Trotter-based quantum algorithm for solving transport equations with vector norm scaling

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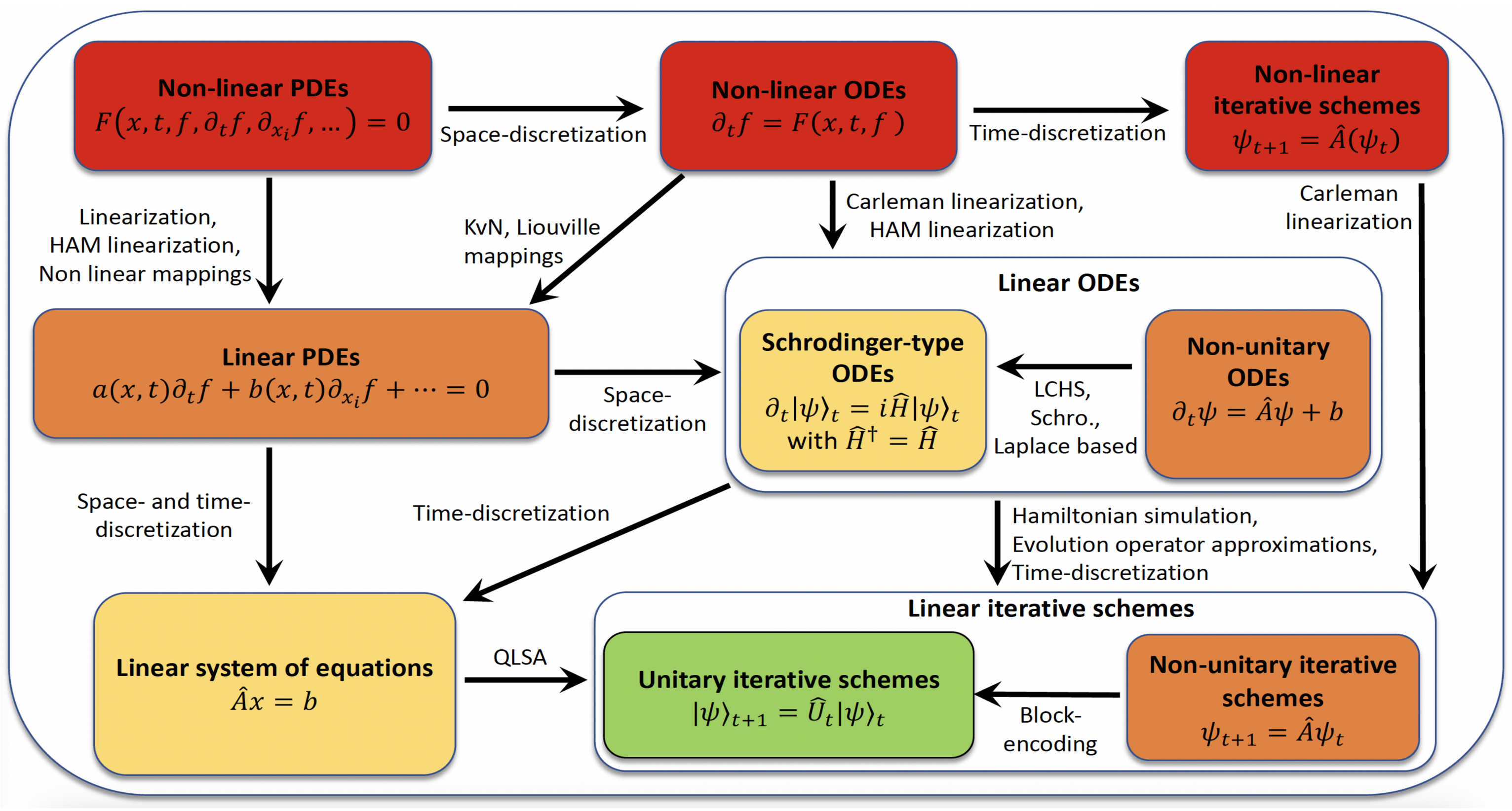
How to solve differential equations on digital fault-tolerant quantum computers ?

Differential equations are mathematical tools to model physical phenomena.
Quantum gates are linear and unitary:
⟶**Non-linear problems**: linearization or linear embeddings.
⟶**Non-unitary problems**: block-encoding.
Two strategies:
⟶Map the problem to a **linear system of equations** that requires inversion.
⟶Map the problem to a **Schrödinger-type ODE**.

To pave the way for practical implementation, the primary prerequisite is the development of efficient quantum numerical schemes:
⟶**Efficient quantum routines**.
⟶**Numerical analysis**.



Transport equation & quantum numerical scheme

Let $\vec{c} = \vec{c}(x,t)$ be a time-dependent vector field defined on $[0,1]^d \times [0,T] \to \mathbb{R}^d$ for a final time $T > 0$. Consider the following multidimensional anisotropic transport equation with $\vec{x} \in [0,1]^d, t \in [0,T]$:

$$\begin{aligned} \partial_t f + \vec{c}(x,t)\cdot\vec{\nabla} f = 0,\\ f(\vec{x}, t=0) = f_0(\vec{x}). \end{aligned} \tag{1}$$

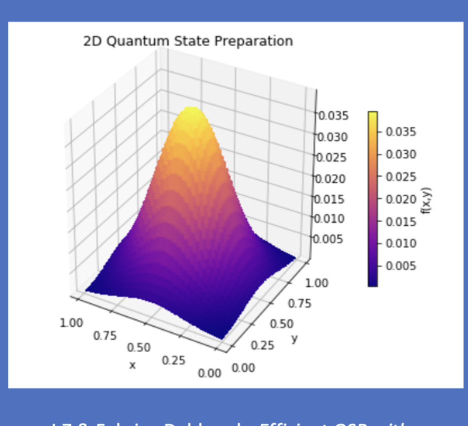
We assume that $\vec{c}$ is bounded, $\forall j, \partial_{x_j} c_j = 0$ (strong incompressibility), and we impose periodic boundary conditions.
⟶ **Space discretization**: $[0,1]^d \to X_j \in \{0/N_j, 1/N_j, \dots, (N_j-1)/N_j\}$, with $N_j = 2^{n_j}$.
Centered Finite Difference: $\partial_{x_j} f(\vec{x},t) \to \frac{\sum_{k=-p}^{p} a_k f(\vec{x}+k\vec{x}_j,t)}{\Delta x_j} + O(\Delta x_j^{2p})$,
⟶ **Real-space encoding**: $|f\rangle_t = \sum_{\vec{X}} f(\vec{X},t)|\vec{X}\rangle$. The multidimensional transport equation Eq.(1) can now be recast as an ordinary differential equation:

$$\frac{d|\tilde{f}\rangle_t}{dt} = -i\Big(\sum_{j=1}^{d} \hat{c}_j(t)\hat{D}_j\Big)|\tilde{f}\rangle_t, \tag{2}$$

which has solution: $|\tilde{f}\rangle_t = \hat{\mathcal{T}} e^{-i\int_0^T \left(\sum_{j=1}^d \hat{c}_j(s)\hat{D}_j\right)ds}|f_0\rangle$ ⟶ **Trotterization**.

1) Quantum State Preparation

$f_0 \to |f_0\rangle = \frac{1}{||f_0||}\sum_{\vec{x}} f_0(\vec{x})|\vec{x}\rangle$



J.Z & Fabrice Debbasch, *Efficient QSP with Walsh Series*, **Phys. Rev. A** 109, 042401

2) Evolution

N_t time-steps

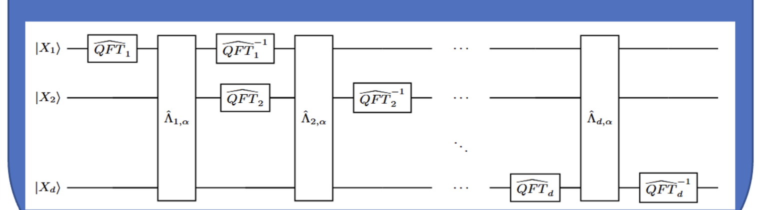
$|\tilde{f}_s\rangle_T = \prod_{l=1}^{N_t}\left(\prod_{j=1}^{d} e^{-i\widehat{c_j}(l\Delta t)\hat{D}_j\Delta t}\right)|f_0\rangle,$

$|f_0\rangle \to |\tilde{f}_g\rangle_T = \prod_{l=1}^{N_t}\left(\prod_{j=1}^{d} e^{-i\int_{l\Delta t}^{(l+1)\Delta t}\widehat{c_j}(s)ds\hat{D}_j}\right)|f_0\rangle,$

Diagonalization in Fourier space

$e^{-i\widehat{c_j}(l\Delta t)\hat{D}_j\Delta t} = \widehat{QFT}^{-1} e^{-i\widehat{c_j}(l\Delta t)\hat{d}_j\Delta t}\widehat{QFT}$

Routines: Diagonal unitaries, Quantum Fourier transforms

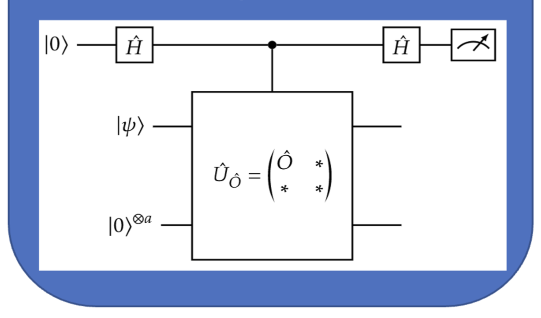


3) Measurement of observables of interests

$|\tilde{f}_\alpha\rangle_T \to \langle\tilde{f}_\alpha|\hat{O}|\tilde{f}_\alpha\rangle_T$

$\hat{O}$ can be designed to estimate fluid moments or fluxes

Hadamard test, Swap test, Quantum amplitude estimation

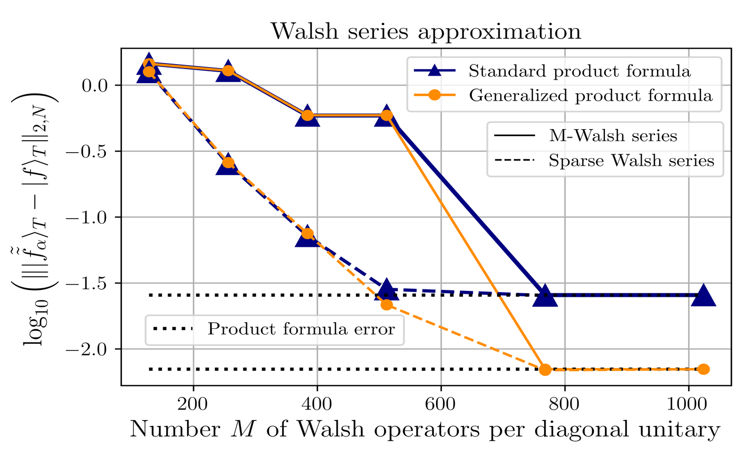


Complexity

Quantum circuit size and depth:

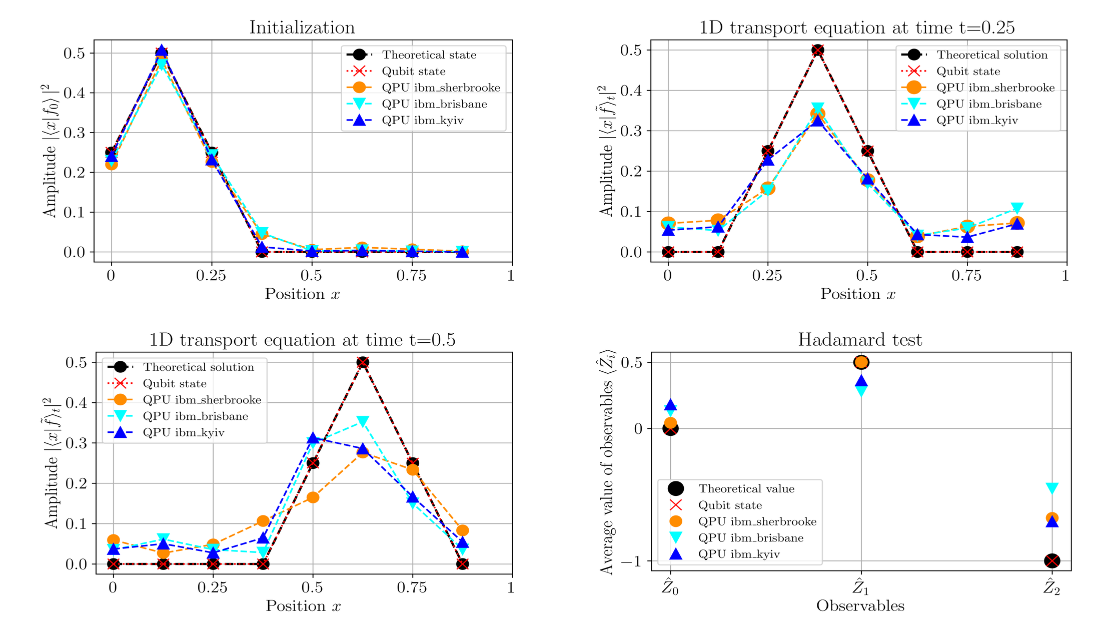
$$O\Big(\frac{C_{\text{QSP}}}{\epsilon} + \frac{d^3T^2(C_{\text{diag}} + 2C_{\text{QFT}})}{\epsilon^2} + \frac{C_{\text{observable}}}{\epsilon}\Big).$$

Gate count for the exact implementation of n-qubit routines: $C_{\text{QSP}} = O(2^n), C_{\text{diag}} = O(2^n), C_{\text{QFT}} = O(n^2), C_{\text{obs}} = O(4^n)$.
⟶ Series expansion to leverage the structure of the problem.
⟶ Efficient quantum circuits based on Walsh-Hadamard series to approximate diagonal unitaries depending on differentiable functions:
$e^{i\hat{f}} \simeq e^{i\sum_j a_j\hat{w}_j} = \prod_j e^{ia_j\hat{w}_j}$, where $w_j(x) = (-1)^{j.x}$ and $\hat{w}_j = \bigotimes_{i=1}^n(\hat{Z}_i)^{j_i}$: depth-accuracy trade-offs.



Hardware simulations

One-dimensional convection equation $\partial_t f + c\partial_x f = 0$ on IBM's QPU: size ~ 250, depth ~ 150, $n = 4$ qubits.



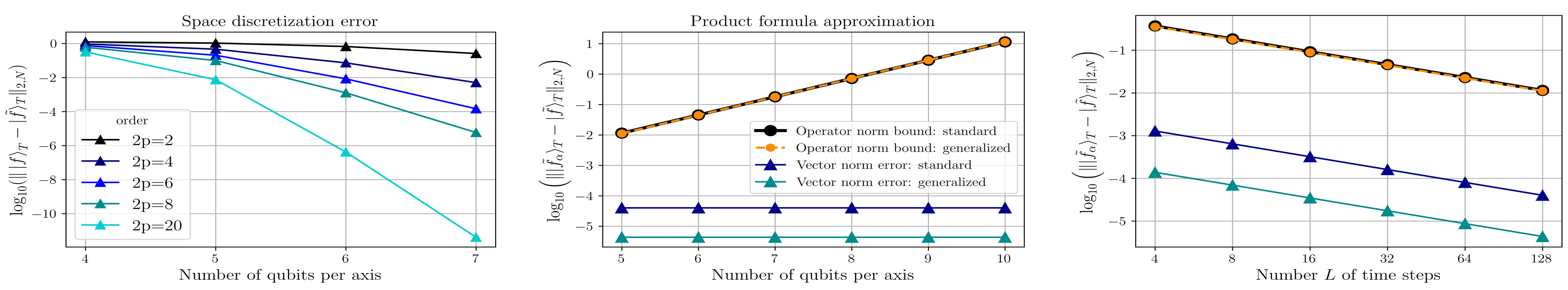
Vector norm analysis

The quantum numerical scheme deals with seven distinct sources of error:

$$\begin{aligned} |O_T - \langle\tilde{O}_T\rangle| \leq& \overbrace{|O_T -_T \langle f|\hat{O}|f\rangle_T|}^{\text{Quadrature error}} + \overbrace{|\langle\tilde{O}_T\rangle -_T \langle\tilde{\tilde{f}}_\alpha|\tilde{\hat{O}}|\tilde{\tilde{f}}_\alpha\rangle_T|}^{\text{Statistical measurement error}} + \overbrace{\|\hat{O} - \tilde{\hat{O}}\|_2}^{\text{q.c. approx.}} \\ &+ 2\|\hat{O}\|_2\Big(\underbrace{\||\tilde{\tilde{f}}_\alpha\rangle_T - |\tilde{f}_\alpha\rangle_T\|_{2,N}}_{\text{q.c. approximation}} + \underbrace{\||\tilde{f}_\alpha\rangle_T - |\tilde{f}\rangle_T\|_{2,N}}_{\text{Product formula error}} + \underbrace{\||\tilde{f}\rangle_T - |f\rangle_T\|_{2,N}}_{\text{Space discretization}} + \underbrace{\||\tilde{f}_0\rangle - |f_0\rangle\|_{2,N}}_{\text{Q.S.P error}}\Big), \end{aligned} \tag{3}$$

Space discretization error: $\||f\rangle_t - |\tilde{f}\rangle_t\|_{2,N} \leq tK\sum_{j=1}^d ||c_j||_\infty(\Delta x_j)^{2p} \longrightarrow n_j = \frac{\log_2(TdK||c_j||_\infty/\epsilon)}{2p}$.
Trotter error: $\|(e^{i(\hat{A}+\hat{B})\Delta t} - e^{i\hat{A}\Delta t}e^{i\hat{B}\Delta t})|f\rangle\| \leq \frac{\Delta t^2}{2}\|[\hat{A},\hat{B}]|f\rangle\| \leq \frac{\Delta t^2}{2}\|[\hat{A},\hat{B}]\| \leq \Delta t^2\max(\|\hat{A}\|,\|\hat{B}\|)^2$

Scaling with n:	$O(1)$	$O(1)$	$O(4^n)$	$O(4^n)$
Cumulative error after N_T time steps:		$O(\frac{T^2}{N_T})$	$O(\frac{T^2}{N_T}4^n)$	$O(\frac{T^2}{N_T}4^n)$



Non-linear Hamiltonian ODEs

For $j = 1,\dots,d$: $\frac{dx_j(t)}{dt} = c_j(\vec{x},t)$ ⟶ Liouville equation Eq.1. The average position of f gives an approximation of the solution of the non-linear ODE. Lotka-Volterra system: