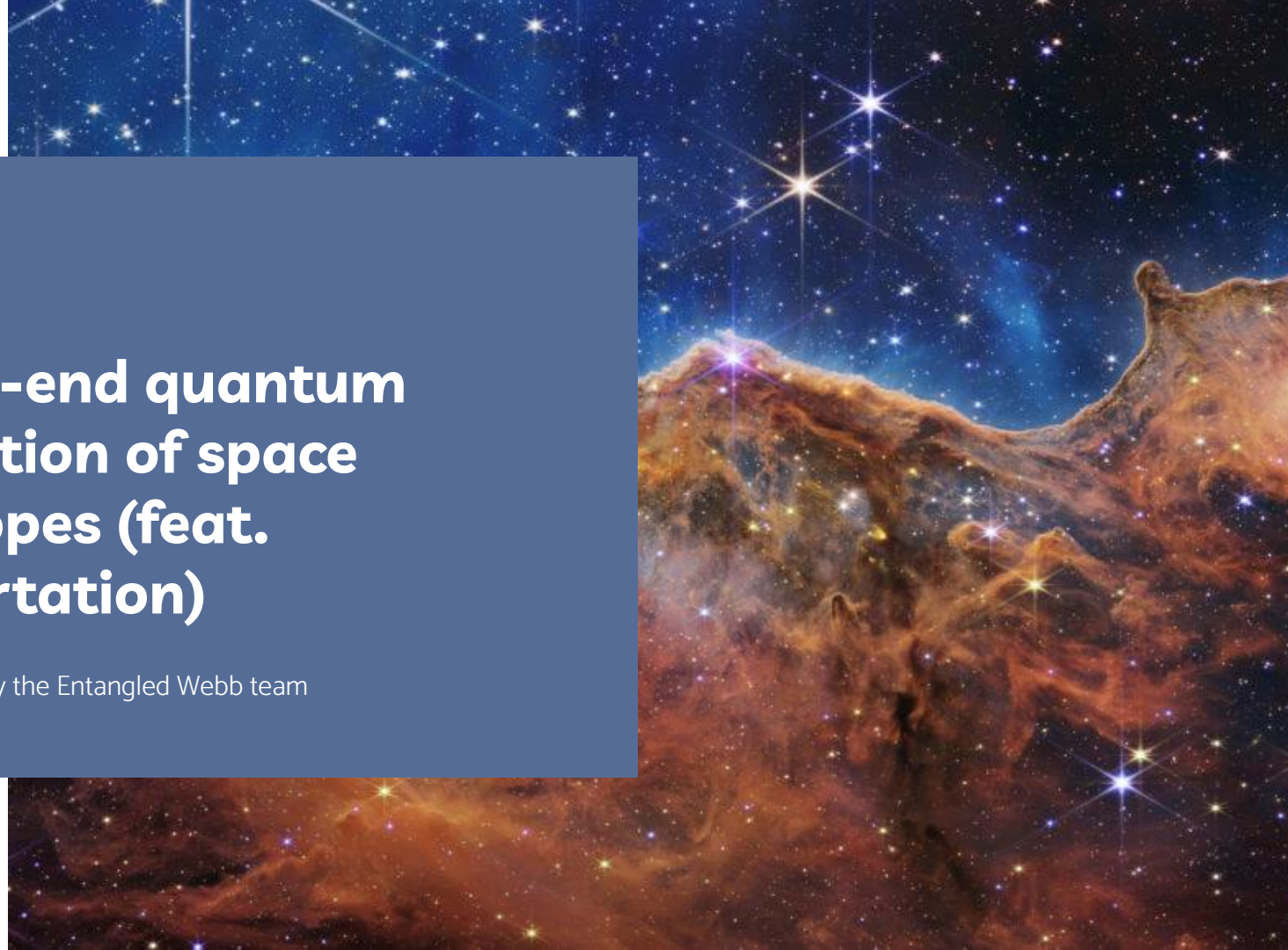
End-to-end quantum simulation of space telescopes (feat. teleportation)

A presentation by the Entangled Webb team



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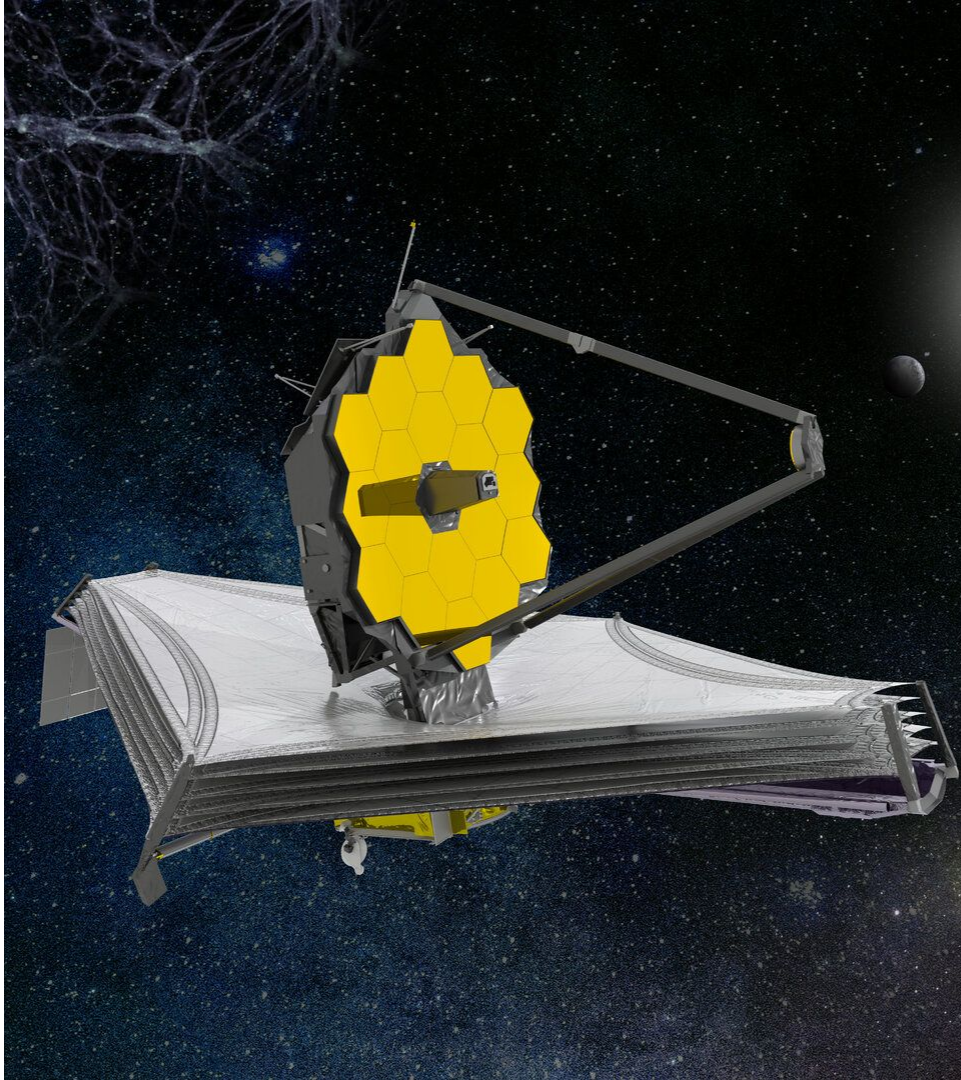

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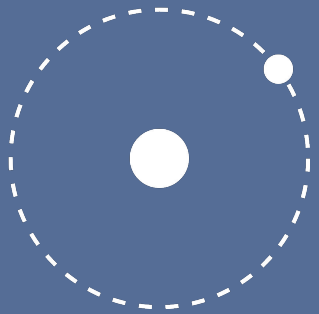
Our system

We assume the satellite to have a circular orbit around the earth with a period of 6 months. This simplifies the problem, because we can describe the position with only one parameter.



Position encoding

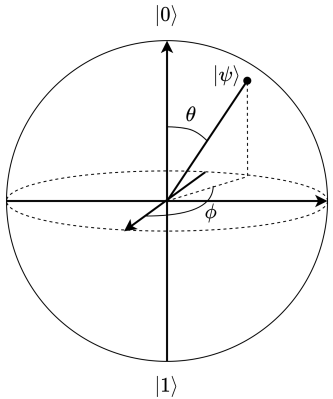
To encode the position of the telescope, we can do it on a real amplitude of a qubit such that

$$|\psi\rangle = x\,|0\rangle + y\,|1\rangle, \quad x^2 + y^2 = 1$$

this is a natural choice, because the radius does not change. Meaning that we can encode the position using pure states.

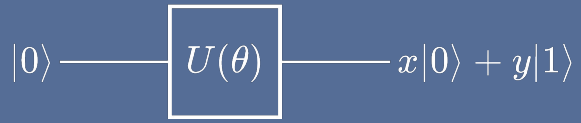
Rotating the state

We can do a rotation with respect to the y axis in the Bloch sphere, so that the amplitudes will stay as real numbers.



Preparing the state

In practice, we prepare the state using a rotation gate, and then feed it into the HHL algorithm. More details in the Jupyter notebook.



THE FAST ALGORITHM

Linear equation solver

The equation that we want to solve is

$$Ax = b$$

$$A = \begin{pmatrix} 1 & \frac{2\pi\Delta t}{T} \\ -\frac{2\pi\Delta t}{T} & 1 \end{pmatrix} \qquad b = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$$

$$x = \begin{pmatrix} x(t+\Delta t) \\ y(t+\Delta t) \end{pmatrix}$$

Matrix condition

The matrix should be Hermitian so that it can be converted into a unitary operator

$$A = A^{\dagger}$$

Problem equation updated

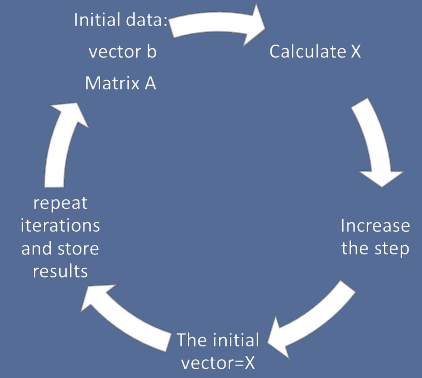
Transforming our matrix into a 4x4 matrix

$$A = \begin{pmatrix} 0 & 0 & 1 & \frac{2\pi\Delta t}{T} \\ 0 & 0 & -\frac{2\pi\Delta t}{T} & 1 \\ 1 & -\frac{2\pi\Delta t}{T} & 0 & 0 \\ \frac{2\pi\Delta t}{T} & 1 & 0 & 0 \end{pmatrix}.$$

The new matrix will do the following transformation

$$\begin{pmatrix} x(t) \\ y(t) \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 0 \\ x(t+\Delta t) \\ y(t+\Delta t) \end{pmatrix}$$

Process



Adjusting Qiskit code

THE FAST ALGORITHM

Circuit for HHL

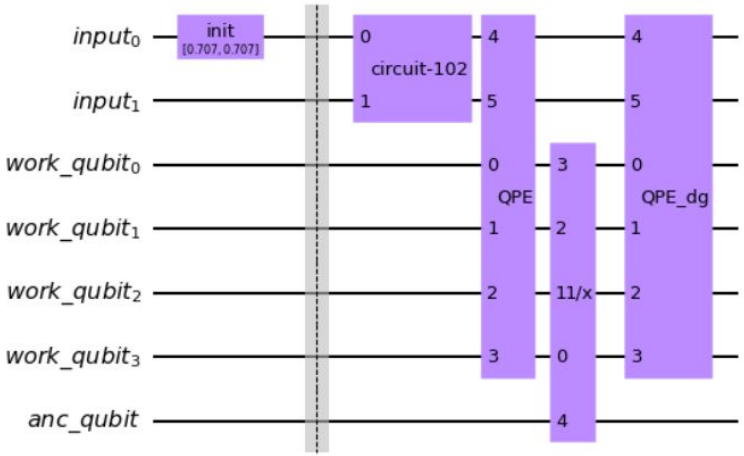


Figure 1. The first two qubits are used to encode the input vector. The work qubits store the eigenvalues of the A. The last qubit is the ancilla qubit. The output is obtained from the first two qubits at the end of the operation.

ODE result

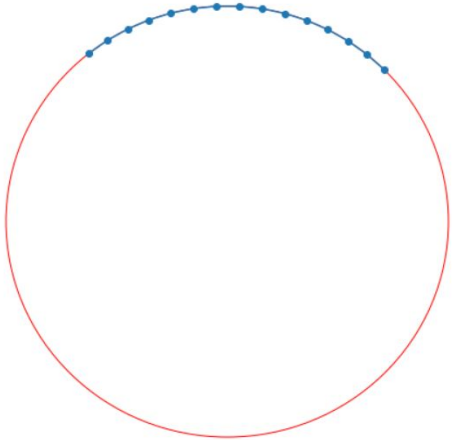


Figure 2. The blue points are our ODE results, the first point is our initial state, starting at x = y = 1/√2. We did a counterclockwise rotation for a quarter of a circle, and it traces our reference circle with a radius of 1. The initial state and the number of iteration can be modified in the Jupyter notebook.

INPUT ENCODING

How to encode n satellites

To encode the coordinates of n satellites, we need to get our qubits in a superposition state so that we can use the amplitudes. To do this, we apply a Hadamard gate to each qubit. Then, by calculating the angles corresponding to the coordinates, we rotate the qubits by that angle and obtain the amplitudes corresponding to the coordinates. We ensure that the rotation is applied to different amplitudes by using X gates between rotations.

How many qubits for n satellites?

If we have n satellites, that gives us 2n coordinates. Since the number of amplitudes of N qubits is 2^N, the number of coordinates must be less than or equal to the number of amplitudes to cover all coordinates.

$$2n \leq 2^N$$

$$log(2n) \leq log(2^N)$$

$$1 + log(n) \leq N$$

O(n) vs O(log(n))

Here we compare computation complexity of solving linear systems on a classical computer which is O(n) and a quantum computer which is O(log(n)).

$$10 \times 10 = 10^2$$

$$10^{12} \times 10^{12} = 10^{24}$$

Classical Computer:

$10^2 \quad in \quad 1\ second$

$10^{24} \quad in \quad 10^{22}\ seconds$

Quantum Computer:

$log(10^2) \quad in \quad 1\ second$

$log(10^{24}) \quad in \quad 12\ seconds$

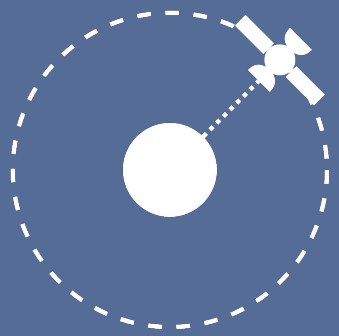
Lower bound on complexity & future of diff-eq solvers

- Each H gate is considered as 1 step and each U gate is considered as N steps since we control N-1 qubits and have 1 target qubit. Therefore we have 1+log(n) steps from H gates, nlog(n) steps from U gates and approximately kn steps, with k being a positive integer, from X gates. In this case, we can say that our circuit has O(nlog(n)) complexity in terms of n.
- What this complexity tells us is if we manage to find an efficient way to encode the input, quantum computers will be able to solve differential equations much faster than classical computers. This will help us simulate complex problems in less time.

TELEPORTATION

Our system

We assume we have a satellite that is going to give us the positions of other satellite in form of quantum states. To process it, we have to teleport the quantum state back to earth.



Photonic qubits

We need to use entangled qubits to do quantum teleportation. In our case, one should be sent to the satellite and one should stay at MIT. Photonic qubits will be very suitable for this application, since they are moving at the speed of light! We can encode the states using polarization of photons. The entangled states are prepared using spontaneous parametric down conversion (SPDC).

Signal transmission

We can put our theoretical satellite in a sun-synchronous orbit. The reason is because we don't need to send signals all the time. By using sun-synchronous orbit, we can send qubits at certain time of the day. The classical bits can be sent to earth using radio signals.

Summary

We are going to do quantum teleportation using several steps:

- Prepare the states using SPDC
- Send them to the satellite using lasers
- The satellite measures its qubits
- The satellite sends the measurement result back to earth using radio signals

Source: https://arxiv.org/abs/1707.00934

Practical Applications Q1

A highly functional quantum computer can be used to solve equations that classical computers are not able to solve efficiently or at all. In many cases, classical computers can only obtain approximations using numerical methods and by simplifying the systems they describe. The Liouville equation is one of them.

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} \stackrel{\text{def}}{=} \sum_{j=1}^{N} \left(\nabla_{r_j} H \cdot \nabla_{p_j} \rho - \nabla_{p_j} H \cdot \nabla_{r_j} \rho \right)$$

N is the number of particles being considered, H is the total energy of the system, ϱ is a probability density function that describes the state of the system, and the subscripts r and p are the position and momentum of the particles, respectively. Using ϱ, physical properties of the system that characterize its state can be found.

The protein folding problem can be solved if the Liouville equation is solved as its solutions would describe the shapes of proteins if they are seen as collections of N atoms [2]. More effective drugs can be designed if the structure of proteins and their interactions are fully understood. Thus, one should be interested in finding the exact solutions and considering realistic cases.

[2] Dix, D.B., Mathematical Models of Protein Folding. *Department of Mathematics, University of South Carolina www. math. sc. edu/~ dix/fold. pdf.*

Practical Applications Q2

In some cases, it is possible to use linear systems to approximate nonlinear processes [3]. Due to the large number of degrees of freedom that proteins have, the number of potential conformations is extremely large, but many proteins tend to find an equilibrium state, or their native structures, very quickly. Also, the energy of the system dissipates as it evolves and reaches an equilibrium state. Those facts lead us to believe that in some cases the nonlinear features of our system can be approximated, and the system can be modeled by a system of linear differential equations as those features vanish. Therefore, a quantum algorithm similar to the one introduced in [3] might be powerful enough to solve the Liouville equation when it is used to analyze realistic cases.

To implement a similar approach, our system of nonlinear partial differential equations can be mapped to an infinite dimensional system of linear differential equations. By truncating that infinite dimensional system, quantum algorithms used to solve linear differential equations can be implemented. One of those algorithms is the HHL algorithm which was implemented in task one to model the orbit of a satellite. As mentioned above, one of the key ideas would be to approximate the nonlinearities of the initial state of the system, and as those disappear use only linear equations to understand the folding process and equilibrium state. Within the next twenty years these ideas will be tested.

[3] Liu, J.P., Kolden, H.Ø., Krovi, H.K., Loureiro, N.F., Trivisa, K. and Childs, A.M., 2021. Efficient quantum algorithm for dissipative nonlinear differential equations. *Proceedings of the National Academy of Sciences*, *118*(35), p.e2026805118.

Practical Applications Q3 & Q4 & Q5

To solve the Liouville equation, we'll need to know the probability density function ϱ. The density function can be acquired from the position r_j and momentum p_j of the protein.

We want to collect the data as quantum states, one way to do it is to use a quantum sensor to measure our protein sample directly. That means we need to find a method that enables us to do so.

Currently, there are several methods to determine the structure of a protein. The one that we think has the most potential to use as a quantum sensor is X-ray crystallography. The advantage of this method are the following:

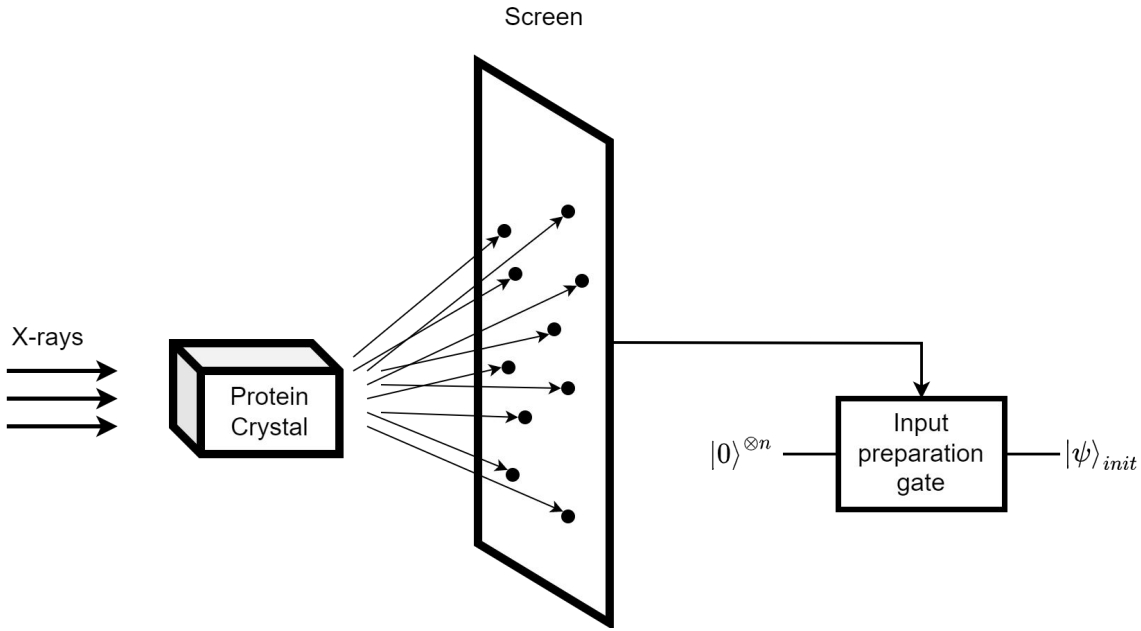
- The images are sharp, and we can use this to get a 3D image [4]
- The data collection is more sensitive compared to another method [5]
- The signals that we get is in the form of photons. Meaning we can shine the X-ray multiple times for our quantum measurements (Will be elaborated in the next slide)

[4] U.S. Department of Health and Human Services. The Structures of Life. July 2007
[5] Viadiu, Hector. "Why do we need crystals?" UCSD Lecture. November 2011

Practical Applications Q5

Here's how we think the quantum sensor will look like. The X-ray will shine on our protein sample. The scattered X-ray beams will then be captured by the screen. Using those signals, we can then prepare our state.

The input preparation gate might involve quantum Fourier transform, since we usually use Fourier transform to get the positions of the atoms.



Practical Applications Q5

Even though X-ray crystallography method might allow us to prepare the initial state by using quantum sensing, we also have to consider several drawbacks of this method:

- We need to prepare the protein crystal. That is because in order to get a high quality image, we have to keep the atoms still. The crystal itself has to be very pure and high quality, otherwise we can't get a clear image. Also, we might not be able to crystallize every protein..
- The distance between two atoms cannot be to small, otherwise we need a very high energy X-ray beam.

We think this method of preparing the input states using quantum sensing might help in some cases. For example if we have a strain of unknown protein, we can use this method to prepare the inputs and directly simulate it using the algorithm that we described earlier. We can also prepare many input states for different simulation run by doing the quantum sensing multiple times.

[4] U.S. Department of Health and Human Services. The Structures of Life. July 2007
[5] Viadiu, Hector. "Why do we need crystals?" UCSD Lecture. November 2011

Practical Applications Q6

The transmission of the information received by the X-ray crystallography will be done through multiple signals that will be linked into our quantum computer. Ideally, the signals would be used to activate gates. The information will include the positions of the atoms of the crystal as well as their momentum, and these inputs will be interpreted as qubits to insert them to the algorithms of differential equation resolution.

As our quantum sensor's precision results from the sensitivity of quantum states to minor changes in the environment other measures could be taken in order to reduce noise and disturbing signals. In case the quantum computer is located far from our quantum sensing, the information could be transmitted using local quantum networks.

Impacts Q7

Levinthal's paradox states that finding the native folded state of a protein by a random search among all possible configurations can take an enormously long time. Yet proteins can fold in seconds or less. Thus, classical computers can't solve it through sampling. One could also use classical molecular dynamics to drive the folding process. However, the quality of the available classical force fields, as well as the computer power needed to solve the corresponding equations of motion are not sufficient to model the folding process.

Folding@home is a distributed computing project aimed to help scientists develop new therapeutics for a variety of diseases by the means of simulating protein dynamics. This includes the process of protein folding and the movements of proteins, and is reliant on simulations run on volunteers' personal computers. So far, it's only able to model relatively short protein chains — chains much smaller than a typical protein found in a body.

An improved version of our end-to-end application would be able to provide a significant speed up to this process. The application can begin to chip away at Levinthal's Paradox and work out how these molecular machines fold so quickly and perform their catalytic functions.

Solutions to Real life problems Q7

MEDICINE

The breakthrough could help researchers understand how misfolded proteins cause diseases like Alzheimer's disease and design drugs that can target a particular topological region of a protein where chemical reactions take place.

VACCINE DEVELOPMENT

By understanding the exact shape of the problem protein, we can design drug molecules which will efficiently affect only the problem protein. This will result in highly effective drugs with no side effects.

CROP IMPROVEMENT

Researchers are also exploring ways to introduce synthetic proteins that will increase crop yields and make plants more nutritious.

NOVEL SOLUTIONS

In the longer term, predicting protein structure will also help design synthetic proteins, such as enzymes that digest waste or produce biofuels.

Dix, D.B., Mathematical Models of Protein Folding. *Department of Mathematics, University of South Carolina www. math. sc. edu/~ dix/fold. pdf.*