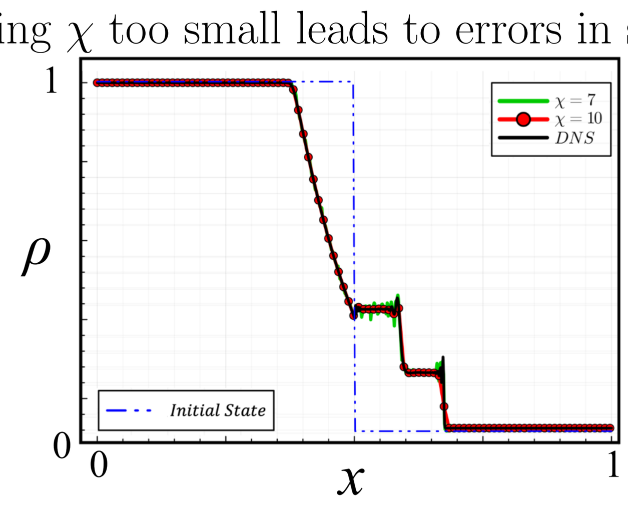
$S^{\pm}$ are global raising/lowering operators on the binary string, and $s_n^{\pm}$ are local raising/lowering operators on the *nth* qubit.

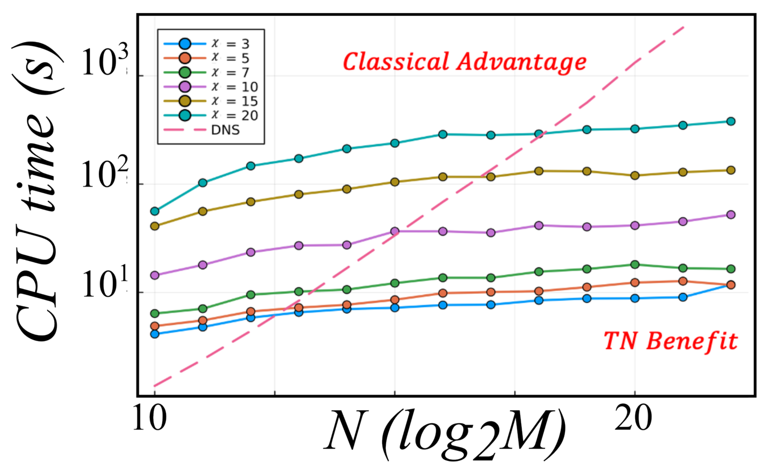
3. Compressible flows

Compressible flows governed by Euler equations. Each variable encoded as separate MPS with bond dimension χ. Time evolve via finite difference schemes and Macormack evolution.

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0\,,$$
$$\frac{\partial\rho\mathbf{u}}{\partial t} + \nabla\left[\rho\mathbf{u}\mathbf{u}^T + p\right] = 0\,,$$
$$\frac{\partial E}{\partial t} + \nabla\cdot\left[(E+p)\mathbf{u}\right] = 0\,.$$

Standard test case of Sod Shock [3]. Initial (dashed blue) discontinuity left to evolve, leading to shock formation. Only small χ required to reproduce dynamics, leading to data compression Truncating χ too small leads to errors in simulation.





True benefit comes via scaling. Conventional solvers scale with grid points (M) i.e. $\sim M$. TN solvers scale logarithmically with M and polynomially in χ, i.e. $\sim \chi^\alpha \log_2 M$.

Can allow TNs to simulate dense grids which would be infeasible with direct simulations, provided χ can be limited without large errors. This appears to be the case for many PDEs !

References

[1] Ulrich Schollwöck. In: *Annals of Physics* 326.1 (2011). [2] Martin Kiffner and Dieter Jaksch. 2023. arXiv: 2303.03010. [3] Gary A Sod. In: *J Comp Phys* 27.1 (1978). [4] Woo Jin Kwon et.al. In: *Phys. Rev. Lett.* 117 (24 2016).

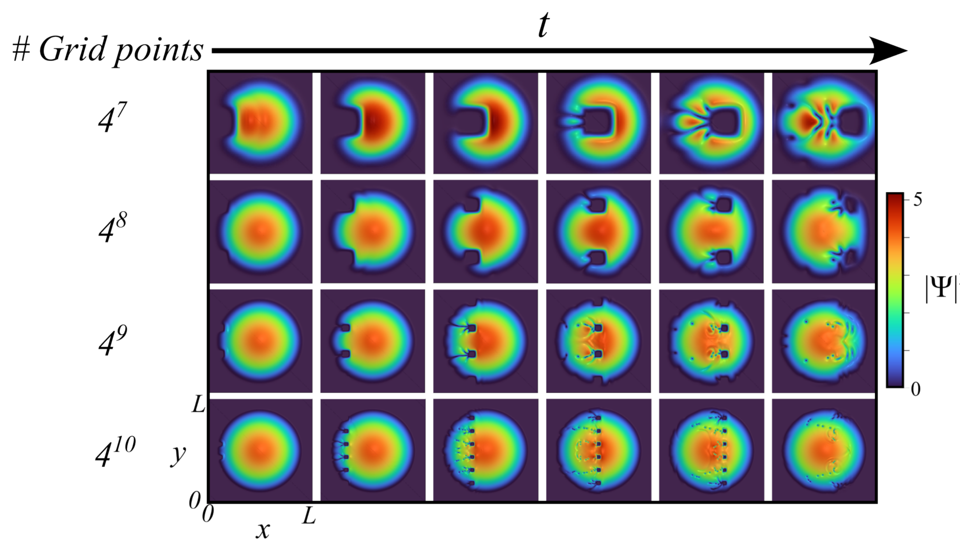
4. Quantised Vortices

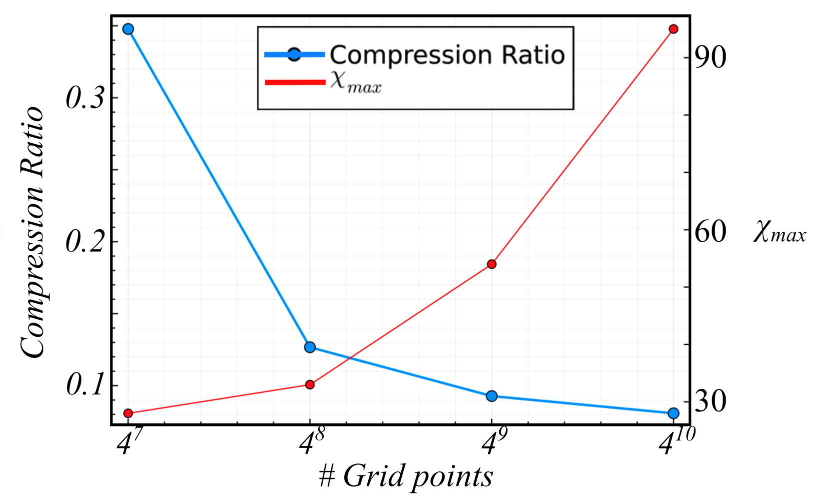
New Journal of Physics 28 023203

Dynamics of Bose-Einstein condensate (BEC) governed by the Gross-Pitaevskii Equation,

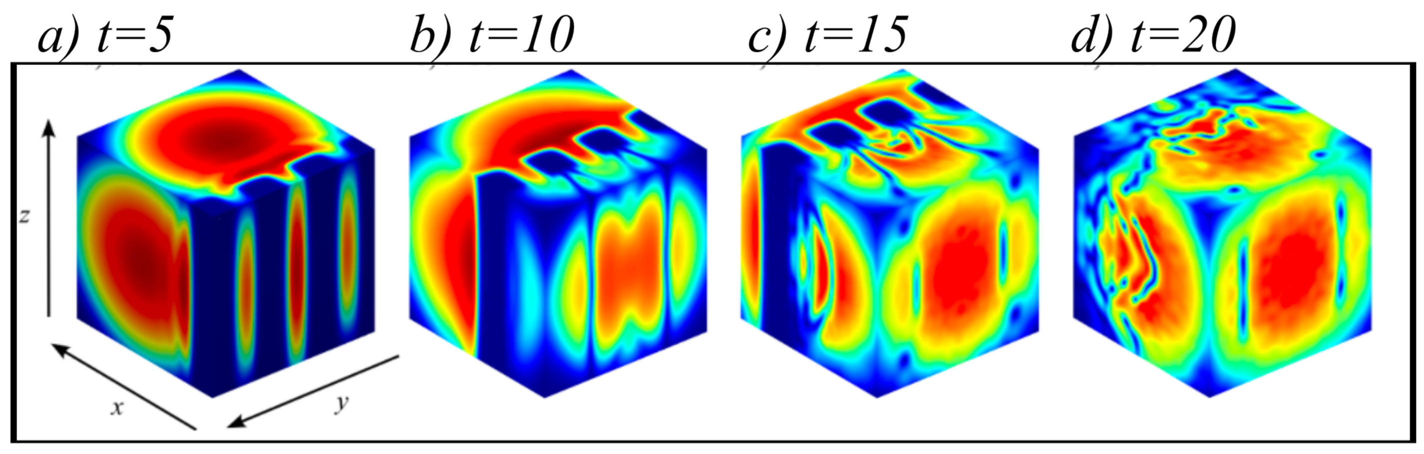
$$i\hbar\frac{\partial\Psi}{\partial t} = (1 - i\gamma)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,t) - \mu + g|\Psi|^2\right]\Psi\,.$$

Apply an external potential $V(x,t)$, which sweeps through and generates vortices behind [4]. Perform MPS simulations for increasing grid density, resolving finer and finer vortices, making use of adaptive χ, based on desired error.





Plot resulting χ as function of grid-points for fixed error (10^{-12}). Observe polynomial increase in χ as function of grid density. Defined compression as ratio of number of terms in MPS simulation to that of a direct simulation. **Huge degrees of compression available for large, dense spatial grids.** Less than 10% resources required for $2^{10}\times 2^{10}$ grid.



Can extend to 3D simulations. Shown dynamics of $2^7\times 2^7\times 2^7$ spatial grid with fixed $\chi = 64$. Corresponds to compression to **4% numerical parameters** compared to direct simulations.

5. Plasma Physics

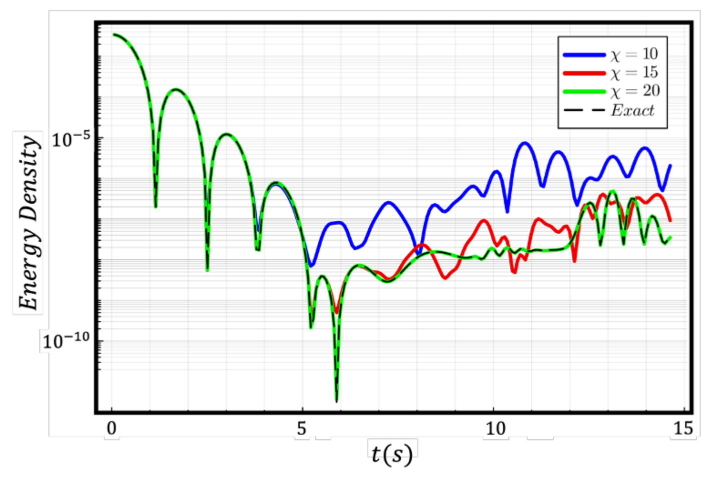
arXiv:2512.15924

Plasmas governed by Vlasov-Maxwell or Magnetohydrodynamics,

Vlasov–Maxwell

$$\frac{\partial f_s(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_r f_s + \frac{q_s}{m_s}\mathbf{F}\cdot\nabla_v f_s = 0\,,$$
$$\frac{\partial\mathbf{E}}{\partial t} = c^2\nabla\times\mathbf{B} - \frac{1}{\epsilon_0}\mathbf{J}\,,$$
$$\frac{\partial\mathbf{B}}{\partial t} = -\nabla\times\mathbf{E}\,.$$

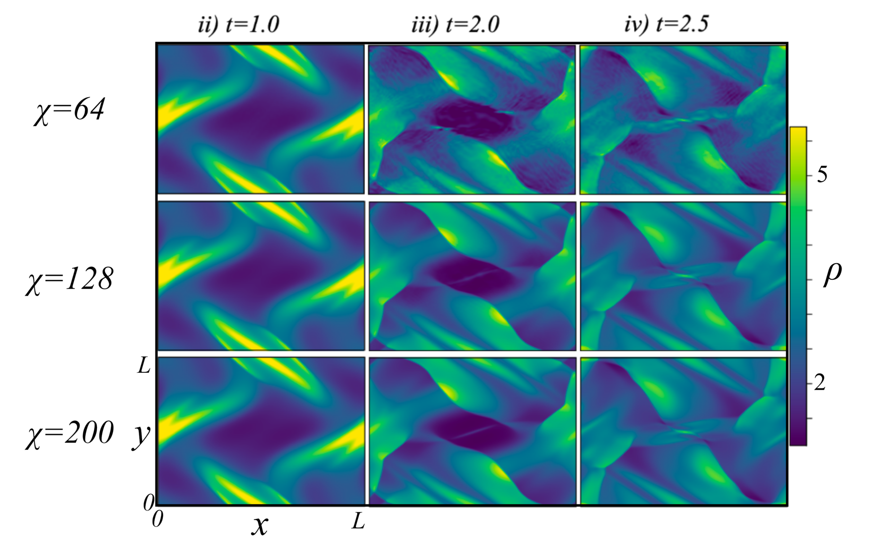
VM models phase space distribution $f(\mathbf{x},\mathbf{v},t)$. Must encode spatial **and** velocity dimensions into MPS. Electric ($\mathbf{E}$) and Magnetic ($\mathbf{B}$) fields represented as MPS and evolved via Maxwells equations. VM leads to fewer equations, but higher dimensionality, (more tensors per MPS).



MHD

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\mathbf{u})\,,$$
$$\frac{\partial(\rho\mathbf{u})}{\partial t} = -\nabla\left[\rho\mathbf{u}\mathbf{u}^T + (p + \tfrac{1}{2}B^2)\,I_{3\times 3} - \mathbf{B}\mathbf{B}^T\right]\,,$$
$$\frac{\partial E}{\partial t} = -\nabla\cdot\left[\left(\frac{\gamma}{\gamma-1}p + \tfrac{1}{2}\rho u^2\right)\mathbf{u} - (\mathbf{u}\times\mathbf{B})\times\mathbf{B}\right]\,,$$
$$\frac{\partial\mathbf{B}}{\partial t} = \nabla\times(\mathbf{u}\times\mathbf{B})\,.$$

MHD derived from VM. Used for stellar formation and large scale turbulence modelling. MHD treats plasma as a compressible fluid in real space only, with a fluid density $\rho(\mathbf{x})$ and velocity $\mathbf{u}(\mathbf{x})$. Each of dynamical variables encoded as MPS, giving more simultaneous equations, but lower dimensionality.



Across both VM and MHD formalisms, MPSs can efficiently capture underlying physics and recreate dynamics with **small bond dimensions (high compression ratios)**

Conclusions + Future directions

- TNs can be applied to **wide range of PDEs**, most notably for fluid and plasma dynamics
- Data compression via **removing correlations as opposed to discarding length scales**
- Further development underway to allow TNs to simulate in spatially dense regimes impossible with direct simulations
- Can extend to **curvilinear grids**. Research ongoing for further complex topologies and enhancement of solvers beyond finite difference.
- Alternative TN geometries may present further opportunities for data compression.