Q-SITE-Classiq-Open-Challenge

Dhawal Verma

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Team name:Quantum Ninja

1 Introduction

The given equation is

$$\frac{d^2x(t)}{dt^2} + \omega^2 x(t) = 0$$

with the initial conditions:

$$x(0) = 1, \quad \frac{dx(0)}{dt} = 1$$

which is a second order differential equation. The paper "Quantum algorithm for solving linear differential equations: Theory and experiment (Tao Xin et. al,2020)" deals with the linear differential equation. So, we need to reduce the above differential equation to system of first-order differential equation. Then we reformed it as vector set of differntial equation, to became able to apply the algorithm described in the paper. This involves introducing auxiliary variables to transform the equation into a system of first-order differential equations.

Step-by-Step Reduction

Introduce a New Variable:

Let

$$v(t) = x'(t)$$

This transforms the original second-order equation into two first-order equations:

$$\frac{dx(t)}{dt} = v(t)$$

$$\frac{dv(t)}{dt} = -\omega^2 x(t)$$

Express in Vector Form:

Define the state vector $X(t)$ as:

$$X(t) = \begin{pmatrix} x(t) \\ v(t) \end{pmatrix}$$

The system can now be written as:

$$\frac{dX(t)}{dt} = MX(t) \tag{1}$$

Where the system matrix A is:

$$M = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}$$

Analytical Solution

The analytical solution to this system is:

$$X(t) = e^{Mt} X(0)(1)$$

For the given initial conditions:

$$X(0) = \begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Thus, the solution becomes:

$$X(t) = e^{Mt} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

According to the paper, the analytical solution of a general simple LDE like,

$$\frac{dx(t)}{dt} = Mx(t) + b$$

can be written as:

$$x(t) = e^{Mt} x(0) + \left(e^{Mt} - I\right) M^{-1} b \tag{2}$$

This expression involves matrix exponential and inversions. On comparing with equation (1), b = 0, so now we only have to consider x(0) and M for encoding, that will be used by quantum algorithm.

2 Algorithm Framework

The inexact approximation include an approximation order, k, when the solution X(t) is expanded according to Taylor series, as follows,

$$X(t) \approx \sum_{m=0}^{k} \frac{(Mt)^m}{m!} X(0)$$

The vectors $X(0)$ can be described by quantum states $|X(0)\rangle = \sum_j \frac{X_j(0)}{\|X(0)\|}|j\rangle$ where $X_j(0)$ is the j-th elements of these vectors, $|j\rangle$ is the N-dimensional computational basis, and $\|\cdot\|$ is the modulus operation.

Further, the matrix M can be described by the operator A defined as:

$$A = \sum_{i,j} \frac{M_{ij}}{\|M\|} |i\rangle\langle j|.$$

Hence, the k-th order approximate solution converts to:

$$|X(t)\rangle \approx \sum_{m=0}^{k} \|X(0)\| \frac{(\|M\|At)^m}{m!} |X(0)\rangle \tag{3}$$

up to normalization.

In the paper, two cases are present based on the unitary nature of matrix M. As for the matrix considered here,

$$M = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}$$

for $\omega = 1$, is non-unitary.

3 Implementation

Now, we need to prepare state corresponding to $|X(0)\rangle$ and description of operator A.

For the calculation of 2-norm of X(0) and M, we will use Frobenius norm.

Given $X(0) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, the norm of $X(0)$ is:

$$\|X(0)\| = \sqrt{1^2 + 1^2} = \sqrt{2}$$

and given $M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ with $\omega = 1$, the Frobenius norm of M is:

$$\|M\|_F = \sqrt{0^2 + 1^2 + (-1)^2 + 0^2} = \sqrt{2}$$

The size of matrix M is 2×2, means we are dealing with two dimensional system. Thus, $j = \{0, 1\}$
We can represent

$$|X(0)\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

Also, the operator A is written as,

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Classiq supports this feature of preparing state, providing State Preparation method that includes prepare amplitudes function. The entanglement can be done using the hadamard transform, the decoding will be done by reversely applying all the operators, and the final step is measurement of the work qubits in subspace using execute.

Calculation and Analysis

After we solve the equation, the kinetic energy and potential energy can be calculated using, inplace prepare amplitudes. We can implement the optimization method provided by Classiq to keep the gate count minimum.

Insight

One insight is, that the matrix M can be written in term of Pauli matrices, as $M = i\sigma_y$. This leads to simple evolution of the state following the equation (2), for b = 0:

$$X(t) = e^{Mt}X(0) = e^{i\sigma_y t}X(0) \tag{4}$$

where σ_y is a Pauli matrix representing the rotation of qubit about the Y-axis in Bloch Sphere. This approach is an exact one mathematically, but implementation by algorithm results in approximation as it involves the sub-division of time, t and Trotterization. Also the algorithm discussed in the paper is itself Trotterization method, but at a more general level.

In our algorithm, we need ancillary qubits to realize the nonunitary evolution in Eq. (3) in a unitary way. The number of ancilla qubits is 1 + log(k + 1), where k is the approximate order in Eq. (2) and 1 more qubit for the encoding of quantum state $|X(0)\rangle$.