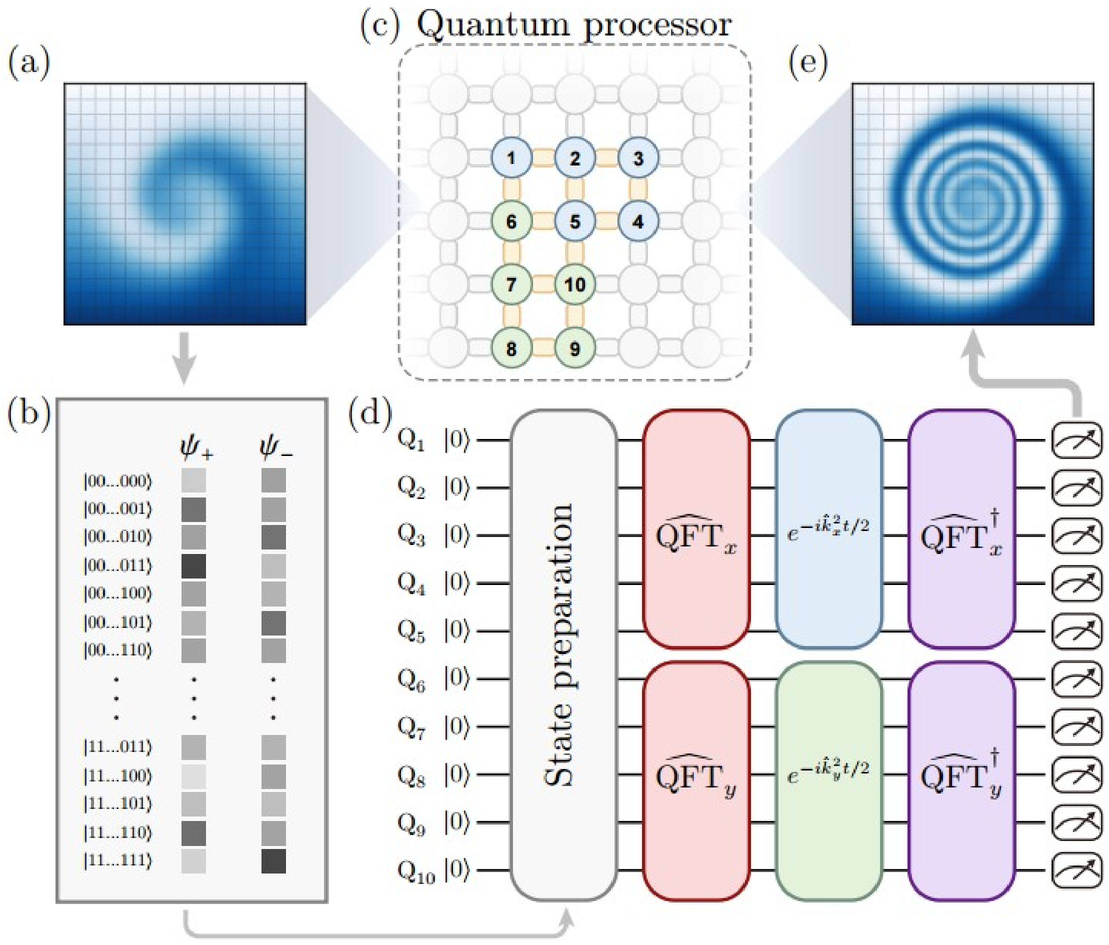
Research Experience 2

Quantum computing and fluid mechanics

Abstract

Quantum computing has emerged to be the next disruptive technology since Feynman pointed out the enormous potential of quantum simulation. Compared to conventional digital computing, quantum computing can dramatically reduce the execution time. We attempt to use quantum computing to solve fluid mechanics problems.

How to proceed ?



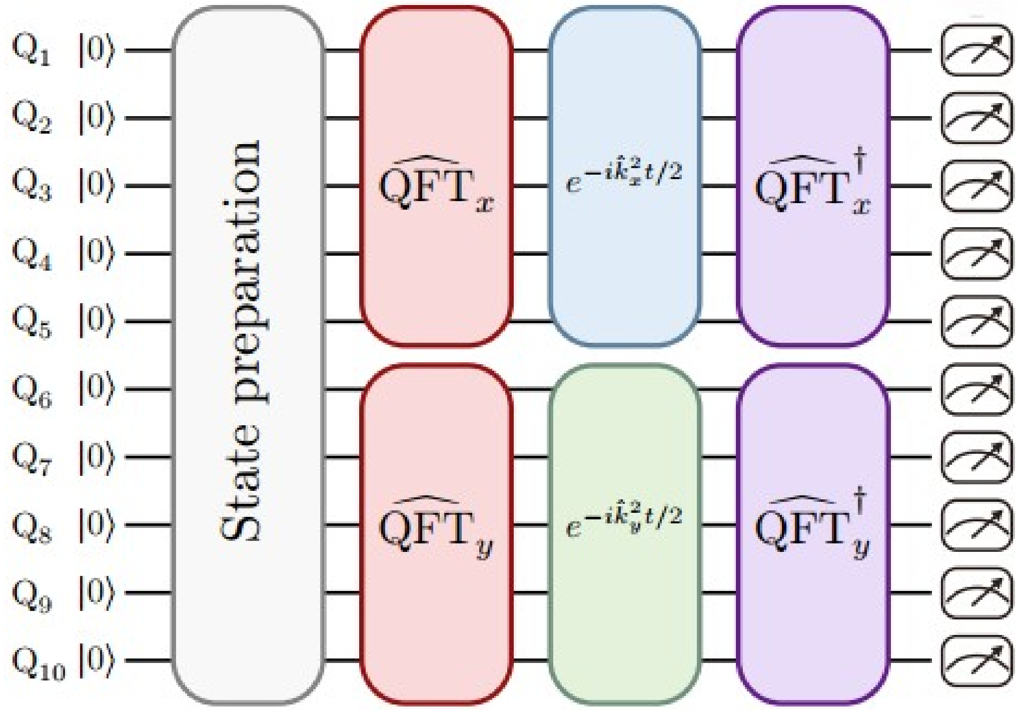
(1) Encoding the physical information of fluid into quantum state information. **[(a),(b)]**

(2) Linearizing the Navier-Stokes equations or transport equations, or transforming them into the Schrödinger form, and then constructing quantum circuits for computation based on the specific forms (sometimes requiring a Fourier transform of the quantum states). **[(c),(d)]**

(3) Extracting the physical information of the fluid from the resulting quantum states. **[(e)]**

Some of my research

Finding a universal form of quantum circuits that can compute a wider variety of equations.



A senior in the same research group has studied the form . Allowing it to be decomposed into basic quantum gate circuits.

$$e^{-i\hat{k}_\alpha^2 t/2} = \exp\left\{-\frac{it}{2}\left[-\frac{1}{2}\left(I_{2^{n_\alpha}} + \sum_{j=1}^{n_\alpha} 2^{n_\alpha-j}\hat{Z}_j\right) + 2^{n_\alpha}\hat{Z}_1\right]^2\right\}$$

Building on my senior's research, I discovered that the square of k can be replaced with a polynomial form of k, which can further be approximated through a Taylor expansion for a general form.

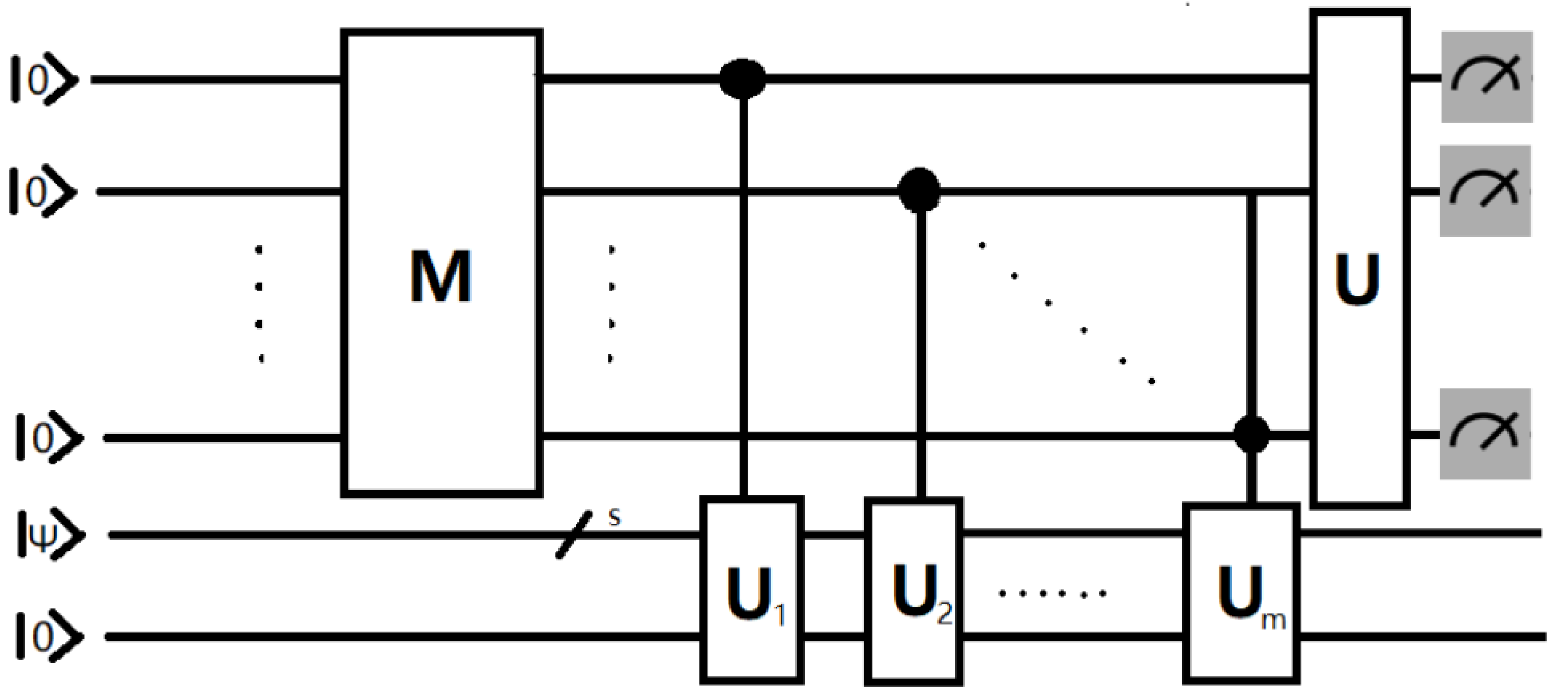
$$e^{-\frac{t}{2}(\hat{Z}_1\hat{Z}_2\cdots\hat{Z}_n)} = C_{n-1}\cdots C_2C_1\left[I_{2^{m-1}}\otimes R_z(\theta)\right]C_1C_2\cdots C_{n-1} \qquad \text{(a)}$$

$$\hat{k}_\alpha = -\frac{1}{2}\left(I_{2^{n_\alpha}} + \sum_{j=1}^{n_\alpha} 2^{n_\alpha - j}\hat{Z}_j\right) + 2^{n_\alpha}\hat{Z}_1 \qquad \text{(b)}$$

Where C_i is the CNOT gate that controls the n-th qubit with the i-th qubit as the control.

With the help of (a) and (b), we can decompose expressions of the form $e^{-iP(k)/2}$ into basic quantum gate circuits, where P is a polynomial.

Another discovery: a method was found to extract physical information from multiple quantum states simultaneously



The original measurement method required constructing multiple quantum circuits for measurement. However, the newly discovered method allows obtaining results through multiple measurements using a single quantum circuit. For detailed information, please refer to [Quantum Measurement.pdf] on my personal website.

Recent work

We consider problems with boundary conditions. For different boundary conditions, there are fast diagonalization methods for the matrices corresponding to the difference schemes. We can base our quantum computation on this approach to address boundary value problems.

Dirichlet-Dirichlet (DD):	$u(\alpha) = u_\alpha,$	$u(\beta) = u_\beta,$
Dirichlet-Neumann (DN):	$u(\alpha) = u_\alpha,$	$u'(\beta) = u'_\beta,$
Neumann-Neumann (NN):	$u'(\alpha) = u'_\alpha,$	$u'(\beta) = u'_\beta,$
Periodic (P):	$u(\alpha) = u(\beta).$	

$$\mathcal{T}_n^{(DD)} = \begin{bmatrix} 2 & -1 & \cdots & 0 \\ -1 & 2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 \\ 0 & \cdots & -1 & 2 \end{bmatrix}$$

$$\begin{aligned} \mathcal{T}_n^{(DN)} &= \mathcal{T}_n^{(DD)} - e_n e_{n-1}^T, \\ \mathcal{T}_n^{(NN)} &= \mathcal{T}_n^{(DD)} - e_n e_{n-1}^T - e_1 e_2^T, \\ \mathcal{T}_n^{(P)} &= \mathcal{T}_n^{(DD)} - e_1 e_n^T - e_n e_1^T. \end{aligned}$$

Fast diagonalization of different numerical schemes

For the four schemes, we can decompose them quickly :

$$\mathcal{T}_n^{(DD)} s(\theta_j) = 4\sin^2(\theta_j/2) s(\theta_j), \qquad \theta_j = \frac{j\pi}{n+1},$$

$$[V_n^{(DD)}]_{kj} = \sin\left(\frac{kj\pi}{n+1}\right) \qquad \lambda_j = 4\sin^2\left(\frac{j\pi}{2(n+1)}\right)$$

$$\mathcal{T}_n^{(DN)} \cdot s(\theta_j) = 4\sin^2(\theta_j/2) \cdot s(\theta_j), \qquad \theta_j = \frac{(2j-1)\pi}{2n},$$

$$s(\theta_j) = (sin\theta_1, sin\theta_2, \ldots, sin\theta_n)^T$$

$$[V_n^{(DN)}]_{kj} = \sin\left(\frac{k(2j-1)\pi}{2n}\right) \qquad \lambda_j = 4\sin^2\left(\frac{(2j-1)\pi}{4n}\right)$$

$$D = Diag(\lambda_1, \lambda_2, \ldots, \lambda_N)$$

$$\mathcal{T}_n^{(NN)} \cdot c(\theta_j) = 4\sin^2\left(\frac{\theta_j}{2}\right) \cdot c(\theta_j), \qquad \theta_j = \frac{(j-1)\pi}{n-1}.$$

$$[V_n^{(NN)}]_{kj} = \cos\left(\frac{(k-1)(j-1)\pi}{n-1}\right) \qquad \lambda_j = 4\sin^2\left(\frac{(j-1)\pi}{2(n-1)}\right)$$

Handling computational problems

$$\frac{d\vec{u}}{dt} = T\vec{u} \qquad \frac{d(V\vec{u})}{dt} = VT\vec{u} = D(V\vec{u})$$

Define $\vec{x} = V\vec{u}$, then: $\quad \dfrac{d\vec{x}}{dt} = D\vec{x}, \quad D$ is a diagonal matrix

By applying appropriate methods (such as block-encoding or Fourier transform) to the diagonal matrix, we can transform it into a unitary diagonal matrix related to the wavenumber. Then, we can construct a quantum circuit composed of basic quantum gates for computation using the previous method.

Current difficulties:

1. The analysis of eigenvalue decomposition for higher-order numerical schemes has not been conducted yet, and it is unclear whether they have a unified format.
2. In problems with boundary conditions, the use of block-encoding and

Summary and discussion

In our research, we have studied various issues related to using quantum computing methods to solve problems encountered in computational fluid dynamics. For example, how to efficiently extract physical information from quantum states, how to transform different types of equations into a form suitable for quantum computing, and how to address boundary value problems, among others.

Reference

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