Introduction to Simulation Algorithms for Open Quantum Systems

Xiantao Li (Pennsylvania State University)

Collaboration with (C. Wang, Z. Ding, L. Lin, W. He, T. Li, Z. Li, K. Wang)

Outline

- Classical algorithms
  - Non-Hermitian time evolution
  - SDE based algorithms
  - Structure-preserving method
- Quantum algorithms
  - Kraus form of the CPTP map
  - Dilated Hamiltonian
- Application to control problems

Lindblad Dynamics

System-bath coupled dynamics

$H_{tot} = H_S \otimes I_B + I_S \otimes H_B + \lambda H_I$

$\rho_S(t) = tr_B\left(U_{tot}(t)\rho_S(0) \otimes \rho_B U_{tot}(t)^\dagger\right)$

Carmichael 2002

$$\frac{d}{dt}\rho = -i[H_S + \Lambda, \rho] + \sum_j L_j \rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\}$$

Lindblad-Gorini-Kossakowski-Sudarshan

semigroup $M(t)$: $\rho(t) = M(t)\rho(0)$

Classical algorithms

Monte-Carlo trajectory (Breuer-Petruccione).

- Non-Hermitian Hamiltonian $D = H_S - \frac{i}{2}\sum_{j=1}^{m} L_j^\dagger L_j$
- $|\psi(t+\Delta t)\rangle = e^{-\mathrm{i}\Delta t D}\,|\psi(t)\rangle. p = 1 - ||\,\psi(t+\Delta t)||^2$
- With some probability, the system jumps to $\frac{L_j|\psi(t)\rangle}{\langle\psi(t)|L_j^\dagger L_j|\psi(t)\rangle^{\frac{1}{2}}}$
- Interpretation via a jump SDE

$$d\psi_t = -i\left(H_S - \frac{i}{2}\sum_{j=1}^{m} L_j^\dagger L_j + \frac{i}{2}\sum_{j=1}^{m}\left|\left|L_j\psi\right|\right|^2\right)\psi dt + \sum_{j=1}^{m}\left(\frac{L_j|\psi(t)}{\left|\left|L_j|\psi(t)\right|\right|^2} - \psi\right)dN_j$$

It is possible to apply regular time discretization (Platen&Bruti-Liberati).

Classical algorithms

SDE based approach

- Unravel Lindblad: $id\psi = (H_S - \frac{i}{2}\sum_{j=1}^{m} L_j^\dagger L_j)\psi dt + \sum_{j=1}^{m} L_j \psi dW_j$
- SDE solver (e.g., Euler-Maruyama, or general weak Ito-Taylor)
- $\rho(t) = E[|\psi(t)\rangle\langle\psi(t)|]$
- Preserves CP, needs less memory, but requires more samples

Runge-Kutta?

- Example: $\frac{\mathrm{d}}{\mathrm{dt}}\rho = -\frac{1}{2}\{LL^\dagger, \rho\} + L^\dagger \rho L$
- Euler's method: $\rho(t+\Delta t) \approx \rho(t) - \frac{\Delta t}{2}\{LL^\dagger, \rho\} + \Delta t L^\dagger \rho L$
- not preserve CP!

Structure preserving classical algorithms

- A structure-preserving method (Cao-Lu 2021)
- Decompose a Lindbladian: $\mathcal{L} = \mathcal{L}_D + \mathcal{L}_J$

$$\mathcal{L}_D = \left[-iH - \frac{1}{2} \sum_{j=1}^{m} L_j^\dagger L_j \,, \quad \cdot \right]; \mathcal{L}_J \rho = \sum_{j=1}^{m} L_j \rho L_j^\dagger$$

Duhamel's principle (Plenio-Knight 1998)

$$\rho(t) = e^{t\mathcal{L}_D} \rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_D} \mathcal{L}_J \rho(t_1) dt_1$$

$$\rho(t) = e^{t\mathcal{L}_D} \rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_D} \mathcal{L}_J e^{t_1 \mathcal{L}_D} \rho(0) dt_1 + O(t^2)$$

- $e^{t\mathcal{L}_D}$: Taylor expansion. The integrals: numerical quadrature.
- Overall this can be expressed in Kraus form

Quantum algorithms

- Kliesch et al. 2011. $O\left(\frac{t^2}{\epsilon}\right)$ complexity.
- Childs-Li 2017. $O\left(\frac{t^{\frac{3}{2}}}{\sqrt{\epsilon}}\right)$.
- Cleve-Wang 2017. $O\left(\mathrm{tpolylog}\frac{t}{\epsilon}\right)$.
  - First-order approximation in Kraus form:
  - $\mathcal{E}\rho = A_0\rho A_0^\dagger + \sum_{j=1}^m A_j\rho A_j^\dagger$.
  - $A_0 = I - i\Delta t H - \frac{\Delta t}{2}\sum_{j=1}^m L_j^\dagger L_j,\ A_j = \sqrt{\Delta t} L_j$
  - A compression scheme is required.

Block-encode A_j: $A_j \approx s_j(\langle 0| \otimes I)U_j(|0\rangle \otimes I)$

$$|\mu\rangle \propto \sum_j s_j|j\rangle.$$

$$W = \sum_j |j\rangle\langle j| \otimes U_j|\mu\rangle|0\rangle \otimes I.$$

$$\sum_j |j\rangle A_j|\psi\rangle \approx I \otimes \langle 0| \otimes I) \sum_j |j\rangle\langle j| \otimes U_j|\mu\rangle|0\rangle\,|\psi\rangle$$

$$|\rho_{new}\rangle = (A_0|\psi\rangle, \cdots, A_j|\psi\rangle),$$

$\mathcal{E}\rho = \mathrm{tr}_A(|\rho_{new}\rangle\langle\rho_{new}|)$

Boost the prob. using oblivious amplitude amplification for isometries.

Reduction to a Kraus form (Li-Wang 2023)

- Duhamel expansion: $\rho(t) = e^{t\mathcal{L}_D}\rho(0) + \int_0^t e^{(t-t_1)\mathcal{L}_D}\mathcal{L}_J e^{t_1\mathcal{L}_D}\rho(0)dt_1 + \int_0^t \int_0^{t_1} \cdots$
- Gaussian quadrature $(s_1, s_2, \cdots, s_q), (w_1, w_2, \cdots, w_q)$ $\int_0^1 f(t)dt = \sum_{j=1}^q w_j f(s_j) + O\left(\frac{q\|f^{2q}\|}{(2q)!2^{4q-1}}\right)$.
- $\int e^{(t-t_k)\mathcal{L}_D}\mathcal{L}_J e^{(t_k-t_{k-1})\mathcal{L}_D} \cdots \rho(0)dt_1 \cdots dt_k$
$$\approx \sum_{j_1=1}^{q}\sum_{j_2=1}^{q}\cdots\sum_{j_k=1}^{q} w_{j_k}, w_{(j_k,j_{k-1})}, \cdots w_{(j_k,\cdots j_1)} F_k\left(s_{j_k}, s_{(j_k,j_{k-1})}, \cdots s_{(j_k,\cdots j_1)}\right) + O\left(\frac{\|G\|^{2q} 2^{2k} t^{2q+k}}{(k-1)!(2q)!}\right)$$
- The sum of the coefficients $\sum_{j_1}\sum_{j_2}\cdots\sum_{j_k} w_{j_k}, w_{(j_k,j_{k-1})}, \cdots w_{(j_k,\cdots j_1)} = \frac{\mathrm{t}^{\mathrm{k}}}{(\mathrm{k}+1)!}$
- Truncation: $K, q = \frac{\log 1/\epsilon}{\log\ \log 1/\epsilon}$.
- The algorithm yields an approximate $\rho(t) = e^{t\mathcal{L}}\rho(0)$, with error within ϵ using $O(t\|\mathcal{L}\|_{be}\mathrm{polylog}\frac{\mathrm{t}}{\epsilon})$ queries and $O(tm\|\mathcal{L}\|_{be}\mathrm{polylog}\frac{\mathrm{t}}{\epsilon})$ additional 1- and 2-qubit gates.

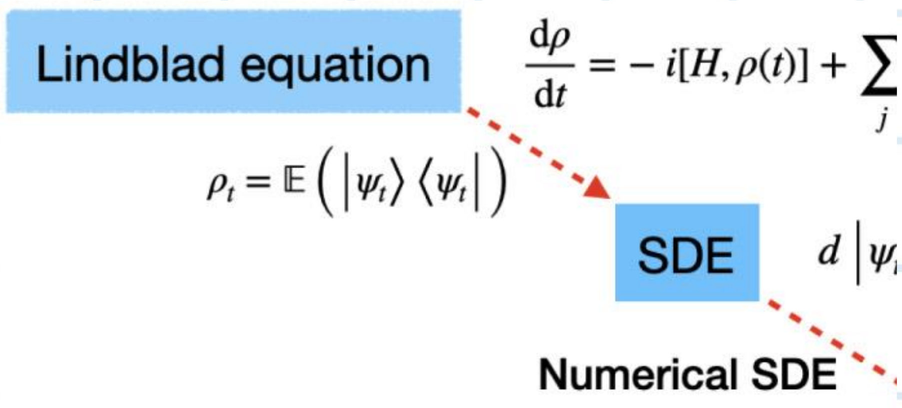
Quantum algorithms via Hamiltonian simulation

- First-order approximation (Cleve-Wang 2017)

$$\rho(t) = tr_A(e^{-i\sqrt{\Delta t}\widetilde{H}}|0\rangle\langle 0| \otimes \rho_S(0)e^{i\sqrt{\Delta t}\widetilde{H}}) + O(\Delta t^2)$$

- Dilated Hamiltonian

$$\widetilde{H} = \begin{bmatrix} \sqrt{\Delta t}H_S & L_1^\dagger & L_2^\dagger & \cdots & L_m^\dagger \\ L_1 & & & & \\ L_2 & & & & \\ \vdots & & & & \\ L_m & & & & \end{bmatrix}$$



- Hamiltonian simulation $U(t) = e^{-i\sqrt{\Delta t}\widetilde{H}}$.
- There are many algorithms for simulating $U(t)$
- Can we extend this to higher order?

Kraus from from unravelling

- Stochastic Schrödinger (unravelling)

$$id\psi = (H_S - \frac{i}{2}\sum_{j=1}^{M} L_j^\dagger L_j)\psi dt + \sum_{j=1}^{M} L_j \psi dW_j$$

- $\rho(t) = E[|\psi(t)\rangle\langle\psi(t)|]$ satisfies exactly the Lindblad equation
- Ito-Taylor expansion (Platen-Kloeden)
- $\psi(\Delta t) = \psi(0) + \sum_{\alpha\in\Gamma_k} L_{j_1} L_{j_2} \cdots L_{j_{|\alpha|}} \psi(0) I_\alpha$. I_α: stochastic integrals.
- Example: $\psi(\Delta t) = \psi(0) + \Delta t D\psi(0) + \frac{\Delta t^2}{2} D^2\psi(0) + \sum_j L_j \int_0^{\Delta t} dW_{t_1}^j + \sum_j L_j D \int_0^{\Delta t}\int_0^{t_1} dt_2 dW_{t_1}^j + \cdots$
- Approximate density operator

$$\rho(\Delta t) = A_0 \rho_n A_0^\dagger + \sum_j A_j \rho_n A_j^\dagger + O(\Delta t^{k+1}).\ A_j = O(\sqrt{\Delta t}, \Delta t, \Delta t\sqrt{\Delta t}, \cdots)$$

- Another approach to generate a Kraus form

From Kraus to Hamiltonian dynamics
Ding-Li-Lin 2024

- From Kraus for Stinespring

$$A_0\rho_n A_0^\dagger + \sum_j A_j\,\rho_n A_j^\dagger = \mathrm{tr}_\mathrm{A}\left(\begin{bmatrix} A_0 & \cdot & \cdots & \cdot \\ A_1 & \cdot & \cdot & \cdot \\ \vdots & \cdot & \ddots & \vdots \\ A_J & \cdot & \cdots & \cdot \end{bmatrix} \left|\,|0\rangle\langle 0|\,\otimes \rho_S(0)\right| \begin{bmatrix} A_0 & \cdot & \cdots & \cdot \\ A_1 & \cdot & \cdot & \cdot \\ \vdots & \cdot & \ddots & \vdots \\ A_J & \cdot & \cdots & \cdot \end{bmatrix}^\dagger\right)$$

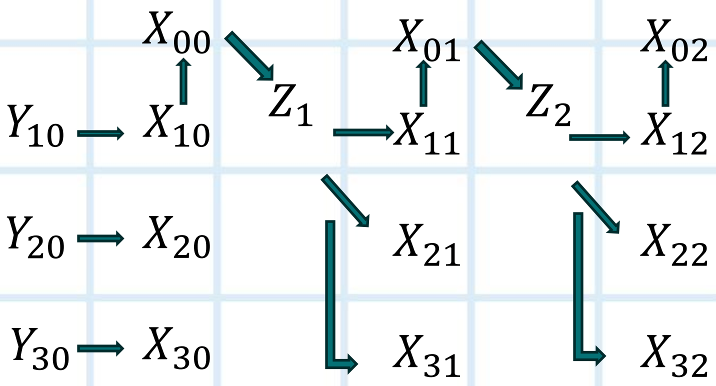
- Generate the Stinespring form using Hamiltonian simulations

$$\begin{bmatrix} A_0 & \cdot & \cdots & \cdot \\ A_1 & \cdot & \cdot & \cdot \\ \vdots & \cdot & \ddots & \vdots \\ A_J & \cdot & \cdots & \cdot \end{bmatrix} = e^{-i\sqrt{\Delta t}\,\widetilde{H}}, \qquad \widetilde{H} = \begin{bmatrix} \sqrt{\Delta t} H_{0,0} & \times & \cdots & \times \\ H_{0,1} & 0 & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ H_{0,J} & 0 & \cdots & \cdot \end{bmatrix}$$

- **Main theorem:** There exists a dilated Hamiltonian defined with $O(k \log J)$ ancilla qubits such that $\rho_S(\Delta t) = tr_A(e^{-i\sqrt{\Delta t}\widetilde{H}}|0\rangle\langle 0| \otimes \rho_S(0)e^{i\sqrt{\Delta t}\widetilde{H}}) + O(\Delta t)^{k+1}$.

The Dilated Hamiltonian

- Expand operators in the Kraus form: $F_j = \Delta t^{\alpha_j} Y_{j,0} + \Delta t^{\alpha_j+1} Y_{j,1} + \Delta t^{\alpha_j+2} Y_{j,2} + \cdots +$
- Expand operators in the dilated Hamiltonian: $H_j = \Delta t^{\beta_j} X_{j,0} + \Delta t^{\beta_j+1} X_{j,1} + \Delta t^{\beta_j+2} X_{j,2} + \cdots +$



First order dilated Hamiltonian solves a modified Lindblad

$$\tilde{H} = \begin{bmatrix} \sqrt{\Delta t} H_S & L_1^\dagger & L_2^\dagger & \cdots & L_m^\dagger \\ L_1 & & & & \\ L_2 & & & & \\ \vdots & & & & \\ L_m & & & & \end{bmatrix} \rightarrow \frac{d}{dt}\rho = \mathcal{L}\rho + \Delta t E_1 \rho + \Delta t^2 E_2 \rho + \cdots$$

$\tilde{H}$ ⟵ Near identity transformation

- Motivated by shadow Hamiltonians and canonical transformations
- Extension to time-dependent Lindbladians: $\tilde{H}$ contains time derivatives of H_S and V_j.

Other quantum algorithms

- Schlimgen et al. 2021, 2022: unitary decomposition.
- Patel-Wilde 2023: Wave matrix Lindbladian
- Di Bartolomeo, 2023, quantum noise formalism
- Pocrnic et al. 2023: repeated interactions.
- Chen et al. 2023. Block encode the Lindbladian
- Chen et al. 2024; David et al. 2024. q-DRIFT type idea

Application: optimal control (He-Li-Li-Li-Wang-Wang 2024)

- Lindblad equation with a system control

$$\frac{d}{dt}\rho = -i\left[H_0 - \sum_{j=1}^{N_C} u_j(t)\mu_j\,,\rho\right] - \frac{1}{2}\sum_j\{L_j^\dagger L_j,\rho\} + \sum_j L_j\rho\, L_j^\dagger.$$

- The control is applied to the system only
- The objective function

$$\max J[u]\,, J = tr\big(O\rho(T)\big) - \frac{\alpha}{2}\sum_{j=1}^{N_C}\int_0^T |u_j(t)|^2 dt.$$

- Unlike closed systems, open quantum systems may not be controllable (Altafini J. Math. Phys. 2003).
- We treat it as an optimization problem.

Simulating time-dependent Lindblad

- Duhamel's principle + Kraus form

- Interaction picture

- L_1-time scaling

Estimating the cost function

- To determine the optimal control variables, we optimize the cost function using its gradient
- We use a quantum gradient estimation algorithm[2].

➢ The efficiency depends on the smoothness of $J[u]$

➢ Discretize the control variables to N time steps → a finite dimensional problem

➢ Lindblad simulation algorithm: $\rho(T) = tr_E(|\rho_T\rangle\langle\rho_T|)$. $\to J[u] = \langle\rho_T|O \otimes I|\rho_T\rangle$.

➢ Phase oracle $O_f|x\rangle|0\rangle = e^{if(x)}|x\rangle|0\rangle$, converted from a probability oracle using $f = \frac{1-J_1[u]}{2}$.

- **Theorem.** Suppose we have the access to the phase oracle, then the quantum gradient algorithm outputs g such that $\|g - \nabla J\| < \epsilon$ with probability at least $1-\gamma$ using $\tilde{O}\left(\frac{N_C T}{\epsilon}\log\frac{N}{\gamma}\right)$ queries to O_f and $\tilde{O}\,(N)$ additional 1- and 2-qubits gates.

2. Gilyén-Arunachalam-Wiebe 2019

Optimization

- **The gradient descent** algorithm: $x_{t+1} \leftarrow x_t - \alpha_t \nabla f(x_t)$ is guaranteed to reach stationary point. But it may get stuck at local stationary points
- **Perturbed gradient descent**[3] : If the gradient ∇f is L-Lipschitz and it is estimated with variance $\sigma^2 = \epsilon^2$, and the learning rate is $\alpha_t < \Theta\left(\frac{1}{L}\right)$, then the PSGD visits a stationary point satisfying ϵ first- and second-order optimality condition with probability at least $1 - \delta$ at least once with the following number of iterations $O\left(\frac{L}{\epsilon^2} \log \frac{1}{\delta}\right)$.
- **Perturbed Accelerated Gradient Descent**[4]

➢ based on Nesterov's accelerated gradient descent

➢ Introduce a Gaussian perturbation when $|\nabla f| < \epsilon$.

➢ a negative curvature exploitation step

➢ Finds a first- and second-order ϵ-stationary point within $O\left(\frac{1}{\epsilon^{\frac{7}{4}}}\right)$ iterations.

3. Jin et al. JACM 2021; 4. Jin et al PMLR, 2018

Overall complexity

- **First-order stationary point ($\|\nabla J\| < \epsilon$).** $O\left(\frac{N_C T \|\mathcal{L}(t)\|_{be,\infty}}{\epsilon^{\frac{23}{8}}}\right)$ queries to the operators in the Lindbladian.
  - The sampling error in the gradient estimation can be easily incorporated in the convergence analysis.
- **First- and second-order stationary point** ($\|\nabla J\| < \epsilon,\ \|\nabla^2 J\| > -\vartheta\sqrt{\epsilon}$). $O\left(\frac{N_C T^{\frac{7}{4}} \|\mathcal{L}(t)\|_{be,\infty}}{\epsilon^5}\right)$ queries to the operators in the Lindbladian.
  - The sampling error in the gradient estimation has to be much less than ϵ in order to maintain the convergence of AGD.

Summary

- Quantum algorithms for Lindblad
  - Duhamel's --> Kraus form
  - Kraus form → Stinespring → shadow Hamiltonians
  - Extension to non-Markovian? (Li-Wang 2023).
  - Open: Non-Markovian without weak coupling..
- Quantum optimal control
  - Closed quantum system (Li-Wang 2023)
  - Open quantum system.
  - Open: Control landscape → better optimization complexity?