Solving Differential Equations using Quantum Computation

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PH515 Basics of quantum computation

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Outline

Outline

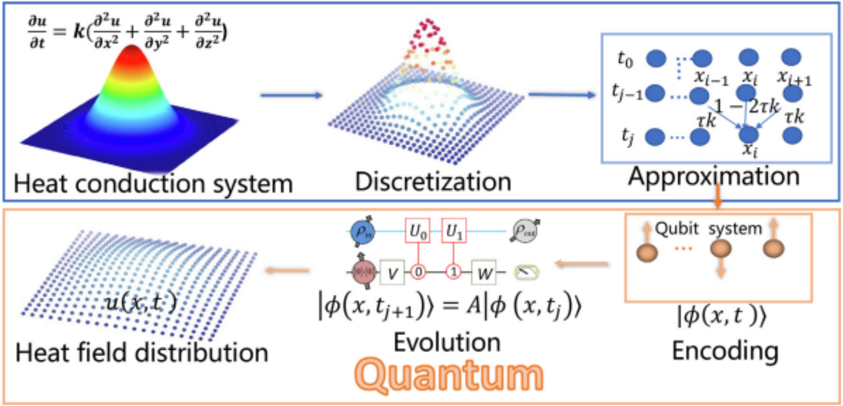
Objectives

Solving DEs using QC algorithms

In this presentation, we will look at

- quantum algorithm based on the finite difference method to solve the 1-D heat equation.

Overview of algorithm



Outline

1-D heat equation

1-D Heat equation

Consider the following partial differential equation,

$$\frac{\mathrm{d}u}{\mathrm{d}t} = k\frac{\partial^2 u}{\partial x^2}, \tag{1}$$

with boundary conditions

$$u(x = x_0, t) = C_1; \tag{2}$$
$$u(x = x_n, t) = C_2; \tag{3}$$
$$u(x, t = 0) = f(x); \tag{4}$$

where x_0, x_n are the endpoints in the considered geometric domain

1-D heat equation (contd..)

Dirichlet boundary conditions

$$u(x,t) = v(x,t) + (x - x_0).\frac{C_2 - C_1}{x_n - x_0} + C_1 \tag{5}$$

and consequently

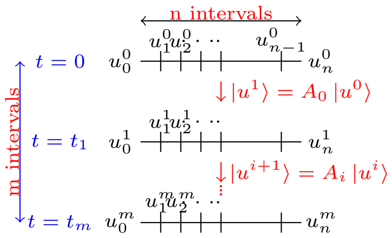
$$\frac{\mathrm{d}v}{\mathrm{d}t} = k\frac{\partial^2 v}{\partial x^2}, \tag{6}$$

with boundary conditions

$$v(x = x_0, t) = 0; \; v(x = x_n, t) = 0; \; v(x, t = 0) = f(x) - (x - x_0).\frac{C_2 - C_1}{x_n - x_0} - C_1; \tag{7}$$

Discretization of solution space

- The time domain ([0, T]) is discretized into m equal time intervals ($[0,t_1]$, $[t_1,t_2]$, ...$[t_{m-1},t_m]$),
- the space is discretized to N equal intervals ($[x_0,x_1]$,$[x_1,x_2]$...$[x_{n-1},x_n]$),
- The corresponding solutions at these points are denoted by v_j^i, where superscript (i$\in \{0,1...,m\}$) denotes time index and subscript (j$\in \{0,1...,n\}$) corresponds to length index.



Linearized time-stepping

Using forward finite different schemes,

$$
\begin{aligned}
v_j^{i+1} - v_j^i &\approx \frac{T}{n}\frac{\mathrm{d}v_j}{\mathrm{d}t} && (8)\\
&= \frac{k.T}{n}\frac{\mathrm{d}^2 v^i}{\mathrm{d}x^2} && (9)\\
&\approx k\frac{T}{n}\frac{\left(v_{j+1}^i + v_{j-1}^i - 2v_j^i\right)}{2\left(\frac{x_m - x_0}{n}\right)^2} && (10)\\
&= k\tau\frac{\left(v_{j+1}^i + v_{j-1}^i - 2v_j^i\right)}{2s^2} && (11)\\
v_j^{i+1} &\approx v_j^i + \alpha\left(v_{j+1}^i + v_{j-1}^i - 2v_j^i\right) && (12)
\end{aligned}
$$

Linearized time-stepping (contd...)

$$v_j^{i+1} \approx v_j^i + \alpha(v_{j+1}^i + v_{j-1}^i - 2v_j^i) \tag{13}$$

$$v_j^0 = f(x_j) - (x_j - x_0)\frac{C_2 - C_1}{x_n - x_0} - C_1 \tag{14}$$

$$\begin{Bmatrix} v_0^{i+1} \\ v_1^{i+1} \\ v_2^{i+1} \\ . \\ . \\ v_n^{i+1} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \alpha & 1-2\alpha & \alpha & \dots & 0 \\ 0 & \alpha & 1-2\alpha & \dots & 0 \\ . & . & . & . & \\ . & . & . & . & . \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{Bmatrix} v_0^i \\ v_1^i \\ v_2^i \\ . \\ . \\ v_n^i \end{Bmatrix} \tag{15}$$

State preparation

We ideally require a state

$$|\psi^i\rangle = \frac{\sum_{j=0}^{n} v(x_j^i)\,|j\rangle}{C} \tag{16}$$

$$|\psi^0\rangle = \sum_{j=0}^{n}(f(x_j) - (x_j - x_0).\frac{C_2 - C_1}{x_n - x_0} - C_1)\,|j\rangle)/C^* \tag{17}$$

and a quantum circuit capable of simulating the following matrix

$$\begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ \alpha & 1-2\alpha & \alpha & \dots & 0 & 0 \\ 0 & \alpha & 1-2\alpha & \dots & 0 & 0 \\ . & . & . & . & & \\ . & . & . & . & . & \\ 0 & 0 & 0 & \dots & \alpha & 1 \end{bmatrix}_{(n+1)\times(n+1)} \tag{18}$$

State preparation (contd..)

Preparation of arbitrary quantum states- Network based approach[a]

[a] Phillip, et al. Quantum Networks for generating arbitrary quantum states

Idea:

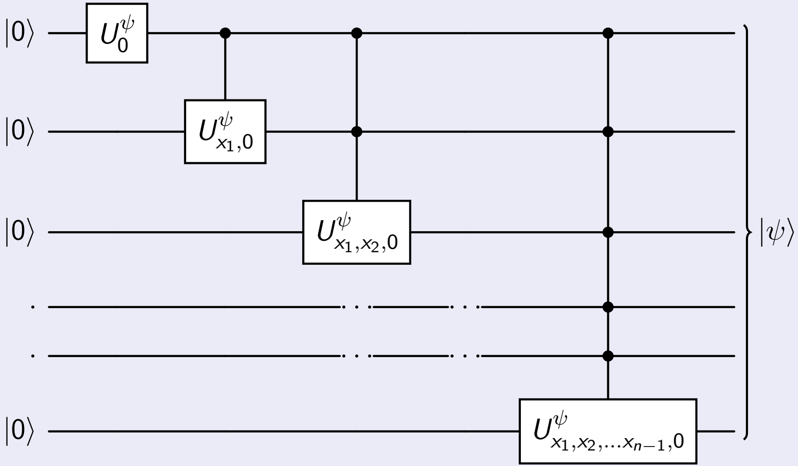
$$|x_1\rangle\,|x_2\rangle \dots |x_{k-1}\rangle\,|0\rangle \xrightarrow{c-U^{\psi}_{x_1,x_2,\dots x_{k-1},0}} |x_1\rangle\,|x_2\rangle \dots |x_{k-1}\rangle\,\left(\frac{p_{x_1,x_2,\dots x_{k-1},0}}{p_{x1,x2,\dots x_{k-1}}}\,|0\rangle + \frac{p_{x_1,x_2,\dots x_{k-1},1}}{p_{x_1,x_2,\dots x_{k-1}}}\,|1\rangle\right) \tag{19}$$

Quantum register ($|\bar{\psi}\rangle$)

$$|\bar{\psi}\rangle\,|0\rangle\,|x_1\rangle \dots |x_{k-1}\rangle \xrightarrow{U_k} |\bar{\psi}\rangle\,|\omega_k\rangle\,|x_1\rangle \dots |x_{k-1}\rangle \tag{20}$$

$$cos^2(2\pi\omega_k) = \left(\frac{p_{x_1,x_2,\dots x_{k-1},0}}{p_{x_1,x_2,\dots x_{k-1}}}\right)^2. \tag{21}$$

$$c - U^{\psi}_{x_1,x_2,\ldots x_{n-1},0}\left(c - U^{\psi}_{x_1,x_2,\ldots x_{n-2},0}\left(\ldots c - U^{\psi}_{x_1,0}\left(U^{\psi}_0 \left|0\right\rangle\right)\left|0\right\rangle \ldots\right)\left|0\right\rangle\right)\left|0\right\rangle = \left|\psi\right\rangle$$



State preparation (contd..)

$$N = 2^{[log_2(n+1)]} \tag{22}$$

$$|\psi^i\rangle = \frac{\sum_{j=0}^{n} v(x_j^i)\,|j\rangle + \sum_{j=n+1}^{N-1} 0\,|j\rangle}{C_{norm}} \tag{23}$$

$$|\psi^{i+1}\rangle = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \alpha & 1-2\alpha & \alpha & \dots & 0 \\ 0 & \alpha & 1-2\alpha & \dots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & 0 & \dots & 1-2\alpha \end{bmatrix}_{N\times N} |\psi^i\rangle \tag{24}$$

Quantum circuit implementation

$$\begin{bmatrix} 1 & 0 & 0 & \dots & . & . & 0 & 0 \\ \alpha & 1-2\alpha & \alpha & \dots & . & . & 0 & 0 \\ 0 & \alpha & 1-2\alpha & \dots & . & . & 0 & 0 \\ . & . & . & \dots & . & . & . & . \\ . & . & . & \dots & . & . & . & . \\ 0 & 0 & 0 & \dots & . & . & 0 & 1 \end{bmatrix}_{N\times N} \tag{25}$$

$$\simeq (1-2\alpha)\boldsymbol{I}_{N\times N} + \alpha \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ . & . & . & . & \\ . & . & . & . & . \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix}_{N\times N} + \alpha \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ . & . & . & . & \\ . & . & . & . & . \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix}_{N\times N} \tag{26}$$

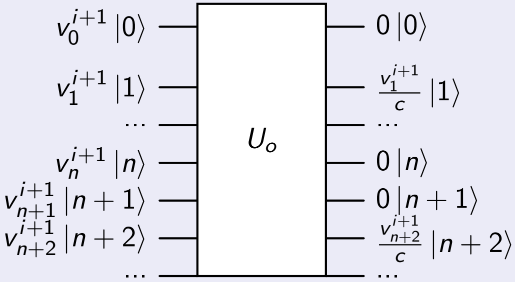
Quantum circuit implementation (contd..)

Error correction

Following the matrix operation, the states at positions 0, n and n+1 ($C = \{0,\ n,\ n+1\}$) must be corrected, this can be done by replacing

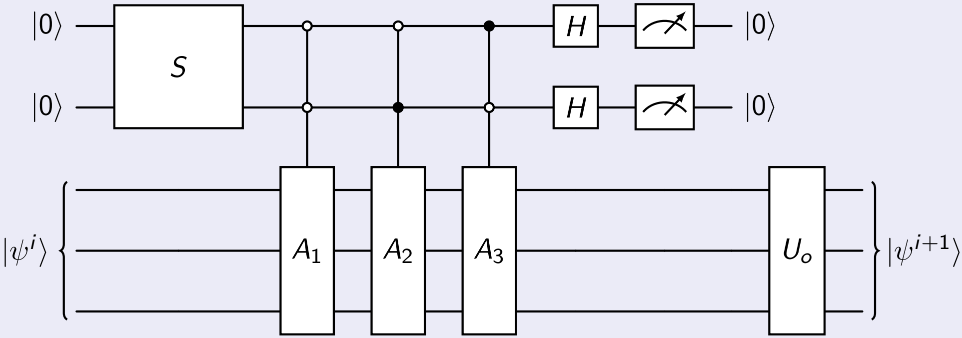
$$|\psi^{i+1}\rangle \xrightarrow{U_0} \left(\boldsymbol{I} - \sum_{p \in C} |p\rangle\langle p|\right)^* |\psi^{i+1}\rangle \qquad (27)$$

Illustration



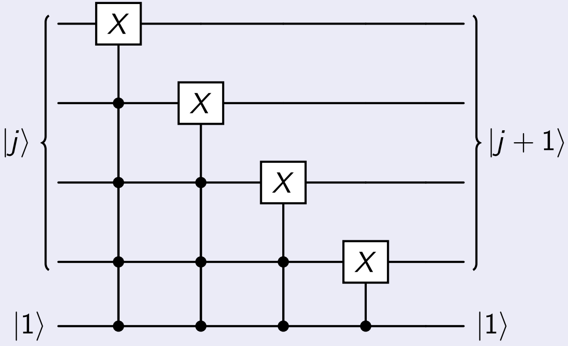
Quantum circuit implementation (contd..)

Heat equation solved based on finite difference method

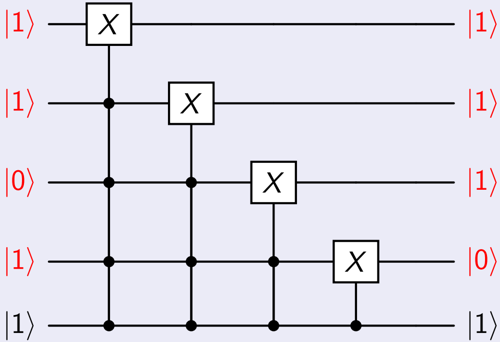


Quantum circuit implementation (contd..)

Decomposition of A_2



Decomposition of A_2 for $|j\rangle = |13\rangle$



Quantum circuit implementation (contd..)

$$|\beta_0\rangle = |\psi^i\rangle \otimes |00\rangle \tag{28}$$

$$|\beta_1\rangle = \boldsymbol{I} \otimes \boldsymbol{S}\,|\beta_0\rangle = |\psi^i\rangle \otimes \frac{((1-2\alpha)\,|00\rangle + \alpha\,|10\rangle + \alpha\,|01\rangle)}{D} \tag{29}$$

$$|\beta_2\rangle = \frac{((1-2\alpha)\boldsymbol{A}_1\,|\psi^i\rangle \otimes |00\rangle + \alpha\boldsymbol{I}\,|\psi^i\rangle \otimes |10\rangle + \alpha\boldsymbol{I}\,|\psi^i\rangle \otimes |01\rangle)}{D} \tag{30}$$

$$|\beta_3\rangle = \frac{((1-2\alpha)\boldsymbol{A}_1\,|\psi^i\rangle \otimes |00\rangle + \alpha\boldsymbol{A}_2\,|\psi^i\rangle \otimes |10\rangle + \alpha\boldsymbol{I}\,|\psi^i\rangle \otimes |01\rangle)}{D} \tag{31}$$

$$|\beta_4\rangle = \frac{((1-2\alpha)\boldsymbol{A}_1\,|\psi^i\rangle \otimes |00\rangle + \alpha\boldsymbol{A}_2\,|\psi^i\rangle \otimes |10\rangle + \alpha\boldsymbol{A}_3\,|\psi^i\rangle \otimes |01\rangle)}{D} \tag{32}$$

Quantum circuit implementation (contd..)

$$|\beta_4\rangle = \frac{((1-2\alpha)\boldsymbol{A_1}|\psi^i\rangle \otimes |00\rangle + \alpha \boldsymbol{A_2}|\psi^i\rangle \otimes |10\rangle + \alpha \boldsymbol{A_3}|\psi^i\rangle \otimes |01\rangle)}{D} \tag{33}$$

$$|\beta_5\rangle = ((1-2\alpha)\boldsymbol{A_1}|\psi^i\rangle \otimes (|00\rangle + |01\rangle + |10\rangle + |11\rangle) \tag{34}$$

$$+ \alpha \boldsymbol{A_2}|\psi^i\rangle \otimes (|00\rangle + |01\rangle - |10\rangle - |11\rangle) \tag{35}$$

$$+ \alpha \boldsymbol{A_3}|\psi^i\rangle \otimes (|00\rangle - |01\rangle + |10\rangle - |11\rangle))/D^* \tag{36}$$

$$|\beta_6\rangle = \frac{((1-2\alpha)\boldsymbol{A_1} + \alpha \boldsymbol{A_2} + \alpha \boldsymbol{A_3})|\psi^i\rangle}{D} = \boldsymbol{A}|\psi^i\rangle \tag{37}$$

$$|\beta_7\rangle = \boldsymbol{U_0}|\beta^6\rangle = |\psi^{i+1}\rangle. \tag{38}$$

Outline

Comparing quantum and classical algorithms

Three parameters dictate the solution as well as the time complexity of producing a numerical solution to the differential equation,

- N, dimension of the system,
- ϵ, allowed error range of the solution,
- Δ_t, discretization of the time (time-step).

Most efficient Classical algorithms

Time complexity,

- $\sim$ O(poly(N))
- $\sim$ O(poly(log(1/ϵ)))
- $\sim$ O(poly(Δ_t))

Most efficient Quantum algorithms*

Time complexity,

- $\sim$ O(poly(log(N)))
- $\sim$ O(poly(log(1/ϵ)))
- $\sim$ O(poly(Δ_t))

No fast forwarding theorem

Intuition

- For the Hamiltonian evolution of general matrices where the structure (mathematical properties) of the problem is not known, it is not possible to solve it in sub-linear time.
- Consider a dynamical system (e.g. a 1-DoF pendulum), it is required to calculate the position at a given time, provided knowledge about the behaviour of the pendulum, if no information about the behaviour of the pendulum is inferred, it can only be observed by simulating the pendulum till the particular time and measuring it.

Application in solving Non-linear differential equations

Non-linear differential equations

Let us consider the following case,

$$\dot{x} = f(x), \tag{39}$$

f(x) is a nonlinear and C_∞ function of x. Using Taylor's theorem it is possible to express it as power series.

$$\dot{x} = a_0 + a_1 x + a_2 x^2 \dots \tag{40}$$

Application in solving Non-linear differential equations (contd...)

Carlemann linearization

Let us consider the case where $a_{i\neq 2} = 0$ and $a_2 = 1$

$$\dot{x} = x^2 \tag{41}$$

$$\dot{y_1} = y_2$$
$$\dot{y_2} = 2y_3$$
$$\dot{y_3} = 3y_4$$
$$\cdot$$
$$\cdot$$

$$\{\dot{y}_\infty\} = \boldsymbol{A}\{y_\infty\}, \tag{42}$$

where A is a matrix with constant coefficients

Variables

$$y_1 = x;$$
$$y_2 = x^2;$$
$$y_3 = x^3;$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

Thank You!

References

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