Efficient quantum algorithms for nonlinear ODEs and PDEs

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Reference


(Presented by Andrew Childs on Monday)

Quantum computers can offer potential \textit{exponential} speedup for producing the quantum-encoding solutions of

- quantum simulations\(^\dagger\);
- linear systems\(^\ddagger\);
- linear differential equations\(^\S\).

\(^\dagger\) [Lloyd 96; Berry et al. 15; Low, Chuang 17]
\(^\ddagger\) [Harrow, Hassidim, Lloyd 08; Ambainis 12; Childs, Kothari, Somma 15]
\(^\S\) [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$^\dagger$.
- 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 $\ell_2$ ratio of nonlinearities and linear dissipation.
- When $R \geq \sqrt{2}$, there is a worst case such that any quantum algorithm must suffer from $\exp(T)$.

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$^\dagger$[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

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

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

\[
E(u) = D \int |\nabla u|^2 \, dx + \int F(u) \, dx,
\] (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

\[
\frac{dU_i}{dt} = D \sum_{k=1}^{n^d} (\Delta_h)_{ij} U_k + f(U_i), \quad i \in [n^d], \quad i \in [n^d],
\]

\(U_i(t) = u(x_i, t)\) on grids, \(\Delta_h\): 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 \( \frac{dU_i}{dt} = \frac{1}{h^2} (U_{i-1} - 2U_i + U_{i+1}) + U_i - U_i^2. \)

Embedding and truncation

- \( \frac{dU_i}{dt} = \frac{1}{h^2} (U_{i-1} - 2U_i + U_{i+1}) + U_i - U_i^2. \)
- \( \frac{dU_i^2}{dt} = 2U_i \frac{dU_i}{dt} = \frac{2}{h^2} (U_i U_{i-1} - 2U^2_i + U_i U_{i+1}^2) + 2U_i^2 - 2U_i^3. \)
- \( \ldots \ldots \)
- \( \frac{dU_i^N}{dt} \approx \frac{N}{h^2} (U_i^{N-1} U_{i-1} - 2U_i^N + U_i^{N-1} U_{i+1}) + N U_i^N. \)
- Give a linear ODE with variables \( y_j \approx U^j \in \mathbb{R}^{n^{jd}} \) 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 \( n^d + n^{2d} + \cdots + n^{Nd}. \)
We give a linear ODEs $\frac{d\hat{y}}{dt} = A\hat{y}$ with $\hat{y}(0) = \hat{y}_{\text{in}}$, by

$$
\begin{pmatrix}
\hat{y}_1 \\
\hat{y}_2 \\
\vdots \\
\hat{y}_N
\end{pmatrix}
= 
\begin{pmatrix}
A_1^1 & \cdots & A_M^1 \\
A_1^2 & \cdots & \cdots \\
\vdots & \cdots & \cdots \\
A_{N-M+1}^N & \cdots & A_N^N
\end{pmatrix}
\begin{pmatrix}
\hat{y}_1 \\
\hat{y}_2 \\
\vdots \\
\hat{y}_N
\end{pmatrix},
$$

where $\hat{y}_j \approx U^\otimes j \in \mathbb{R}^{n^j_d}$, $\hat{y}_{\text{in}} = [U_{\text{in}}; U_{\text{in}}^\otimes 2; \ldots; U_{\text{in}}^\otimes N]$, and $A_j^{j+k-1}$ 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

\[
\frac{dU_i}{dt} = D \sum_{k=1}^{n^d} (\Delta_h)_{ij} U_k + a_1 U_i + a_2 U_i^2, \quad i \in [n^d].
\]  

(5)

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

Lemma (convergence analysis)

(i) Assume \(R = \frac{|a_2|}{|\lambda_1|} \|U_{in}\| < 1\). The \(\ell_2\) error bound satisfies

\[\|\eta_j(t)\| \leq \|U_{in}\|^j R^{N-1}.\]  

(6)

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

\[\|\eta_j(t)\|_\infty \leq \gamma^j R_D^{N-1}.\]  

(7)

\[\text{[Liu et al. 21]}\]
Carleman Linearization

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

(8)

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

Lemma (convergence analysis)

(i) Assume \( R = \frac{1}{|\lambda_1|\|U_{in}\|} g(\|U_{in}\|) < 1 \). The \( \ell_2 \) error bound satisfies

\[
\|\eta_j(t)\| \leq \|U_{in}\|^j R^{N-1}_{M-1}.
\]

(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 \( \ell_\infty \) error bound satisfies

\[
\|\eta_j(t)\|_\infty \leq \gamma^j R_D^{N-1}_{M-1}.
\]

(10)
Carleman Linearization

Figure: \( \frac{\partial u}{\partial t} = 0.2 \Delta u + 0.2u - u^2, \ u(x, 0) = 0.1 \left(1 - \cos(2\pi x)\right) \) with homogenous Dirichlet boundary condition. Spatial grid number \( n = 16. \ C = 4.4620, \ R_D = 0.5047. \) Left: \( l_\infty \) 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 $q := \frac{\|U_{\text{in}}\|}{\|U(T)\|}$. There is a quantum algorithm that

(i) produces $|U\rangle \sim \sum_k U(kh)|k\rangle$ with $\tilde{O}(T^2 d^2 \|U_{\text{in}}\|^{2N} / \epsilon)$;
(ii) produces $|U(T)\rangle$ with $\tilde{O}(T^2 d^2 q \|U_{\text{in}}\|^{2N} / \epsilon)$.

**Corollary**

Assume $R < 1$ (or assume $R \leq 1$ with $R_D < 1$). The above results can be reduced to $\tilde{O}(T^2 d^2 q / \epsilon)$ and $\tilde{O}(T^2 d^2 / \epsilon)$. 
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\(^\dagger\).
- Maximum Principle: \( \forall t, \|U(t)\|_\infty \leq \gamma \).

Comparison

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

\(^\dagger\) [Liu et al. 21]
Applications

Postprocess the history or final state

We have developed efficient quantum algorithm for producing

$$|U\rangle = \frac{1}{Z_0} \sum_{k \in [m], l \in [n^d]} u(x_l, t_k) |l_1\rangle \ldots |l_d\rangle |k\rangle. \quad (11)$$

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

- 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

\[
\frac{\int_{\Omega_t} \int_{\Omega_\mathbf{x}} |u(\mathbf{x}, t)|^2 \, dtd\mathbf{x}}{\int_0^T \int_{[0,1]^d} |u(\mathbf{x}, t)|^2 \, dtd\mathbf{x}} \sim \frac{\sum_{k\in I_t, l\in I_\mathbf{x}} |u(\mathbf{x}_l, t_k)|^2}{\sum_{k\in [m], l\in [n^d]} |u(\mathbf{x}_l, t_k)|^2}.
\]  

(12)

Let the projector \( P \) associate with indices \( I_t \subset [m] \) and \( I_\mathbf{x} \subset [n^d] \):

\[
P = \sum_{k\in I_t, l\in I_\mathbf{x}} (|l_1\rangle\langle l_1|) \otimes \cdots \otimes (|l_d\rangle\langle l_d|) \otimes (|k\rangle\langle k|).
\]

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

Example: diffusive Lotka-Volterra equations

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D \Delta u + \alpha u - \beta uv \\
\frac{\partial v}{\partial t} &= D \Delta v + \delta uv - \gamma v.
\end{align*}
\]  

(13)

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

Ratio of diffusive energy

We can produce

$$|\nabla_x U\rangle = \frac{1}{Z_1} \sum_{k \in [m], l \in [n^d]} \nabla x_j u(x_l, t_k) |j\rangle |l_1\rangle \ldots |l_d\rangle |k\rangle$$  \hspace{1cm} (14)

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

Quantum circuit for preparing a quantum state encoding partial derivatives
Applications

Ratio of diffusive energy

\[
\frac{\int_{\Omega_t} \int_{\Omega_x} |\nabla_x u(x, t)|^2 \, dt \, dx}{\int_0^T \int_{[0,1]^d} |\nabla_x u(x, t)|^2 \, dt \, dx} \sim \frac{\sum_{k \in I_t, l \in I_x} |\nabla_x u(x_l, t_k)|^2}{\sum_{k \in [m], l \in [n^d]} |\nabla_x u(x_l, t_k)|^2}.
\]  

(15)

Perform \( I - 2P \) with \( \tilde{O}(1/\epsilon) \) to estimate \( \langle \nabla_x U | P | \nabla_x U \rangle \).

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. 
\( \| \nabla_x u \|^2 \) measures the \( L^2 \) total variation distance.
Summary

Takeaways

- Quantum computer can efficiently characterize weak gradient flows in $\tilde{O}(T^2 d^2 / \epsilon)$ when $R_D < 1$ or $R < 1$. $\ell_\infty$ 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 $\tilde{O}(d / \epsilon)$. 
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: $D \int |\nabla u|^2 dx + \int F(u) dx$. 