Hamiltonian Simulation for Allen-Cahn phase-field model by Quantum-Classical Hybrid Approach

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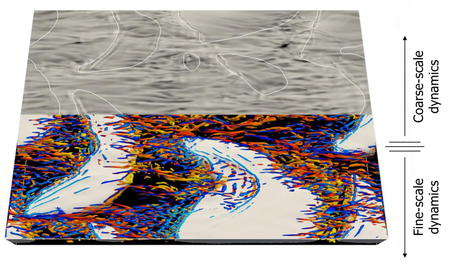
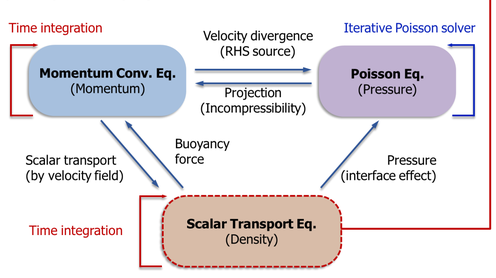
Which quantum algorithms could offer advantage for solving PDEs? (Especially, phase-field model)

Algorithm for two-phase flow simulation

- Solve Navier-stokes (Momentum, Poisson Eqs.) and Scalar Transport (Density) Eq.
- Multi-scale phenomena → Large-gap on time-step (Δt) between two regime
  - ▸Bulk flow advection-diffusion vs interfacial capillary microphysics



< Navier-stoke equations (Bubbly flow) >



< Algorithm of two-phase flow simulation >

Phase-field (Allen-Cahn)

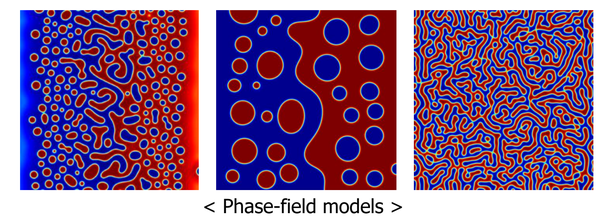
$$\frac{\partial \boldsymbol{\phi}}{\partial t} + (u \cdot \nabla)\boldsymbol{\phi} = -\boldsymbol{M}\mu \qquad \mu = \frac{\delta F}{\delta \phi} = f'(\phi) - \varepsilon^2 \nabla^2 \phi$$

- Chemical potential μ
  - ▸ Naturally incorporate surface tension
- Require relatively small Δt due to stiff gradient energy term $\leftarrow \frac{1}{dx^2}$

Exponential integrators (Matrix Exponential)

$$\frac{\partial \phi}{\partial t} = \boldsymbol{L}\phi + \boldsymbol{N}(\phi) \;\Rightarrow\; \phi(t) = e^{\boldsymbol{L}t}\phi_0 + \int_0^\tau e^{\boldsymbol{L}(t-\tau)}\boldsymbol{N}\big(\phi(\tau)\big)d\tau$$

- Stable with large Δt, accurate linear integration
- Requiring expensive matrix exponential
  - ▸ High cost in HPC (Memory, Communication)



< Phase-field models >

Hamiltonian simulation

$$i\frac{d}{dt}\psi = \hat{H}\psi \quad \Rightarrow \quad \psi = e^{-i\hat{H}t}\psi_0$$

- To solve **time-dependent Schrödinger** equation
- Matrix exponential time evolution natively
  - ▸Removes HPC bottleneck

Requirements for Hamiltonian simulation from quantum computing

Requirement for Quantum Hamiltonian simulation

- Reformulation into Schrödinger-type equation
  - ▸Unitary embedding of non-unitary operators
- Linearization of Nonlinear terms
  - ▸Infeasible for Current NISQ devices
- Physical quantity depend on simulation
  - ▸Not well-suited linearization strategy for fluid simulation

$$i\frac{d}{dt}\psi = \hat{H}\psi \quad \overset{\text{Shape}}{\neq} \quad \frac{d\phi}{dt} = \mathcal{A}\phi$$

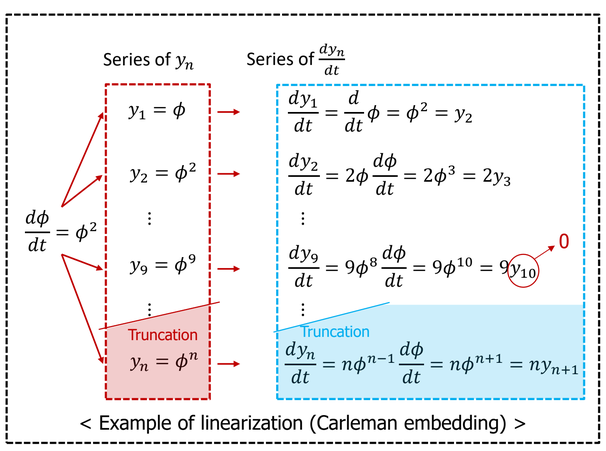
Imaginary number

Operators → Generally non-Hermitian

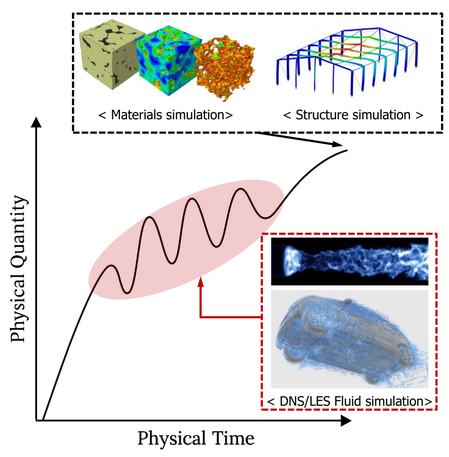
If $A = A^\dagger (= (A^*)^T) \rightarrow e^{-iAt}$ is Unitary

$$A = \begin{pmatrix} 2 & 2+i & 4 \\ 2-i & 3 & i \\ 4 & -i & 1 \end{pmatrix} \qquad A^T = \begin{pmatrix} 2 & 2-i & 4 \\ 2+i & 3 & -i \\ 4 & i & 1 \end{pmatrix} \qquad A^\dagger = \begin{pmatrix} 2 & 2+i & 4 \\ 2-i & 3 & i \\ 4 & -i & 1 \end{pmatrix}$$

< Example of Hermitian operator $(A = A^\dagger)$ >



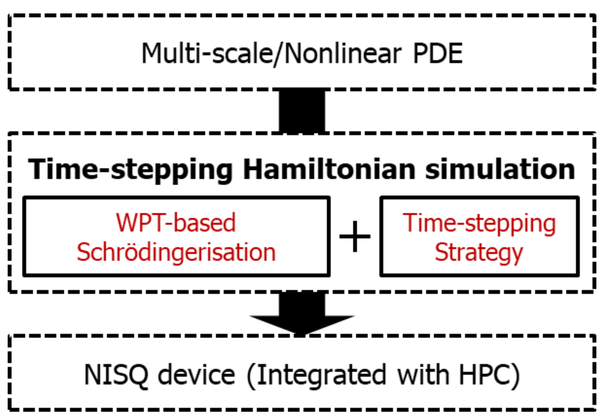
< Example of linearization (Carleman embedding) >



Quantum-Classical hybrid algorithm

Schrödingerisation (Warped Phase Transform)

- Dissipative system (Non-unitary) → conservative system (Unitary)
- Time-stepping strategy for linear treatment of nonlinear term
  - ▸ Time-integrating with Δt from quantum circuit
  - ▸ Updated nonlinear term from classical computer



Proposed Algorithm (Time-stepping Hamiltonian simulation)

Warped Phase Transform (WPT)-based Schrödingerisation

- Reformulate classical PDEs into the Schrödinger equation by introducing an auxiliary variable p
- Operator decomposition: $\mathcal{A} = \mathcal{H}_1 + i\mathcal{H}_2$ naturally accommodates Nonlinear terms in Hermitian operator for Δt

Schrödingerisation procedure

- PDE → ODE (spatial discretization $\mathcal{A}$)
- Decomposition $\mathcal{A}$ into Hermitian
- Warped Phase Transform ($\boldsymbol{\phi} \rightarrow \boldsymbol{\omega}$)
- Fourier transform ($\boldsymbol{\omega} \rightarrow \boldsymbol{\psi}$)

$$\frac{d\phi}{dt} = \mathcal{A}\phi$$
$$\frac{d\phi}{dt} = (\mathcal{H}_1 + i\mathcal{H}_2)\phi = \mathcal{H}_1\phi + i\mathcal{H}_2\phi$$
$$e^{|p|}\frac{\partial \omega}{\partial t} = -\mathcal{H}_1 e^{|p|}\frac{\partial \omega}{\partial p} + i\mathcal{H}_2 e^{|p|}\omega$$
$$\frac{\partial \psi}{\partial t} = -\mathcal{H}_1 i\eta\psi + i\mathcal{H}_2\psi$$
$$\times i \text{ on LHS and RHS}$$
$$i\frac{\partial \psi}{\partial t} = (\eta\mathcal{H}_1 - \mathcal{H}_2)\psi = \mathcal{H}_\eta\psi$$

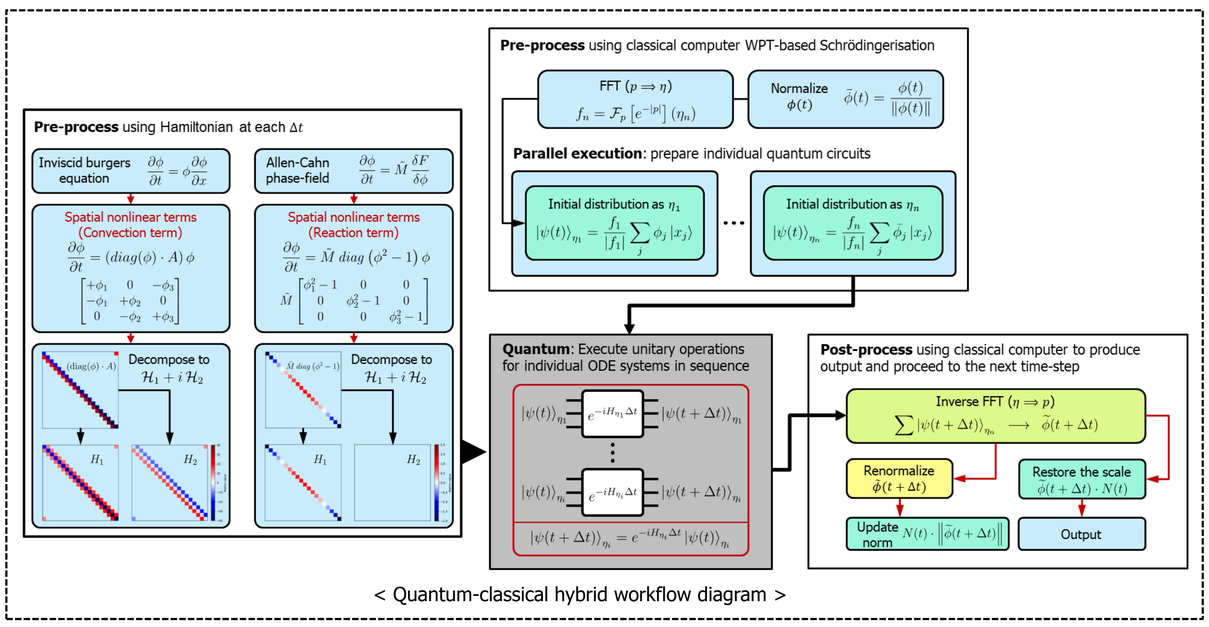
$$\mathcal{A} = \mathcal{H}_1 + i\mathcal{H}_2$$
$$\mathcal{H}_1 = \frac{\mathcal{A} + \mathcal{A}^\dagger}{2} \qquad \mathcal{H}_2 = \frac{\mathcal{A} - \mathcal{A}^\dagger}{2i}$$

$$\omega(t,p) = e^{-|p|}\phi(t)$$
$$\omega = e^{-|p|}\phi \;\Rightarrow\; \phi = e^{|p|}\omega$$
$$\frac{\partial \omega}{\partial t} = e^{-|p|}\frac{d\phi}{dt} \;\Rightarrow\; \frac{d\phi}{dt} = e^{|p|}\frac{\partial \omega}{\partial t}$$
$$\frac{\partial \omega}{\partial p} = -e^{-|p|}\phi \;\Rightarrow\; \phi = -e^{|p|}\frac{\partial \omega}{\partial p}$$

$$\psi(t,\eta) = \int_{-\infty}^{\infty} \omega(t,p)\, e^{-i\eta p}\, dp \qquad \mathcal{F}_p\left[\frac{\partial \omega}{\partial t}\right] = \frac{\partial \psi}{\partial t}$$
$$\mathcal{F}_p\left[\frac{\partial \omega}{\partial p}\right] = \int_{-\infty}^{\infty}\frac{\partial \omega}{\partial p}\, e^{-i\eta p}\, dp \qquad \mathcal{F}_p[\omega] = \psi$$
$$= \underbrace{\left[\omega e^{-i\eta p}\right]_{p=-\infty}^{p=\infty}}_{0} - \int_{-\infty}^{\infty}\omega\,\frac{\partial}{\partial p}\left(e^{-i\eta p}\right)dp = i\eta\psi$$

Quantum-classical hybrid workflow

- Pre-process: WPT-based Schrodingerisation to transform classical PDEs and linearize Nonlinear terms, followed by transpilation into independent quantum circuits
- FFT instead of QFT for reducing qubit requirements for Warped phase variable (lowering entangling gates) → a practical alternative in NISQ devices by reducing overhead
- Quantum computing: Sequential evolution of each decoupled ODE system
- Post-process: Inverse FFT to return to the physical domain, preparation for next step (accumulate the original norm, re-normalizing the evolved state), and output



< Quantum-classical hybrid workflow diagram >

Numerical results (1D/2D Allen-Cahn Phase field model)

Experimental Setup

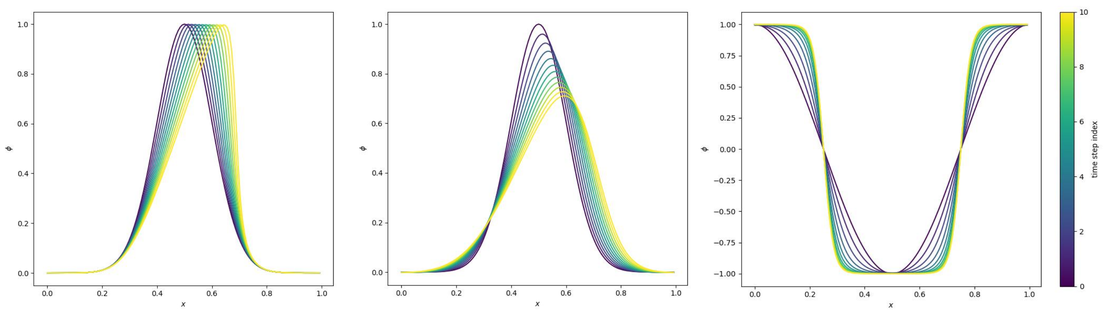
Quantum Framework:
- Qiskit v1.3.0
- Qiskit-Aer v0.15.0
- SciPy v1.11.4

Simulators:
- Noise-free (Statevector simulator)
- *get_statevector* (Qiskit) method

R-CCS Cloud:
- AMD EPYC 9684X (96 Cores @ 2.55 GHz)
- 768 GB DDR4 RAM
- 8 × NVIDIA A100 80 GB GPUs

1D Nonlinear equations (Burgers, Allen-Cahn phase field)

- Gaussian distribution for Burgers cases and single-period cosine for the Allen–Cahn phase-field
  - ▸ Only a 1st-order upwind scheme is used for Burgers equations
- Inviscid Burgers/Burgers → shock formation with and without diffusive effects.
- Allen-Cahn phase field → bi-phasic structure due to the nonlinear reaction term
- Nonlinear terms are effectively updated classically for accurate unitary evolution



< Inviscid Burgers > < Burgers > < Allen-Cahn phase-field >

2D Allen-Cahn phase field

- The results are based on 12 qubits, with 6 qubits for each axis ($p = 2^8$, auxiliary variable).
- A random noise distribution is used for the initial conditions, and the discretization scheme employs 2nd-order central differencing.
- The field evolves toward two energetically favorable states ($\phi = \pm 1$), while the diffusion term, scaled by ϵ^2, smooths the interfaces between phases. In this simulation, ϵ was set to 0.01, resulting in a relatively sharp but finite interface thickness.
- As time progresses, the field separates clearly, revealing interface structures, and the solution stabilizes into a step-like profile—consistent with the expected Allen–Cahn dynamics