QUANTUM ALGORITHMS AND ARCHITECTURES FOR DOMAIN SCIENCE @PNNL

Potential quantum advantage for nonlinear multiscale complex systems

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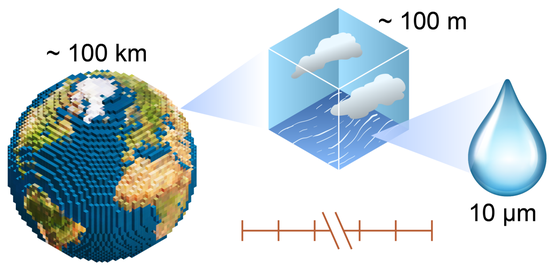
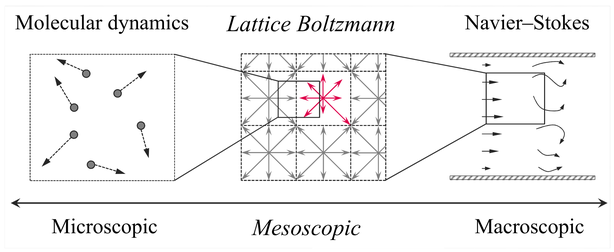
MULTIPHASE TURBULENT TRANSPORT



Multiscale physics requiring high resolution, while covering a wide range of spatiotemporal scales



$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}\cdot(\nabla\mathbf{u}) = -\frac{\nabla p}{\rho} + \nu\nabla^2\mathbf{u} + \mathbf{F}$$

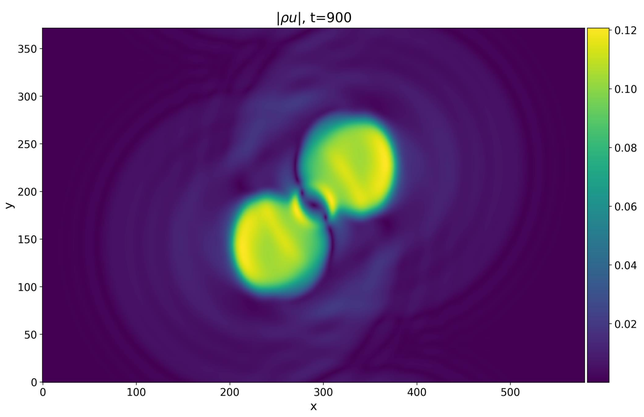
$$\mathbf{u}\cdot(\nabla\mathbf{u})/(\nu\nabla^2\mathbf{u}) \sim \boxed{\mathrm{Re} \gg 1}$$

Transforming the Navier-Stokes equation to the lattice Boltzmann formulation to make an efficient quantum algorithm for turbulence

Can we couple turbulent flows to particle-particle interactions?

$$\partial_t f_m + \mathbf{e}_m \cdot \nabla f_m = -\frac{1}{\tau}(f_m - f_m^{\mathrm{eq}}) + \frac{w_m \mathbf{e}_m \cdot \mathbf{F}}{c_s^2}$$

"Reactions" involving two phases (i.e., droplet collisions) bring additional complications associated with density gradients



Can quantum computing break the curse of dimensionality in reactive nonlinear transport?

NON-LINEAR TO LINEAR TRANSFORMATION

ON CLASSICAL COMPUTER

Original nonlinear system

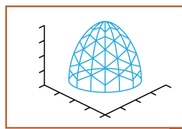
Navier-Stokes

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{\nabla p}{\rho} + \nu\nabla^2\mathbf{u}$$

Many important cases for DOE domain science involve multi-phase transport with strong nonlinearity

$$\frac{dn_k}{dt} = \frac{1}{2}\sum_{\substack{i=1\\ j=k-i}}^{k-1} F_{ij} n_i n_j - \sum_{i=1}^{\infty} F_{ki} n_k n_i$$

Generalized population balance



Spatial and temporal discretization

Carleman embedding into infinite linear system

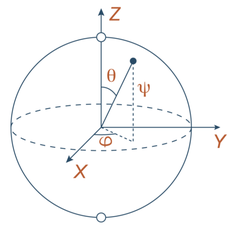
$$\frac{d\mathbf{X}}{dt} = \widetilde{M}\mathbf{X} + \mathbf{C}$$

$$\frac{d}{dt}\begin{bmatrix} a_1 \\ s_1 \\ a_2 \\ s_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} B_0^1 & B_1^1 & B_2^1 & 0 & \cdots \\ 0 & B_0^2 & B_1^2 & B_2^2 & \cdots \\ 0 & 0 & B_0^3 & B_1^3 & \cdots \\ 0 & 0 & 0 & B_0^4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ s_1 \\ a_2 \\ s_2 \\ \vdots \end{bmatrix} + \begin{bmatrix} C_1 \\ C_2 \\ 0 \\ \vdots \end{bmatrix}$$

Finite linear system with truncation

$$\frac{d\mathbf{X}_n}{dt} = \widetilde{M}_n\mathbf{X}_n + C_n$$

$$\widetilde{M}^n = \begin{bmatrix} B_0^1 & B_1^1 & B_2^1 & 0 & \cdots & 0 \\ 0 & B_0^2 & B_1^2 & \cdots & \cdots & B_{n-2}^2 \\ 0 & 0 & B_0^3 & \cdots & \cdots & B_{n-3}^3 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & B_0^n \end{bmatrix}.$$



ON QUANTUM COMPUTER

Linear problem input with initial condition

Initial state preparation

$$O_x : |0\rangle \rightarrow |\mathbf{X}_x\rangle$$

LCHS algorithm

MEASUREMENT

Final quantum results

Computational cost of the quantum algorithm scales logarithmically in the number of grid points *N* in the simulation domain:

Query complexity

$$O\left\{\sqrt{k}\left(\frac{T}{\tau}\right)\mathrm{poly}\left[\boxed{\log N}\,\log\left(\frac{1}{\epsilon}\right), \log\left(\frac{T}{\tau}\right)\right]\right\}$$

compared to polynomial scaling in classical algorithms

Our work provides an efficient quantum algorithmic framework path for multiscale nonlinear complex systems.

Future objectives

1. Circuit-based end-to-end resource estimation
2. Hybrid quantum–classical algorithms
3. Implementation on quantum hardware with *O*(100) qubits

References

https://doi.org/10.1103/PhysRevResearch.7.013036
https://arxiv.org/abs/2509.20668

Motivation

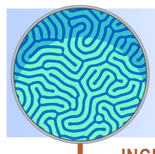
Higher-resolution models will address knowledge gaps in emergent behaviors of multiscale systems

Current classical computing abilities are limited in time and scale due to the large number of degrees of freedom (grid points, species)

Quantum algorithms for classical large-scale dynamic systems are underdeveloped and have potential speed up when dealing with large systems containing many parameters

REACTION–DIFFUSION IN BIOLOGICAL SYSTEMS

CLASSICAL COMPUTER



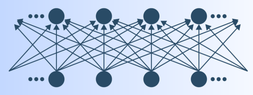
Gierer-Meinhardt (GM) model

One activator and one inhibitor

INCREASING POSSIBLE REACTION COMBINATIONS

QUANTUM COMPUTER

Generalized Turing model



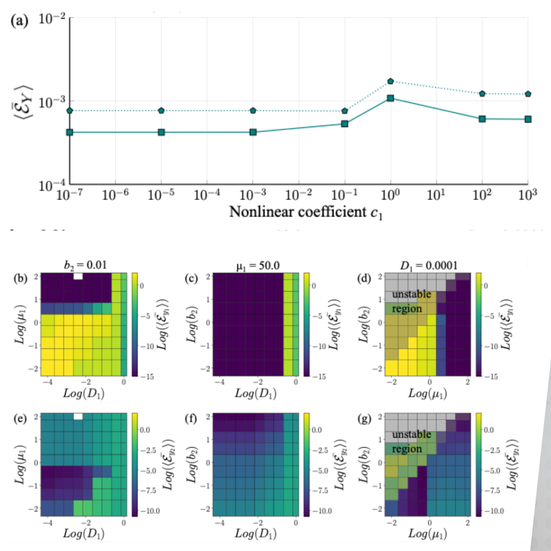
Combinatorial nature of interactions among species and resultant rate constants

Can we couple diffusion with interconnected of biological entities?

Using the Gierer-Meinhardt (GM) model with one activator and one inhibitor as a benchmark:

$$\frac{\partial y_1(x,t)}{\partial t} = D_1\nabla^2 y_1(x,t) - \mu_1 y_1(x,t) + c_1 y_1^2(x,t) y_2(x,t) + b_1$$
$$\frac{\partial y_2(x,t)}{\partial t} = D_2\nabla^2 y_2(x,t) - \mu_2 y_2(x,t) - c_1 y_1^2(x,t) y_2(x,t) + b_2$$

We find that the error between the Carleman solution and RK4 remains small across most stable, biologically relevant parameter regimes.



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