Efficient quantum algorithm for dissipative nonlinear differential equations

Andrew Childs
University of Maryland

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

UMIACS
University of Maryland
Institute for Advanced
Computer Studies

JOINT CENTER FOR
QUANTUM INFORMATION
AND COMPUTER SCIENCE


Jin-Peng Liu
UMD


Herman Kolden
NUST/MIT


Nuno Loureiro
MIT


Hari Krovi
Raytheon BBN


Konstantina Trivisa
UMD

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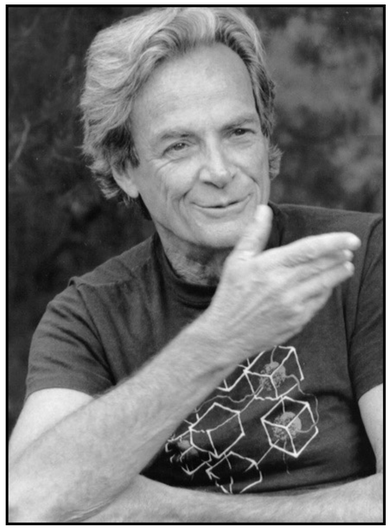
Quantum computers also provide a novel approach to problems in numerical analysis.

Main idea:

- Represent a vector $x \in \mathbb{C}^N$ by a quantum state $|x\rangle$ of $\log_2 N$ qubits.
- Show how to prepare such a state using $\mathrm{poly}(\log N)$ operations.
- Produces a quantum encoding of the solution. Less informative than an explicit solution, but much faster and still potentially useful.

Quantum simulation

Quantum simulation



"… nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

Richard Feynman (1981)
Simulating physics with computers

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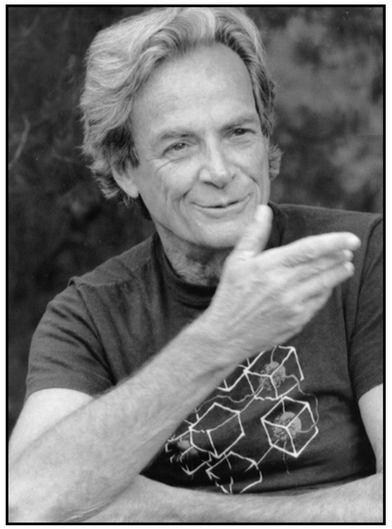

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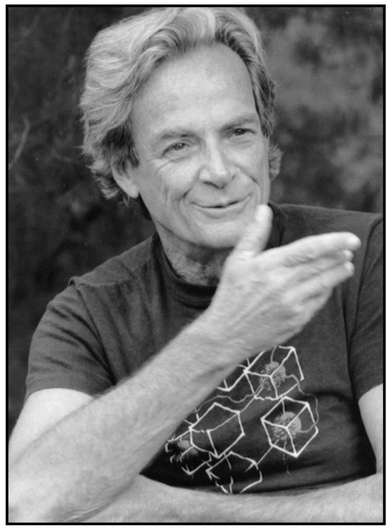

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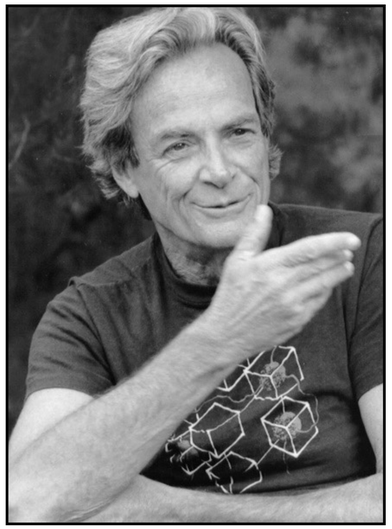

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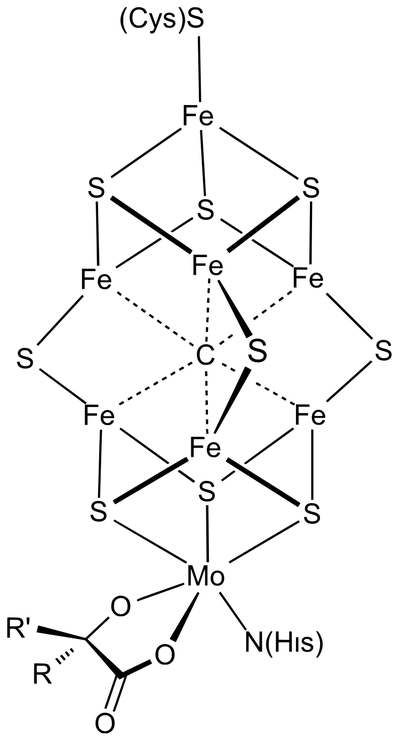
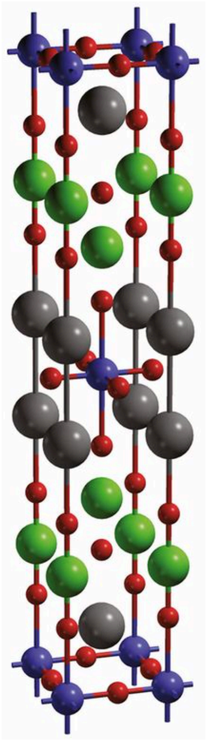
A quantum computer cannot produce a complete description of the state, but by performing measurements, it can answer questions that (apparently) a classical computer cannot

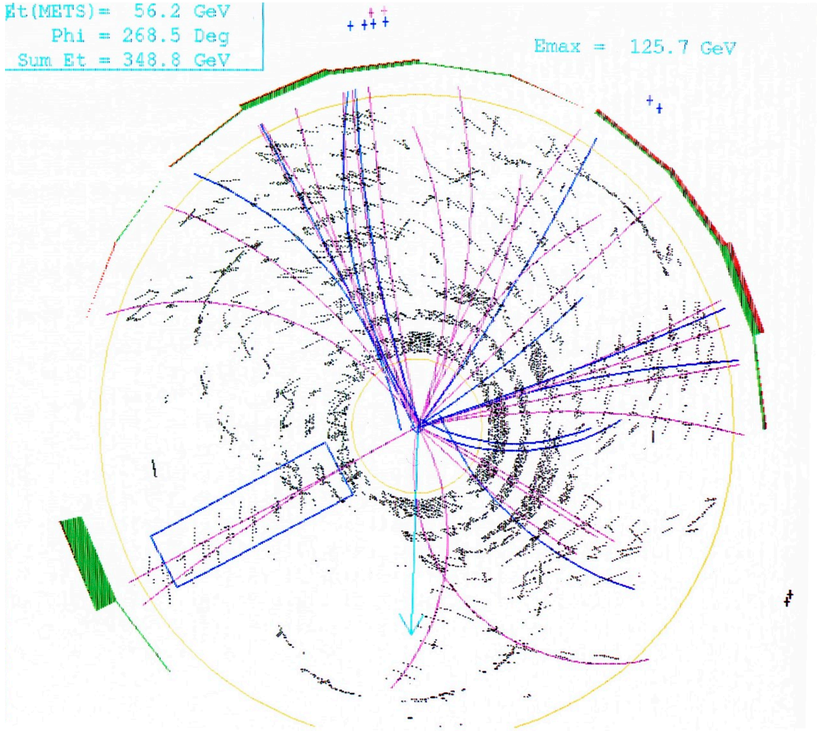
Computational quantum physics



quantum chemistry
(e.g., nitrogen fixation)

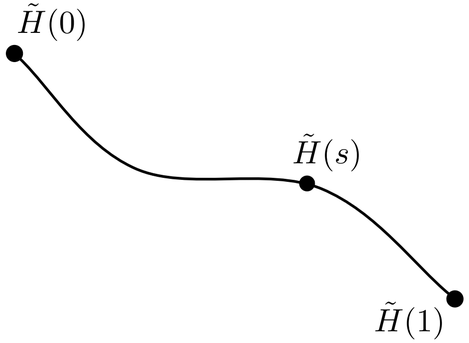


condensed matter physics/
properties of materials

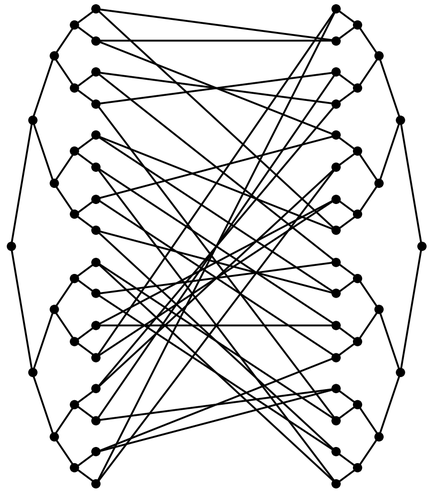


nuclear/particle
physics

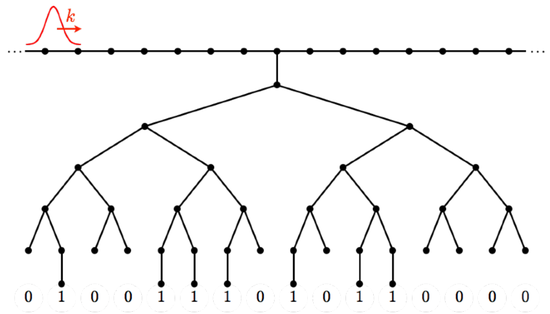
Implementing quantum algorithms



adiabatic optimization



exponential speedup by quantum walk



evaluating Boolean formulas

$$A|x\rangle = |b\rangle$$

linear/ differential equations, convex optimization

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Subsequent improvements do the same with complexity $\kappa\,\mathrm{poly}(\log(1/\epsilon))$ using variable-time amplitude amplification and LCU [Ambainis 12; Childs, Kothari, Somma 17]

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Later work gives improved/generalized algorithms (time-dependent coefficients, BVPs, PDEs)

Nonlinear dynamics

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So maybe there is a fundamental obstacle?

Problem statement

Quantum quadratic ODE problem. Consider an ODE $\frac{\mathrm{d}u}{\mathrm{d}t} = F_2 u^{\otimes 2} + F_1 u + F_0(t)$ with $u(t), F_0(t) \in \mathbb{R}^n,\ F_1 \in \mathbb{R}^{n\times n},\ F_2 \in \mathbb{R}^{n\times n^2}$. Assume we are given an oracle to prepare a quantum state proportional to $u(0) = u_{\mathrm{in}}$, and sparse matrix oracles for $F_0(t), F_1, F_2$. Let the eigenvalues λ_j of F_1 satisfy $\mathrm{Re}(\lambda_n) \le \cdots \le \mathrm{Re}(\lambda_1) < 0$. Parametrize the problem in terms of

$$\mathrm{R} := \frac{1}{|\mathrm{Re}(\lambda_1)|}\left(\|u_{\mathrm{in}}\|\|F_2\| + \frac{\|F_0\|}{\|u_{\mathrm{in}}\|}\right)$$

and assume the values $\|u_{\mathrm{in}}\|, \|F_0(t)\|, \|F_1\|, \|F_2\|, \mathrm{Re}(\lambda_1), \max_t \|F_0(t)\|, \max_t \|F_0'(t)\|$ are known.

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R quantifies the strength of the nonlinearity and driving relative to dissipation.
Qualitatively similar to Reynolds number.

Main result I (algorithm)

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Theorem 1. For $\mathrm{R} < 1$, there is a quantum algorithm for the quantum quadratic ODE problem with query and gate complexity

$$\frac{sqT^2}{\epsilon}\mathrm{poly}\left(\log T, \log n, \log(1/\epsilon)\right)$$

where s is the sparsity of the input, $q := \|u_{\mathrm{in}}\|/\|u(T)\|$, and ϵ is the error in the approximation of $u(T)/\|u(T)\|$.

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Ingredients:

- Carleman linearization (novel convergence analysis)
- Forward Euler discretization
- State preparation procedure
- Condition number and success probability analysis

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In general: $$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} A_1^1 & A_2^1 & & \\ A_1^2 & A_2^2 & \ddots & \\ & \ddots & \ddots & A_N^{N-1} \\ & & A_{N-1}^N & A_N^N \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} + \begin{pmatrix} F_0(t) \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad y_j \approx u^{\otimes j}$$

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Lemma. $N = O\big(\log(T\|F_2\|/\delta)/\log(1/\|u_{\mathrm{in}}\|)\big)$ suffices to approximate the solution within δ.

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Theorem 2. Assume $\mathrm{R} \geq \sqrt{2}$. Then there is an instance of the quantum quadratic ODE problem such that any quantum algorithm for producing a quantum state approximating $u(T)/\|u(T)\|$ with bounded error must have worst-case time complexity exponential in T.

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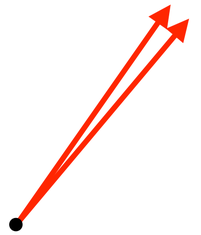
Ingredients:

- Hardness of distinguishing nonorthogonal quantum states



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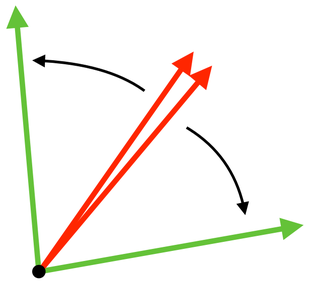
- Hardness of distinguishing nonorthogonal quantum states
- Quadratic ODE that rapidly distinguishes nonorthogonal states



Hardness of state distinguishability

Lemma. Let $|\psi\rangle, |\phi\rangle$ be quantum states with $|\langle\psi|\phi\rangle| = 1 - \epsilon$. Suppose we are either given a black box that prepares $|\psi\rangle$ or a black box that prepares $|\phi\rangle$. Then any bounded-error protocol for determining whether the state is $|\psi\rangle$ or $|\phi\rangle$ must take time $\Omega(1/\epsilon)$.

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Proof:

- If we use the box k times, we produce states with overlap $(1 - \epsilon)^k$.
- These states have trace distance $\Theta(\sqrt{k\epsilon})$.
- By the Helstrom bound, need $k = \Omega(1/\epsilon)$ to distinguish with bounded error.

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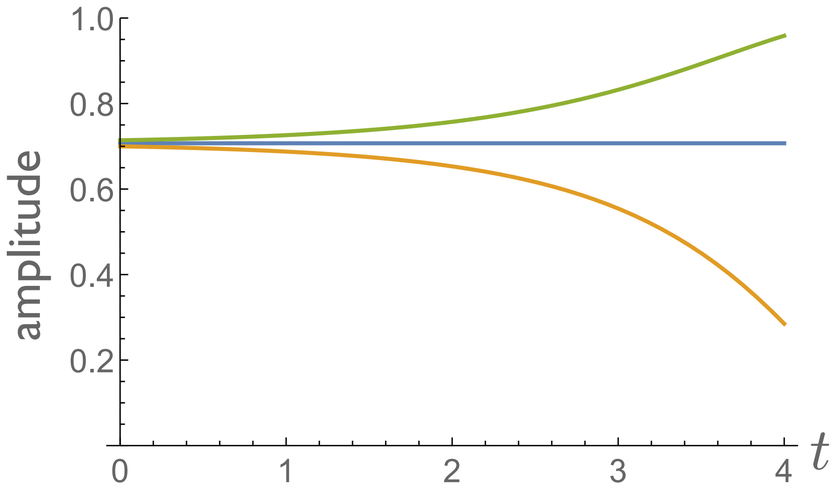

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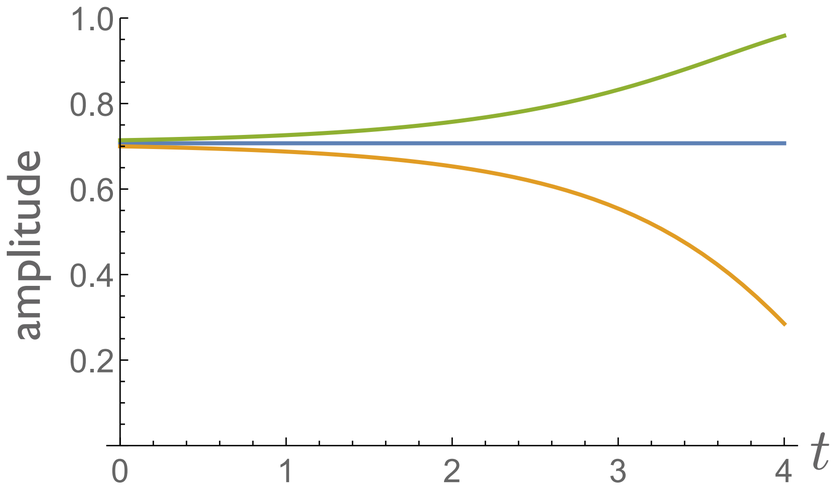

In general, the time to separate states with overlap $1 - \epsilon$ by a constant amount is $O(\log(1/\epsilon))$.

Applications: Epidemiology

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SEIR model of a pandemic:

$$\frac{\mathrm{d}P_S}{\mathrm{d}t} = -\Lambda\frac{P_S}{P} - r_{\mathrm{vac}}P_S + \Lambda - r_{\mathrm{tra}}P_S\frac{P_I}{P}$$
$$\frac{\mathrm{d}P_E}{\mathrm{d}t} = -\Lambda\frac{P_E}{P} - \frac{P_E}{T_{\mathrm{lat}}} + r_{\mathrm{tra}}P_S\frac{P_I}{P}$$
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infected
$$\frac{\mathrm{d}P_I}{\mathrm{d}t} = -\Lambda\frac{P_I}{P} + \frac{P_E}{T_{\mathrm{lat}}} - \frac{P_I}{T_{\mathrm{inf}}}$$

recovered
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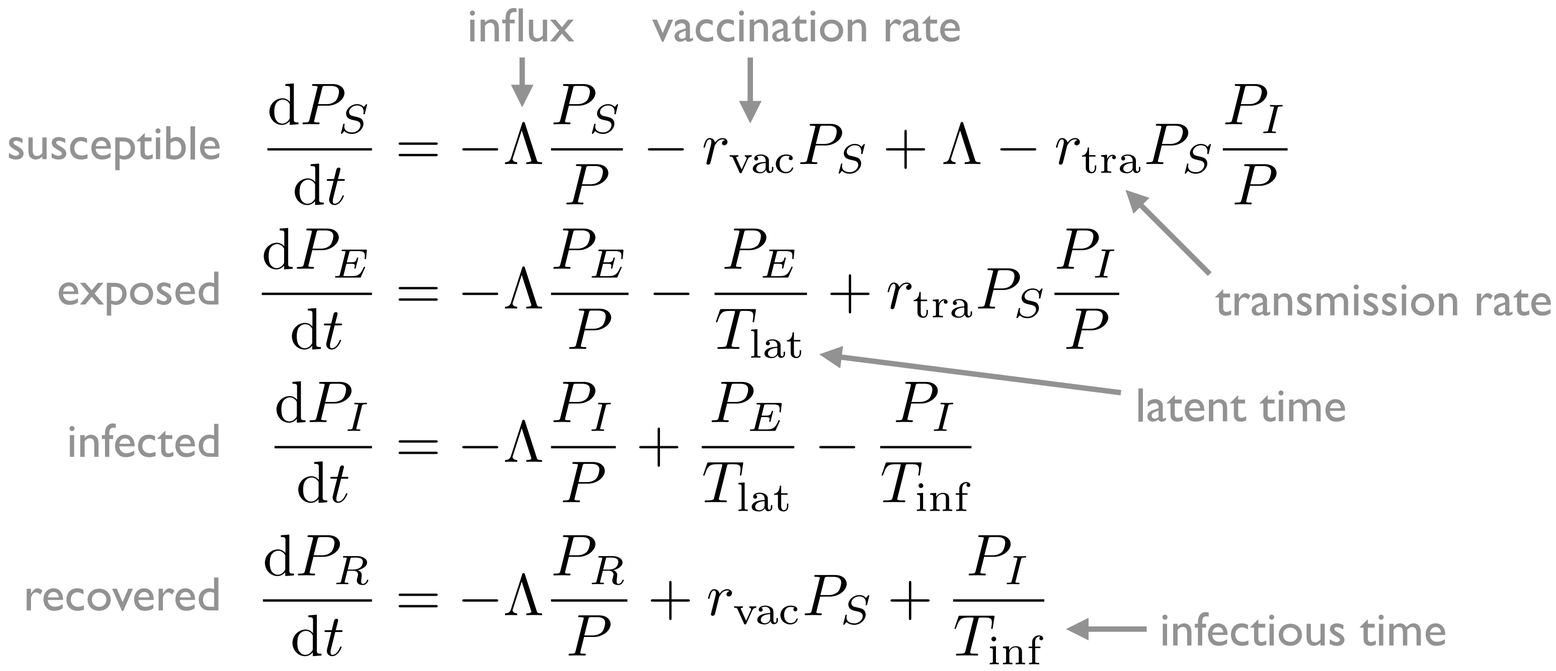

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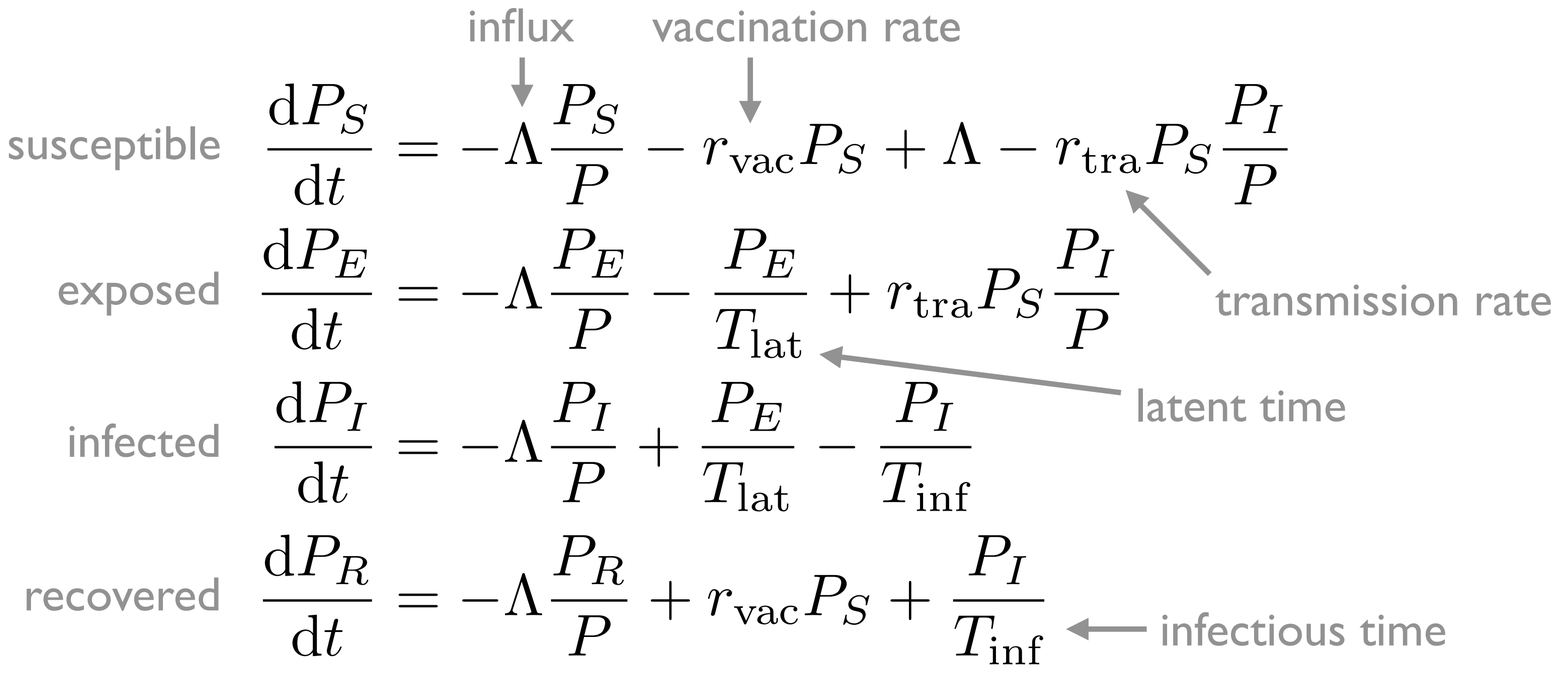

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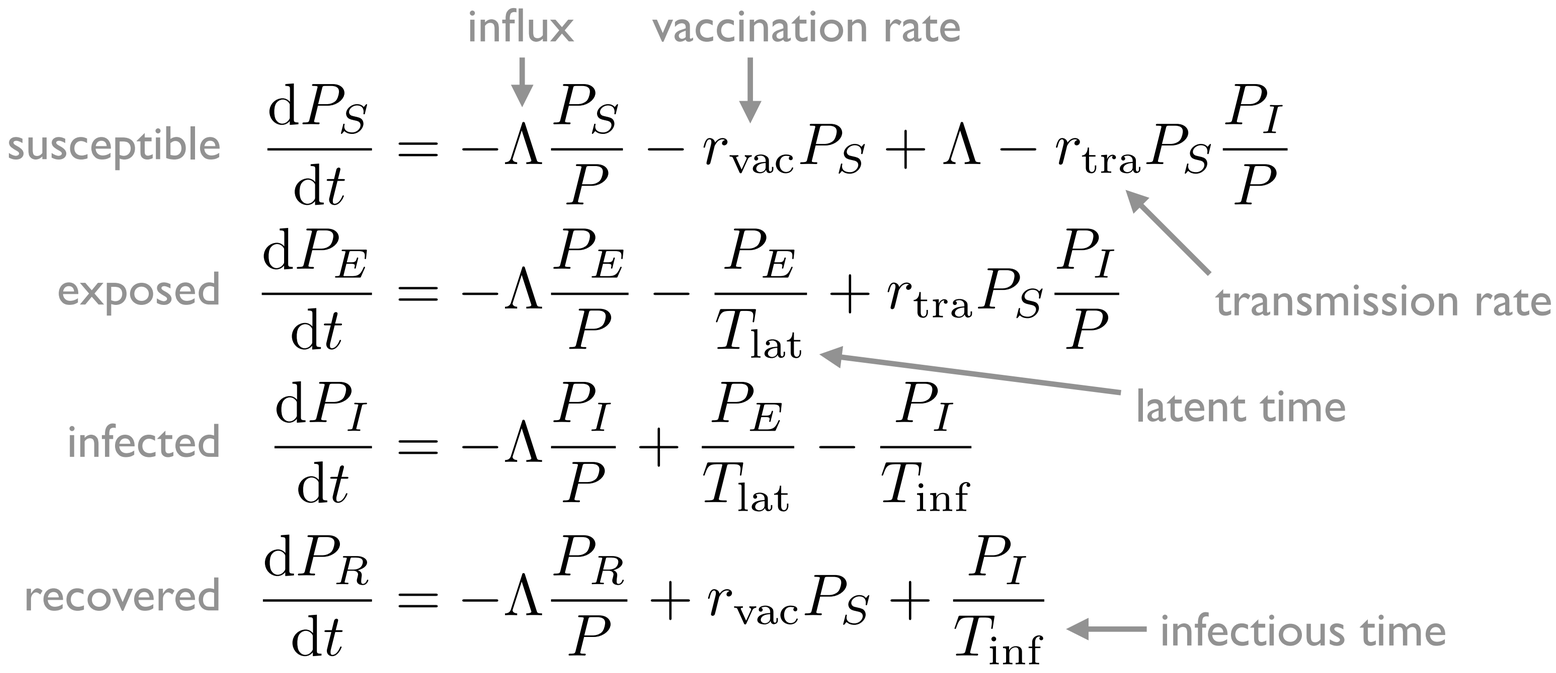

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A high-dimensional version can model many interacting cities

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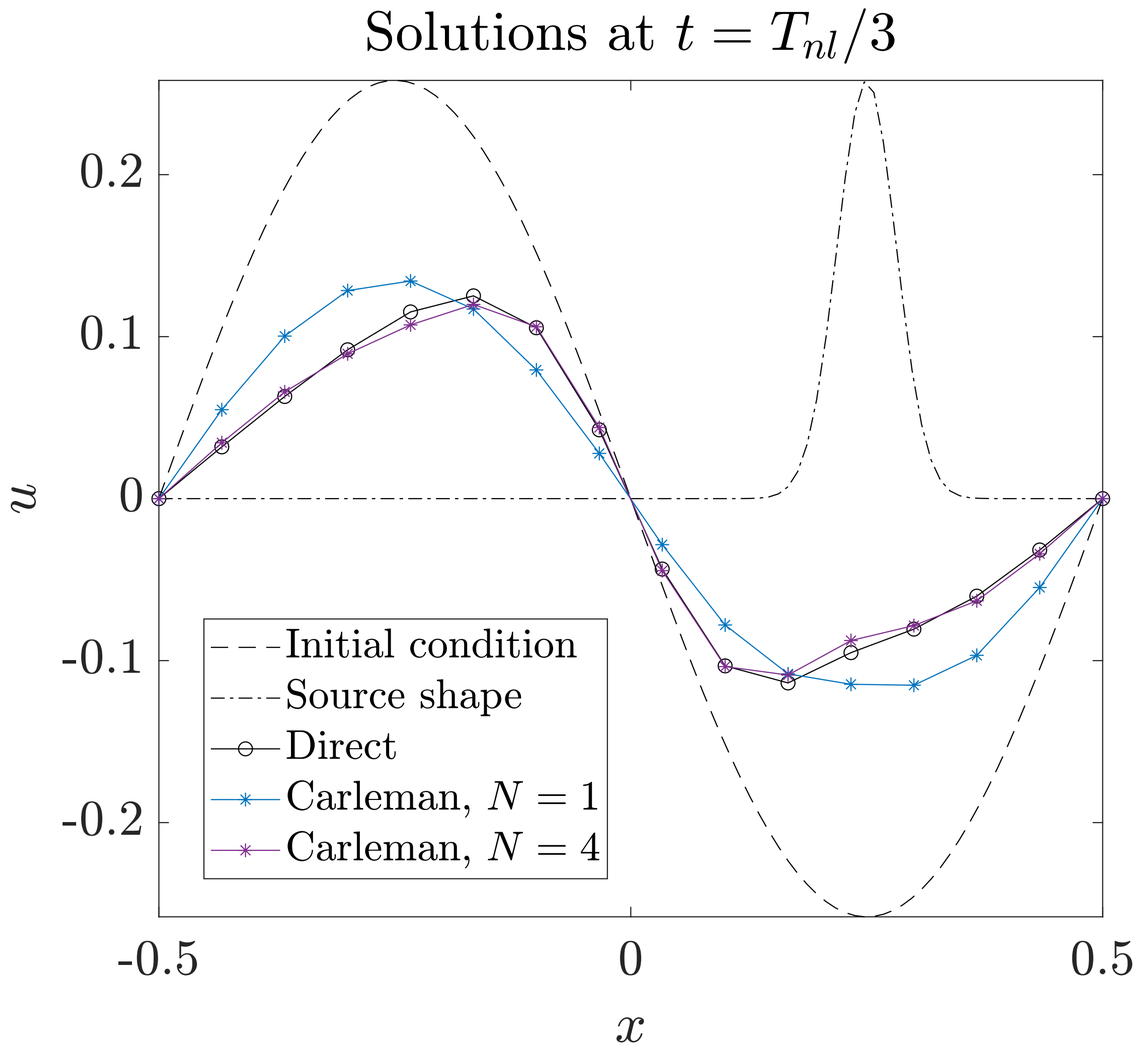
Carleman method shows good convergence even for $\mathrm{R} \approx 40$



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However, numerical evidence suggests that the algorithm may be efficient for certain cases even with R much larger.

Open questions

- What can we say about efficiency/hardness for $1 \leq \mathrm{R} < \sqrt{2}$?
- Our algorithm has complexity quadratic in T. Can this be improved?
- Our algorithm has complexity $\tilde{O}(1/\epsilon)$, whereas other quantum algorithms for simulation/ linear equations/ODEs have complexity $\mathrm{poly}(\log(1/\epsilon))$. Can this be improved?
- Can we identify conditions under which the algorithm is efficient for larger R?
- End-to-end applications