Efficient quantum algorithms for nonlinear ODEs and PDEs

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Reference

- **Jin-Peng Liu**, Herman Øie Kolden, Hari K. Krovi, Nuno F. Loureiro, Konstantina Trivisa and Andrew M. Childs, *Efficient quantum algorithm for dissipative nonlinear differential equations*, Proceedings of the National Academy of Sciences 118, 35 (2021).

  (Presented by Andrew Childs on Monday)

- Dong An, Di Fang, Stephen Jordan, **Jin-Peng Liu**, Guang Hao Low and Jiasu Wang, *Efficient quantum algorithm for nonlinear reaction-diffusion equations and energy estimation*, in preparation.

Quantum Numerical Linear Algebra

Quantum computers can offer potential exponential speedup for producing the quantum-encoding solutions of

- quantum simulations[†];
- linear systems[‡];
- linear differential equations[§].

[†] [LLoyd 96; Berry et al. 15; Low, Chuang 17]
[‡] [Harrow, Hassidim, Lloyd 08; Ambainis 12; Childs, Kothari, Somma 15]
[§] [Berry 14; Berry et al. 17; Childs, Liu 19]

Quantum Scientific Computation

For real-world problems in aeronautics, climate, epidemic, finance...
a challenge is the difference between the linearity of quantum mechanics and nonlinearities in complex systems.

Questions

- Can we provide exponential speedup for nonlinear dynamics?
- Can we postprocess the quantum states to provide meaningful classical information?

Quantum Algorithm for Nonlinear ODEs

Fundamental obstacles

- Direct simulation: represent nonlinearities by multiple copies of quantum states. Need to maintain overall $2^{O(T)}$ copies[†].
- Quantum mechanics with strong nonlinearities can imply poly-time solution for NP-complete and $\#P$ problems[‡].

Solutions[§]

- Carleman linearization for dissipative ODEs with $R < 1$, where R is a ℓ_2 ratio of nonlinearities and linear dissipation.
- When $R \geq \sqrt{2}$, there is a worst case such that any quantum algorithm must suffer from $\exp(T)$.

[†] [Leyton, Osborne 08]

[‡] [Abrams, Lloyd 98; Aaronson 05; Childs, Young 16]

[§] [Liu et al. 21]

Quantum Scientific Computation

Questions

- Can we provide exponential speedup for stronger nonlinear dynamics?
- Can we postprocess the quantum states to provide meaningful classical information?

Inspirations

- Carleman linearization practically works for well-behaved solutions even $R > 1$, e.g. laminar flows†.
- Analog of energy estimation in quantum physics/chemistry.

† [Liu et al. 21]

Reaction-diffusion Equations

$$\frac{\partial u}{\partial t}(\boldsymbol{x},t) = D\Delta u(\boldsymbol{x},t) + f(u(\boldsymbol{x},t)), \quad \boldsymbol{x} \in [0,1]^d. \tag{1}$$

- $f(u) = u - u^2$: biology, ecology, social networks.
- $f(u) = u - u^3$: phase separation, data/image processing.
- $f(u) = \sum_k a_k u^k$: disorder systems, credit valuation adjustment.

$u(\boldsymbol{x},t)$ is the L^2 gradient flow of minimizing the energy functional

$$E(u) = D\int |\nabla u|^2 \mathrm{d}x + \int F(u)\mathrm{d}x, \tag{2}$$

where $\frac{\partial F}{\partial u}(u) = f(u)$. E.g. $f(u) = u - u^3$, $F(u) = \frac{1}{4}(1-u^2)^2$.

Reaction-diffusion Equations

Spatial discretization

$$\frac{\mathrm{d}U_i}{\mathrm{d}t} = D\sum_{k=1}^{n^d}(\Delta_h)_{ij}U_k + f(U_i), \quad i \in [n^d], \tag{3}$$

$U_i(t) = u(\boldsymbol{x_i}, t)$ on grids, Δ_h: Laplacian matrix with Dirichlet/mixed BCs.
Assume polynomial f has roots $\gamma_1 < \cdots < \gamma_M$, $M \geq 2$.

Proposition

Comparison principle. *If $U_i(0)$ lies in $[\gamma_k, \gamma_{k+1}]$, then $\forall\ t$, $U_i(t)$ always stays in $[\gamma_k, \gamma_{k+1}]$.*

Maximum principle. *If $U_i(0)$ lies in $[\gamma_1, \gamma_M]$, then $\forall\ t$, $U_i(t)$ always stays in $[\gamma_1, \gamma_M]$. It indicates that $\|U(t)\|_\infty \leq \gamma := \max\{|\gamma_1|, |\gamma_M|\}$.*

Carleman Linearization

Consider $\frac{\mathrm{d}U_i}{\mathrm{d}t} = \frac{1}{h^2}(U_{i-1} - 2U_i + U_{i+1}) + U_i - U_i^2$.

Embedding and truncation

- $\frac{\mathrm{d}U_i}{\mathrm{d}t} = \frac{1}{h^2}(U_{i-1} - 2U_i + U_{i+1}) + U_i - U_i^2$.
- $\frac{\mathrm{d}U_i^2}{\mathrm{d}t} = 2U_i\frac{\mathrm{d}U_i}{\mathrm{d}t} = \frac{2}{h^2}(U_iU_{i-1} - 2U_i^2 + U_iU_{i+1}^2) + 2U_i^2 - 2U_i^3$.
- $\cdots\cdots$
- $\frac{\mathrm{d}U_i^N}{\mathrm{d}t} \approx \frac{N}{h^2}(U_i^{N-1}U_{i-1} - 2U_i^N + U_i^{N-1}U_{i+1}) + NU_i^N$.
- Give a linear ODE with variables $y_j \approx U^{\otimes j} \in \mathbb{R}^{n^{jd}}$ for $k \in [N]$.

A system of n^d-dim nonlinear ODEs is embedded to a system of linear ODEs with truncation order N, with dimension $n^d + n^{2d} + \cdots + n^{Nd}$.

Carleman Linearization

We give a linear ODEs $\frac{d\hat{y}}{dt} = A\hat{y}$ with $\hat{y}(0) = \hat{y}_{\text{in}}$, by

$$\frac{d}{dt}\begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \vdots \\ \hat{y}_N \end{pmatrix} = \begin{pmatrix} A_1^1 & \cdots & A_M^1 & & \\ A_1^2 & A_2^2 & & \ddots & \\ & \ddots & \ddots & & A_N^{N-M+1} \\ & & \ddots & \ddots & \vdots \\ & & & A_{N-1}^N & A_N^N \end{pmatrix} \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \vdots \\ \hat{y}_N \end{pmatrix}, \qquad (4)$$

where $\hat{y}_j \approx U^{\otimes j} \in \mathbb{R}^{n^{jd}}$, $\hat{y}_{\text{in}} = [U_{\text{in}}; U_{\text{in}}^{\otimes 2}; \ldots; U_{\text{in}}^{\otimes N}]$, and A_{j+k-1}^j encodes k-th order polynomial.

We denote the error from the truncation as $\eta_j(t) := U^{\otimes j}(t) - \hat{y}_j(t)$.

Carleman Linearization

$$\frac{\mathrm{d}U_i}{\mathrm{d}t} = D\sum_{k=1}^{n^d}(\Delta_h)_{ij}U_k + a_1U_i + a_2U_i^2, \quad i \in [n^d]. \tag{5}$$

Assume the largest eigenvalue of $\Delta_h + a_1 I$: $\lambda_1 < 0$, and U_{in} satisfies Maximum Principle, then $\forall t$, $\|U(t)\|_\infty \le \gamma$.

Lemma (convergence analysis)

(i) Assume $R = \frac{|a_2|}{|\lambda_1|}\|U_{\text{in}}\| < 1$*. The* ℓ_2 *error bound satisfies*†

$$\|\eta_j(t)\| \le \|U_{\text{in}}\|^j R^{N-1}. \tag{6}$$

(ii) Assume $R_D = \frac{|a_2|}{|\lambda_1|}\gamma C < 1$*, where* $C = O(d)$ *and independent of* n*. The* ℓ_∞ *error bound satisfies*

$$\|\eta_j(t)\|_\infty \le \gamma^j R_D^{N-1}. \tag{7}$$

† [Liu et al. 21]

Carleman Linearization

$$\frac{\mathrm{d}U_i}{\mathrm{d}t} = D\sum_{k=1}^{n^d}(\Delta_h)_{ij}U_k + a_1 U_i + g(U_i), \quad i \in [n^d]. \tag{8}$$

$g(u) = a_0 + \sum_{k=2}^{M} a_k u^k$. Given $\lambda_1 < 0$, and $\forall t$, $\|U(t)\|_\infty \leq \gamma$.

Lemma (convergence analysis)

(i) Assume $R = \frac{1}{|\lambda_1|\|U_{\text{in}}\|} g(\|U_{\text{in}}\|) < 1$. *The* ℓ_2 *error bound satisfies*

$$\|\eta_j(t)\| \leq \|U_{\text{in}}\|^j R^{\frac{N-1}{M-1}}. \tag{9}$$

(ii) Assume $a_0 = 0$, $R_D = \frac{C}{|\lambda_1|\gamma} g(\gamma) < 1$, *where* $C = O(d)$ *and independent of* n. *The* ℓ_∞ *error bound satisfies*

$$\|\eta_j(t)\|_\infty \leq \gamma^j R_D^{\frac{N-1}{M-1}}. \tag{10}$$

Carleman Linearization

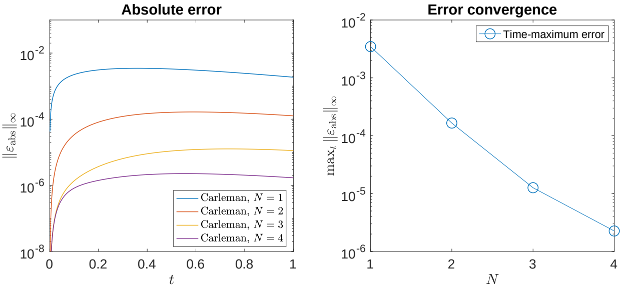


Figure: $\frac{\partial u}{\partial t} = 0.2\Delta u + 0.2u - u^2$, $u(x, 0) = 0.1\,(1 - \cos(2\pi x))$ with homogenous Dirichlet boundary condition. Spatial grid number $n = 16$. $C = 4.4620$, $R_D = 0.5047$. Left: l_∞ norm of the absolute error between the Carleman solutions. Right: convergence of the time-maximum error.

Quantum Carleman Linearization

We linearize the equation with the N-th order truncation, which we solve using the Euler method with step h and QLSA.

Theorem (quantum algorithm)

Assume $R_D < 1$. Let $q := \frac{\|U_{\mathrm{in}}\|}{\|U(T)\|}$. There is a quantum algorithm that
(i) produces $|U\rangle \sim \sum_k U(kh)|k\rangle$ with $\widetilde{O}(T^2 d^2 \|U_{\mathrm{in}}\|^{2N}/\epsilon)$;
(ii) produces $|U(T)\rangle$ with $\widetilde{O}(T^2 d^2 q \|U_{\mathrm{in}}\|^{2N}/\epsilon)$.

Corollary

Assume $R < 1$ (or assume $R \leq 1$ with $R_D < 1$). The above results can be reduced to $\widetilde{O}(T^2 d^2 q/\epsilon)$ and $\widetilde{O}(T^2 d^2/\epsilon)$.

Quantum Carleman Linearization

Why better convergence

- If there is a blow-up solution, the truncation error is generally unbounded. The exponentially increasing error is also used to show the worst-case complexity exponential in time[†].
- Maximum Principle: $\forall t$, $\|U(t)\|_\infty \leq \gamma$.

Comparison

- $R_D \ll R$ if $\gamma \ll \|U_{\text{in}}\|$ for large n and d.
- Assume $R_D < 1$, error decays in R_D^N and cost scales in $\|U_{\text{in}}\|^{2N}$: a trade-off between the approximation and the cost; while there is no dependence of N when $R < 1$.

[†] [Liu et al. 21]

Applications

Postprocess the history or final state

We have developed efficient quantum algorithm for producing

$$|U\rangle = \frac{1}{Z_0} \sum_{k\in[m],\boldsymbol{l}\in[n^d]} u(\boldsymbol{x}_{\boldsymbol{l}}, t_k)|l_1\rangle \dots |l_d\rangle |k\rangle. \tag{11}$$

Postselecting $|U(T)\rangle$ $(T = mh)$ relies on $q = \frac{\|U_{\text{in}}\|}{\|U(T)\|}$.

- For homogeneous systems with $R < 1$, e.g. $f(u) = u - u^3$, the solution decays exponentially in time, i.e. $q = \exp(T)$.
- Given external forces or inhomogeneous BCs, the solution can remain nonzero, decay slowly, or be oscillatory i.e. $q = \text{poly}(T)$.

Applications

Ratio of mean square amplitude

$$\frac{\int_{\Omega_t}\int_{\Omega_{\boldsymbol{x}}} |u(\boldsymbol{x},t)|^2 \,\mathrm{d}t\mathrm{d}\boldsymbol{x}}{\int_0^T\int_{[0,1]^d} |u(\boldsymbol{x},t)|^2 \,\mathrm{d}t\mathrm{d}\boldsymbol{x}} \sim \frac{\sum_{k\in I_t,\boldsymbol{l}\in I_{\boldsymbol{x}}} |u(\boldsymbol{x}_{\boldsymbol{l}},t_k)|^2}{\sum_{k\in[m],\boldsymbol{l}\in[n^d]} |u(\boldsymbol{x}_{\boldsymbol{l}},t_k)|^2}. \tag{12}$$

Let the projector P associate with indices $I_t \subset [m]$ and $I_{\boldsymbol{x}} \subset [n^d]$:
$P = \sum_{k\in I_t,\boldsymbol{l}\in I_{\boldsymbol{x}}} (|l_1\rangle\langle l_1|) \otimes \cdots \otimes (|l_d\rangle\langle l_d|) \otimes (|k\rangle\langle k|)$.

Amplitude estimation: perform $I - 2P$ with $\widetilde{O}(1/\epsilon)$ to estimate $\langle U|P|U\rangle$.

Example: diffusive Lotka-Volterra equations

$$\begin{aligned}\frac{\partial u}{\partial t} &= D\Delta u + \alpha u - \beta uv \\ \frac{\partial v}{\partial t} &= D\Delta v + \delta uv - \gamma v.\end{aligned} \tag{13}$$

Traveling waves in predator-prey, economic cycle, and disease models.

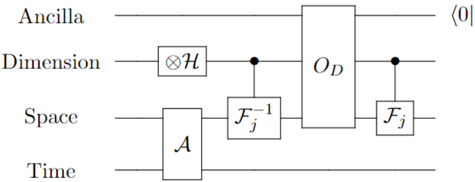
Applications

Ratio of diffusive energy

We can produce

$$|\nabla_{\boldsymbol{x}} U\rangle = \frac{1}{Z_1} \sum_{k \in [m], \boldsymbol{l} \in [n^d]} \nabla_{x_j} u(\boldsymbol{x_l}, t_k) |j\rangle |l_1\rangle \dots |l_d\rangle |k\rangle \tag{14}$$

by performing QFT/IQFT on $|U\rangle$ with cost $\widetilde{O}(d)$.



Quantum circuit for preparing a quantum state encoding partial derivatives

Applications

Ratio of diffusive energy

$$\frac{\int_{\Omega_t}\int_{\Omega_{\boldsymbol{x}}} |\nabla_{\boldsymbol{x}} u(\boldsymbol{x},t)|^2 \, \mathrm{d}t\mathrm{d}\boldsymbol{x}}{\int_0^T \int_{[0,1]^d} |\nabla_{\boldsymbol{x}} u(\boldsymbol{x},t)|^2 \, \mathrm{d}t\mathrm{d}\boldsymbol{x}} \sim \frac{\sum_{k\in I_t, \boldsymbol{l}\in I_{\boldsymbol{x}}} |\nabla_{\boldsymbol{x}} u(\boldsymbol{x}_{\boldsymbol{l}}, t_k)|^2}{\sum_{k\in[m], \boldsymbol{l}\in[n^d]} |\nabla_{\boldsymbol{x}} u(\boldsymbol{x}_{\boldsymbol{l}}, t_k)|^2}. \tag{15}$$

Perform $I-2P$ with $\widetilde{O}(1/\epsilon)$ to estimate $\langle \nabla_{\boldsymbol{x}} U | P | \nabla_{\boldsymbol{x}} U \rangle$.

Example: Allen-Cahn equation

- $\frac{\partial u}{\partial t} = D\Delta u + u - u^3 + F(t)$: phase separation and transition.
- $\frac{\partial u}{\partial t} = D\Delta u + u - u^3 + F(u-u_0)$: data classification, graph cuts, signal or image denoising and reconstruction.

u is the L^2 gradient flow of minimizing a regularized energy functional. $\|\nabla_{\boldsymbol{x}} u\|^2$ measures the L^2 total variation distance.

Summary

Takeaways

- Quantum computer can efficiently characterize weak gradient flows in $\widetilde{O}(T^2 d^2/\epsilon)$ when $R_D < 1$ or $R < 1$. ℓ_∞ aprior estimate is used to improve the linearization and rule out the worst case.
- Nonlinear ODEs/PDEs exhibit rich phenomena. Ratio of energy proportion to amplitude squared and total variation can be estimated in $\widetilde{O}(d/\epsilon)$.

Outlook

Quantum algorithm

- Advection term $f(u, \nabla u)$: N-S equation, Boltzmann equation.
- Non-dissipative systems: nonlinear Schrödinger equations.
- Discrete gradient flows for optimization and control.
- Hermitian/skew-Hermitian linearization.

Postprocessing

- Scattering cross section.
- Time frequency analysis.
- Free energy estimation: $D \int |\nabla u|^2 \mathrm{d}x + \int F(u) \mathrm{d}x$.