量子-古典ハイブリッドスキームを用いた非線形偏微分方程式のための時間ステッピング型ハミルトニアンシミュレーション

Time-stepping Hamiltonian Simulation for Solving Nonlinear PDEs via a Quantum-Classical Hybrid Approach

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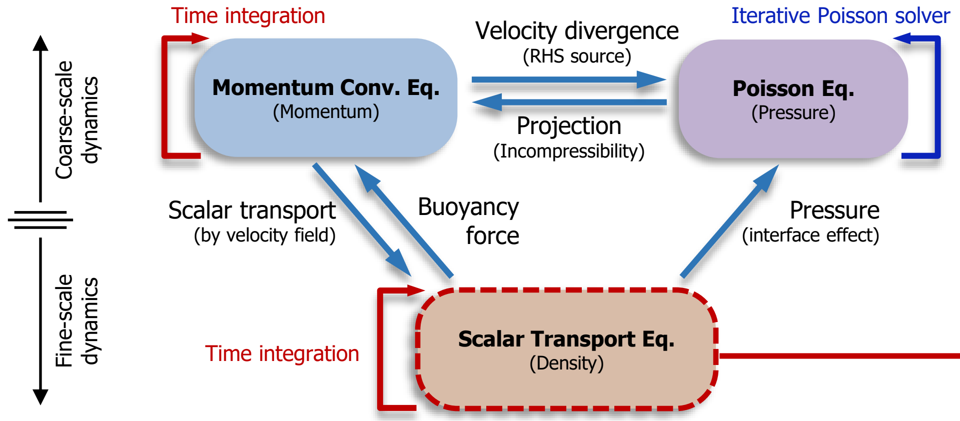
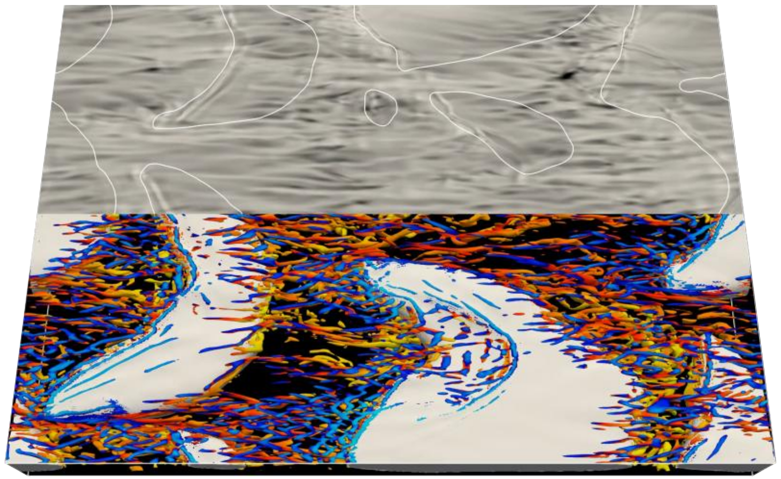
Background

- **Algorithm for two-phase flow**
  - Solve Navier-stokes and Scalar Transport Eqs.
  - Multiscale phenomena → Large-gap on time-step (Δt)
    - ▸ **Flow convection** vs **fine-scale breakup**



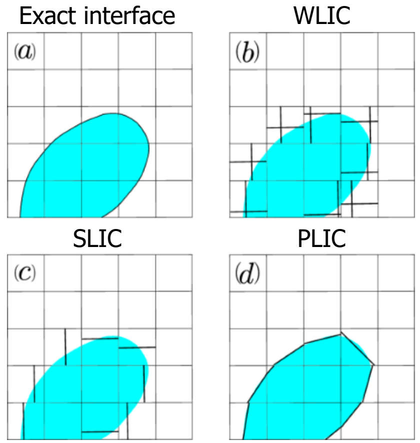


< Navier-stoke equations [1]>

- **Volume of Fluid** (VOF)

$$\frac{\partial \boldsymbol{C}}{\partial t} + (u \cdot \nabla)\boldsymbol{C} = 0$$

- Sharp interface model (SLIC, WLIC, PLIC)
- Advection scheme with interface model
  - ▸ e.g., geometrical advection + PLIC
- Need extra model for surface tension (CSF)



< Various VOF method [2]>

- **Phase-field** (diffuse interface)

$$\frac{\partial \boldsymbol{\phi}}{\partial t} + (u \cdot \nabla)\boldsymbol{\phi} = \boldsymbol{M}\nabla^2 \mu$$

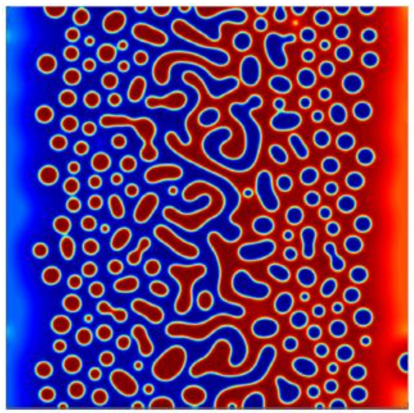
- Diffuse interface Model
  - ▸ Cahn-Hilliard (Cons.), Allen-Cahn (Non-Cons.)
- Chemical potential μ
  - ▸ Naturally incorporate surface tension

$$\mu = \frac{\delta F}{\delta \phi} = f'(\phi) - \varepsilon^2 \nabla^2 \phi$$

Free energy term

Gradient energy term

- Require small-scale Δt
  - ▸ Due to high order derivative ($\boldsymbol{M}\varepsilon^2\nabla^4\phi$)



< Phase-field [3] >

[1] Kim et al., Direct numerical simulation on millimeter-sized air bubble in turbulent channel flow, 2024
[2] Mohan and Tomar, Volume of Fluid Method : A brief Review, 2024
[3] Gomez et al., Accurate, efficient, and (iso)geometrically flexible collocation methods for phase-field models, 2014

Background

- **Exponential integrators** (Matrix Exponential)
  - Linear part : Exact solution (matrix exponential)
  - Nonlinear part : Needs ETD or RK schemes
  - **Stable with large Δt, accurate linear integration**
  - Requiring expensive matrix exponential
    - ▸ High cost in HPC (Memory, Communication)

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

Linear term — Nonlinear term

- **Quantum Hamiltonian simulation**
  - Matrix exponential time evolution natively

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

  - Potentially eliminating limitations
    - ▸ Removes HPC bottleneck
  - Requirements
    - ▸ Feasible on current quantum platforms
    - ▸ Linearization of Nonlinear terms
    - ▸ Unitary embedding of non-unitary operators (Diffusion etc.)

- **Volume of Fluid** (VOF)

$$\frac{\partial \boldsymbol{C}}{\partial t} + (u \cdot \nabla)\boldsymbol{C} = 0$$

  - Sharp interface model (SLIC, WLIC, PLIC)
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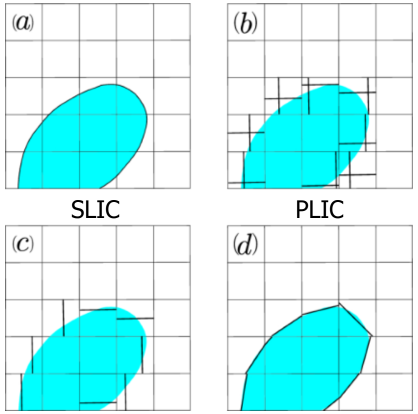

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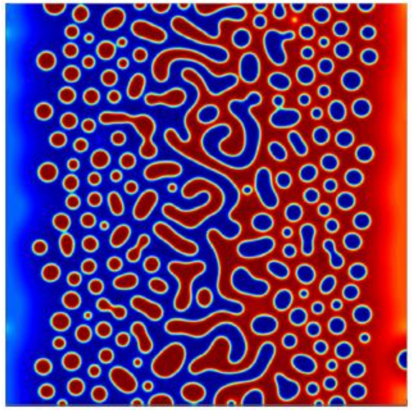


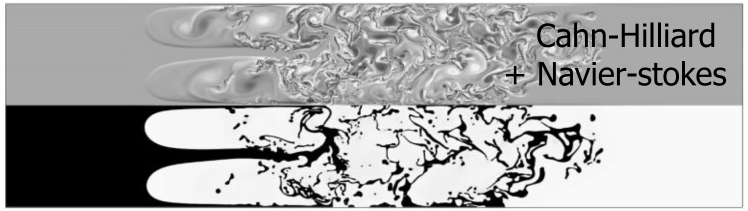
< Phase-field [2] >

[1] Mohan and Tomar, Volume of Fluid Method : A brief Review, 2024
[2] Gomez et al., Accurate, efficient, and (iso)geometrically flexible collocation methods for phase-field models, 2014

Research Objectives

- **Hamiltonian simulation for overcoming stiff time integration in high-order PDEs**
  - Restricting severe when coupled with another physical model (e.g., Navier-stokes)
  - Bypassing such restrictions using **matrix exponential** e^{-At}, implemented as a sequence of quantum gates

High-order PDEs	Microscale Phenomena	Restricting term	Time-step restriction
Cahn-Hilliard	Interface evolution	4th-order derivative ($\nabla^4\phi$)	$dt_{max} \sim dx^4$ 16× smaller
Kuramoto-Sivanshinsky	Instability, Super-diffusion	2nd+4th-order terms ($-\nabla^2 u - \nabla^4 u$)	



- **Growing Hybrid Quantum-HPC platforms**
  - To overcome NISQ limitation supported by HPCs
  - Needs for proper usage of these platforms

- **Limitation of current (Carleman, KvN) Linearization**
  - **Impractical for Current NISQ devices**
    → Exponential growth in state vector, accuracy issue from truncation

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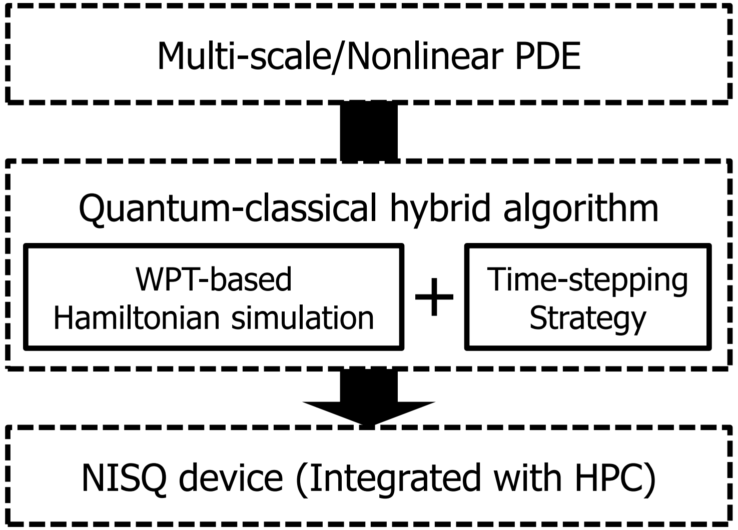
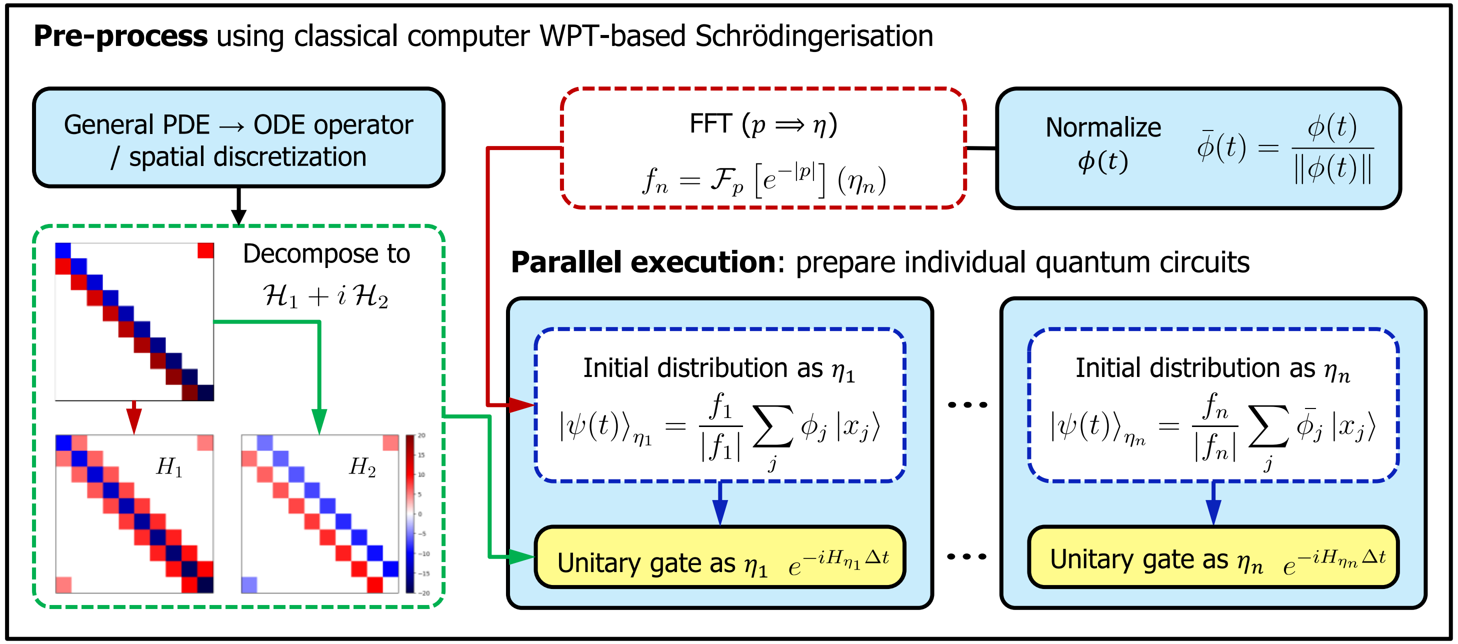
- **We propose Quantum-classical hybrid algorithm**
  - **Warped Phase Transform (WPT)-based Schrödingerisation**
    - Transforming dissipative system (Non-unitary) into a conservative system (Unitary)
    - PDEs can be calculated from quantum computer (Hamiltonian simulation) for linear system
  - **Time-stepping Strategy for linear treatment of nonlinear term**
    - Time-integrating with Δt from quantum circuit
    - Updated nonlinear term from classical computer
  - **Modification for practical calculation in NISQ** (QFT → FFT in WPT)
    - Reducing depth of quantum gates (Initialization, QFT, IQFT for Warped phase variables)
    - Reducing qubit requirements (for Warped phase variables)



Numerical method

- **WPT-based Schrödingerisation [1]**
  - PDE → ODE (spatial discretization $\mathcal{A}$)
  - Decomposition $\mathcal{A}$ into Hermitian
  - Warped Phase Transform ($\boldsymbol{\phi} \rightarrow \boldsymbol{\omega}$)
  - Fourier transform ($\boldsymbol{\omega} \rightarrow \boldsymbol{\psi}$)



$$\frac{d\phi}{dt} = \mathcal{A}\phi$$

$$\downarrow$$

$$\frac{d\phi}{dt} = (\mathcal{H}_1 + i\mathcal{H}_2)\phi = \mathcal{H}_1\phi + i\mathcal{H}_2\phi$$

$$\downarrow$$

$$e^{|p|}\frac{\partial\omega}{\partial t} = -\mathcal{H}_1 e^{|p|}\frac{\partial\omega}{\partial p} + i\mathcal{H}_2 e^{|p|}\omega$$

$$\downarrow$$

$$\frac{\partial\psi}{\partial t} = -\mathcal{H}_1\, i\eta\psi + i\mathcal{H}_2\psi$$

$$\downarrow$$

$$i\frac{\partial\psi}{\partial t} = (\eta\mathcal{H}_1 - \mathcal{H}_2)\psi = \mathcal{H}_\eta\psi$$

$$\mathcal{A} = \mathcal{H}_1 + i\mathcal{H}_2$$

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

$$\omega(t,p) = e^{-|p|}\,\boldsymbol{\phi}(t)$$

$$\omega = e^{-|p|}\phi \quad \Rightarrow \quad \phi = e^{|p|}\omega$$

$$\frac{\partial\omega}{\partial t} = e^{-|p|}\frac{d\phi}{dt} \quad \Rightarrow \quad \frac{d\phi}{dt} = e^{|p|}\frac{\partial\omega}{\partial t}$$

$$\frac{\partial\omega}{\partial p} = -e^{-|p|}\phi \quad \Rightarrow \quad \phi = -e^{|p|}\frac{\partial\omega}{\partial p}$$

$$\psi(t,\eta) = \int_{-\infty}^{\infty}\omega(t,p)\,e^{-i\eta p}\,dp$$

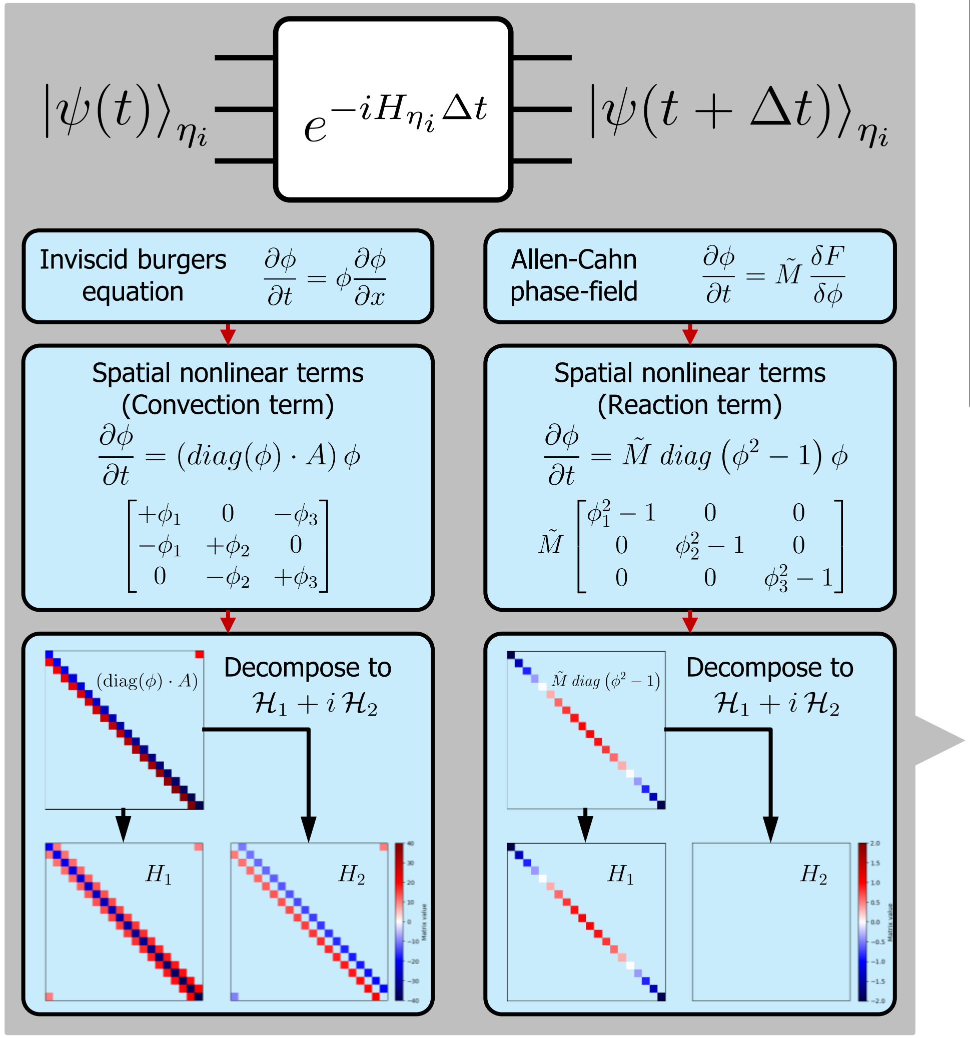
$$\mathcal{F}_p\left[\frac{\partial\omega}{\partial t}\right] = \frac{\partial\psi}{\partial t} \qquad \mathcal{F}_p[\omega] = \psi$$

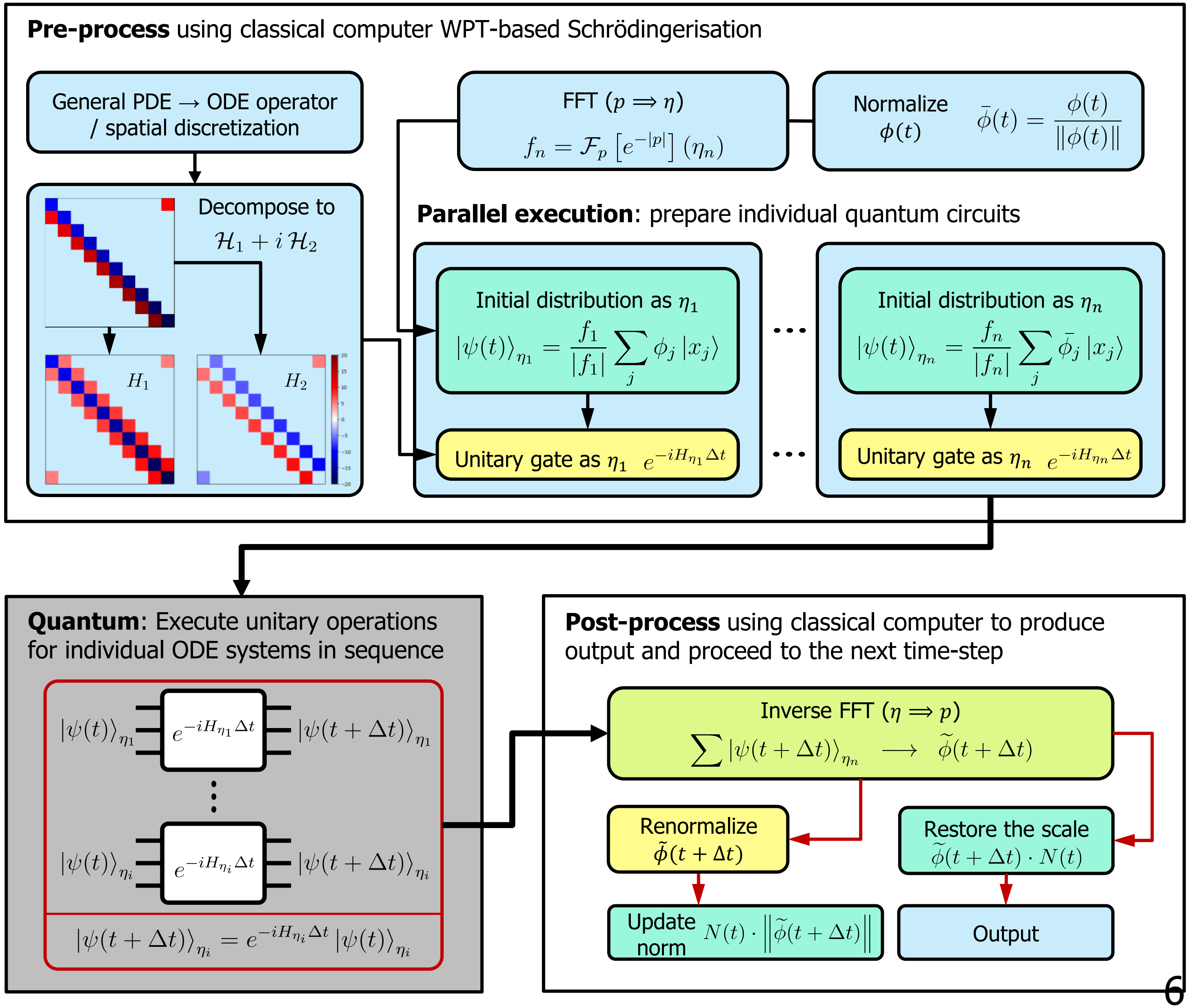
$$\mathcal{F}_p\left[\frac{\partial\omega}{\partial p}\right] = \int_{-\infty}^{\infty}\frac{\partial\omega}{\partial p}e^{-i\eta p}\,dp = i\eta\psi$$

[1] Jin et al., Quantum simulation of partial differential equations via Schrödingerisation, 2022

Numerical method

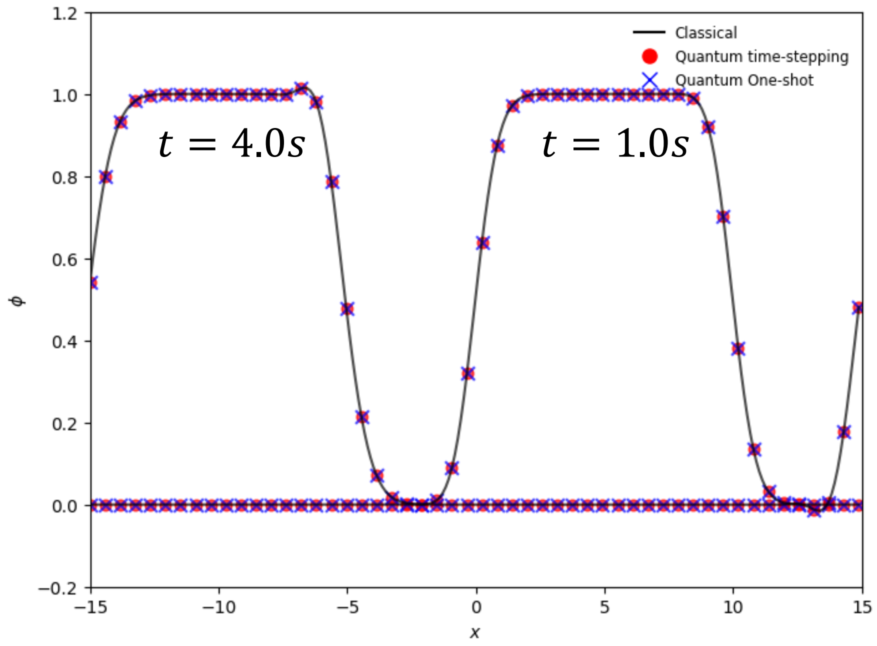
- **Time-stepping Hamiltonian simulation**
  - Evolve $|\psi(t)\rangle$ to target Δt iteratively
  - Assume local linearity of the Nonlinear PDE over Δt
  - Update of the Hamiltonian at each Δt (classical side)





Numerical conditions

- **Quantum Framework**
  - Qiskit v1.3.0
  - Qiskit-Aer v0.15.0
  - Qiskit-Aer-gpu v0.15.0
  - SciPy v1.11.4
- **Simulators**
  - Noise-free (Statevector simulator)
  - Sampling via *get_statevector* (Qiskit)
    - For complex state vector



- **Simulation environment (R-CCS Cloud)**
  - **CPU node**
    - AMD EPYC 9684X
    - 768 GB DDR4 RAM
  - **GPU node**
    - 2 × AMD EPYC 7763
    - 2,048 GB DDR4 RAM
    - 8 × NVIDIA A100 80 GB GPUs

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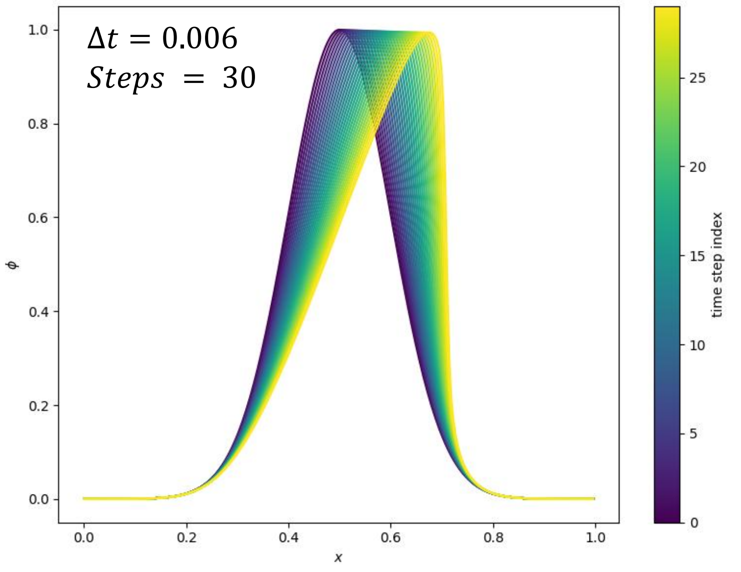

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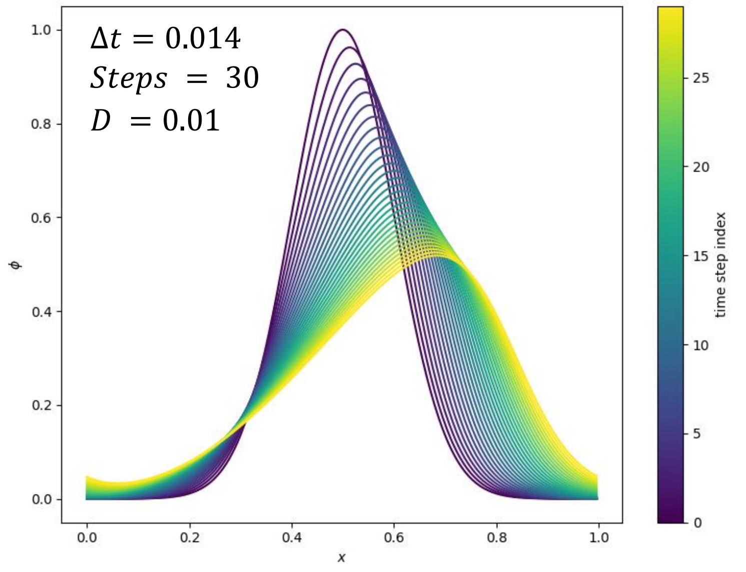
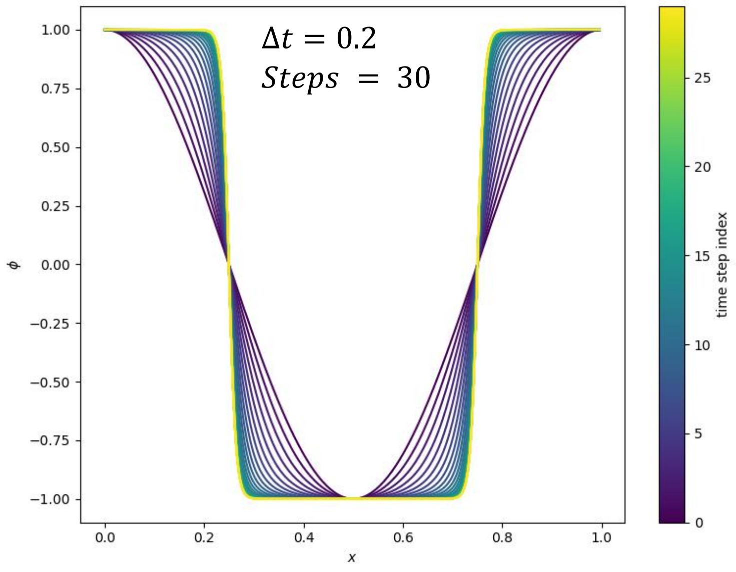


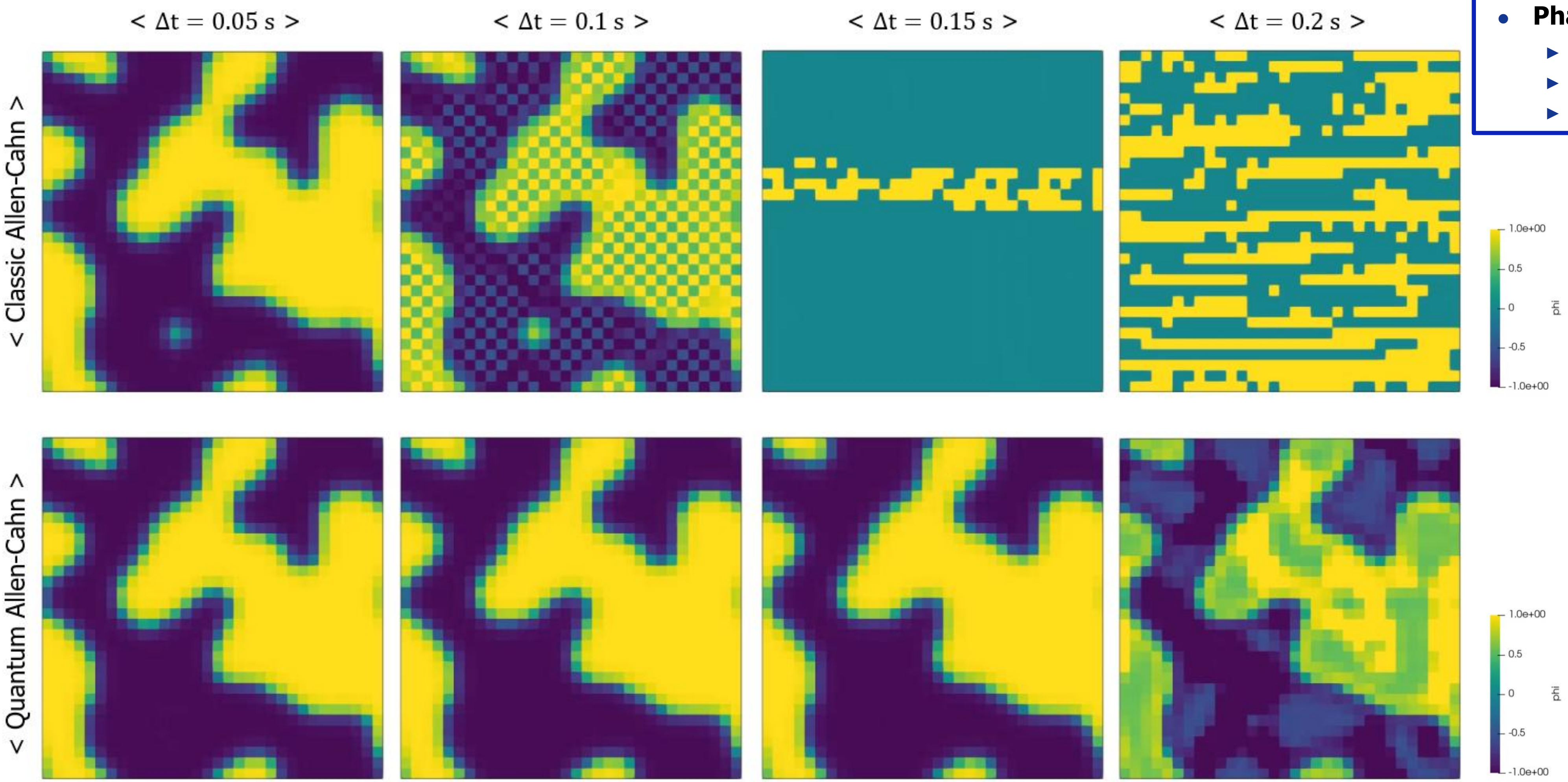
< Allen-Cahn phase-field >



Numerical Results

- **2D Nonlinear equations (Allen-Cahn phase-field)**
  - Classic cases : High-frequency oscillation ($\Delta t = 0.1s$) and diverged ($\Delta t = 0.15s$)
  - Quantum cases : stable until $\Delta t = 0.15s$ and Low-frequency oscillation ($\Delta t = 0.2s$)

- **Initial distribution**
  - Random distribution
  - Periodic boundary condition
- **Resolution**
  - Length $(L_x \times L_y)$: 0.25×0.25
  - Mesh : 10 qubit (Nx, Ny = 2^5)
  - Warped phase variable : $p = 2^7$
- Time-step : 0.03 ~ 0.2 s
- Total time : 4.2 s
- **Phase-field parameter**
  - $\boldsymbol{\epsilon}$ (Interfacial width) : 0.01
  - $\boldsymbol{W}$ (Double-well coef.) : 6.0
  - $\boldsymbol{M}$ (Mobility) : 1.0

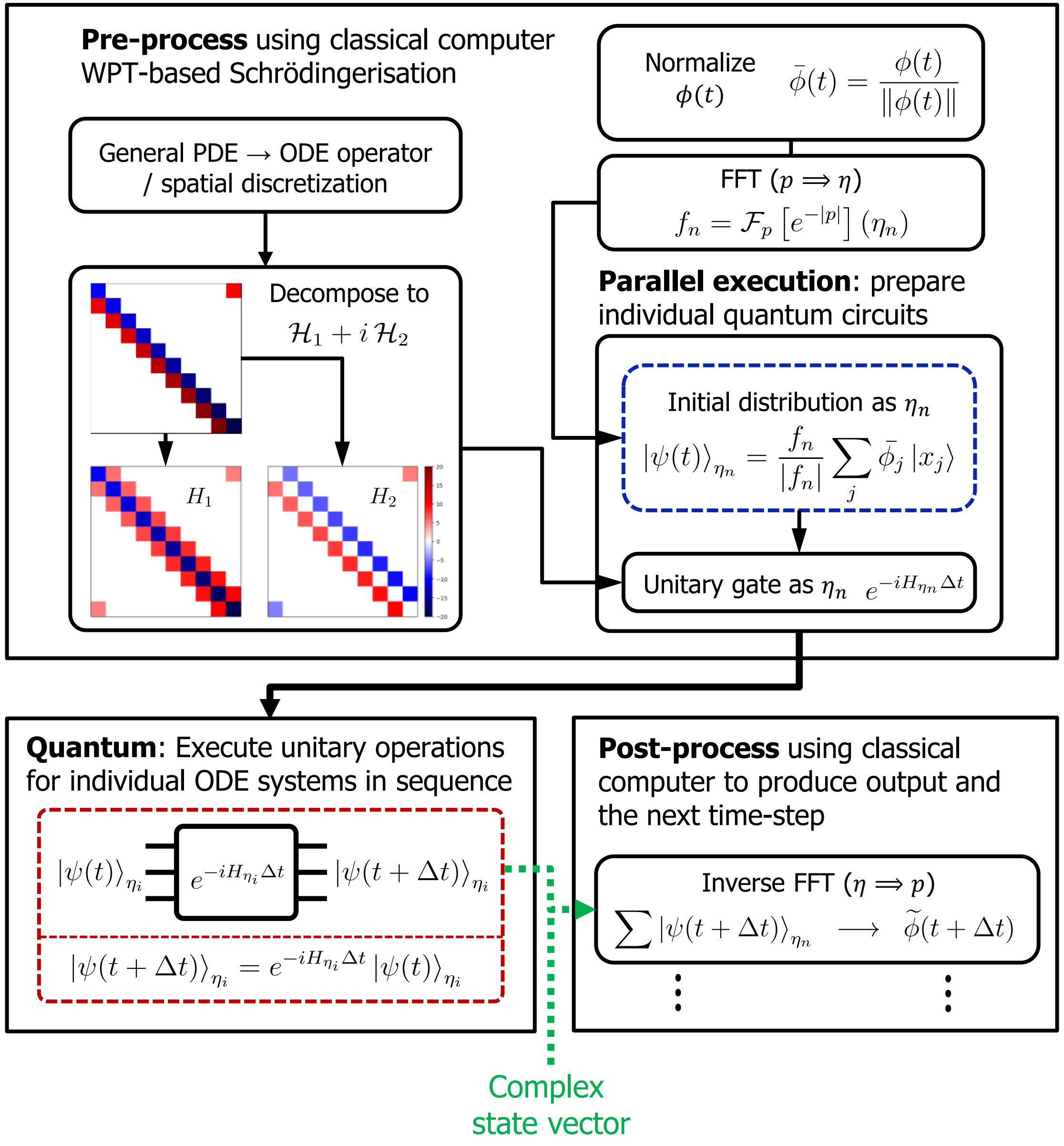


Conclusion

- **In this study, we propose a time-stepping Hamiltonian simulation via WPT-based Schrödingerisation**
  - Robust hybrid quantum-classical approach for addressing Nonlinear PDEs
  - Potential for efficiently simulating Nonlinear dynamics without dimensional inflation

- **Next plan**
  - **Improve algorithm for practical usage on NISQ device**
    - Quantum State Preparation (QSP) to data encoding
    - Explicit Quantum circuit for specific problem
    - Quantum State Tomography (QST) to reconstruct complex state vector
  - **Calculate from Real-device**

- **SC25 Best Research Poster Award**



THANK YOU