End-to-end quantum simulation of space telescopes

WOMANIUM GLOBAL QUANTUM COMPUTING & ENTREPRENEURSHIP PROGRAM

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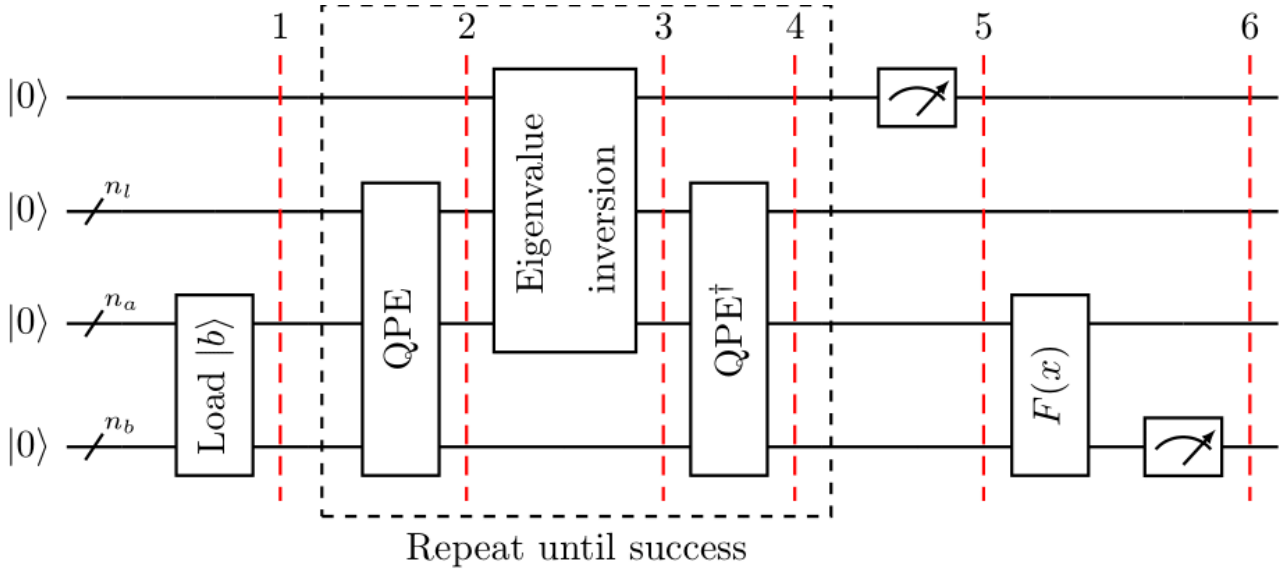
HHL Algorithm

Algorithm description

Solve the linear system $Ax = b$ where A is Hermitian

In case A is not Hermitian, we solve the system $\begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}\begin{pmatrix} 0 \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$ instead.

Application to simulating James Webb Orbit:



HHL Algorithm circuit @ Qiskit

HHL Algorithm

James Webb's Orbit simulation

Differential equation

$$\begin{pmatrix} 0 & -2\pi/T \\ 2\pi/T & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix}$$

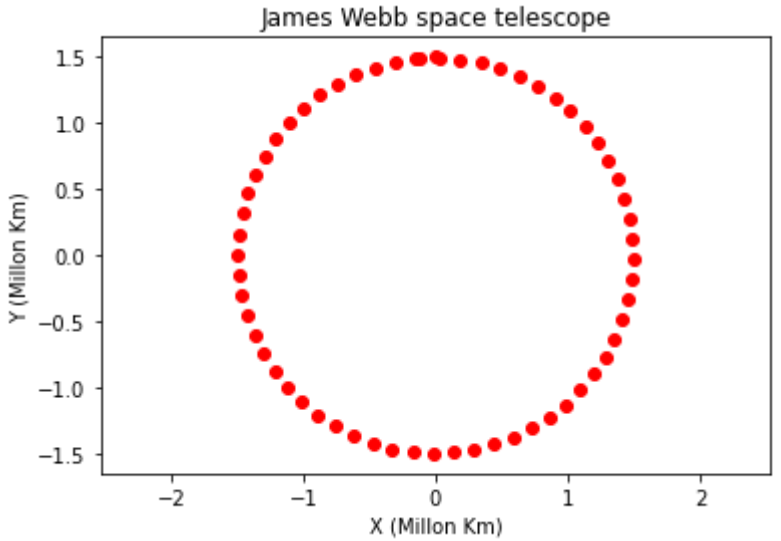
Backward Euler method -> Linear system

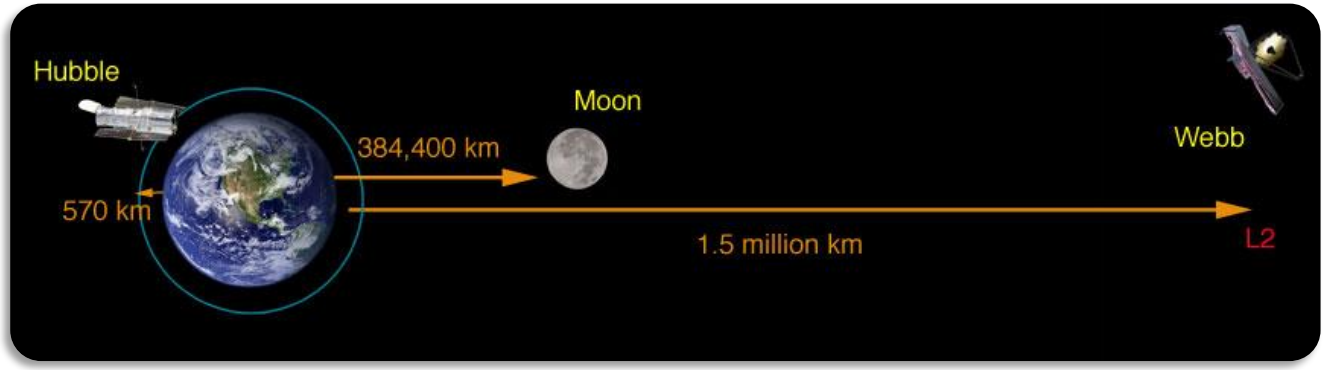
$$\begin{pmatrix} 1 & 2\pi\Delta t/T \\ -2\pi\Delta t/T & 1 \end{pmatrix} \begin{pmatrix} x_i \\ y_i \end{pmatrix} = \begin{pmatrix} x_{i+1} \\ y_{i+1} \end{pmatrix}$$

Simulation parameters

$T = 6\,months\,, \Delta t = 10^{-1}\,,$

$(x_0 \quad y_0) = (0 \quad 1.5)$, duration = T



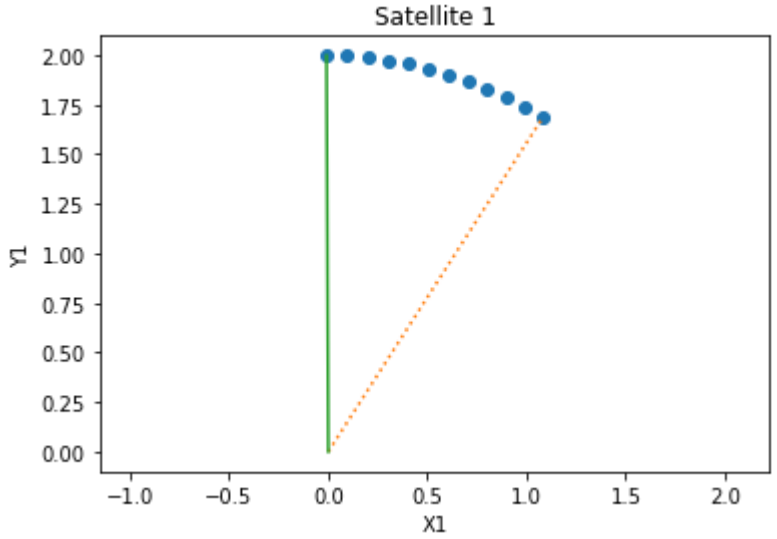


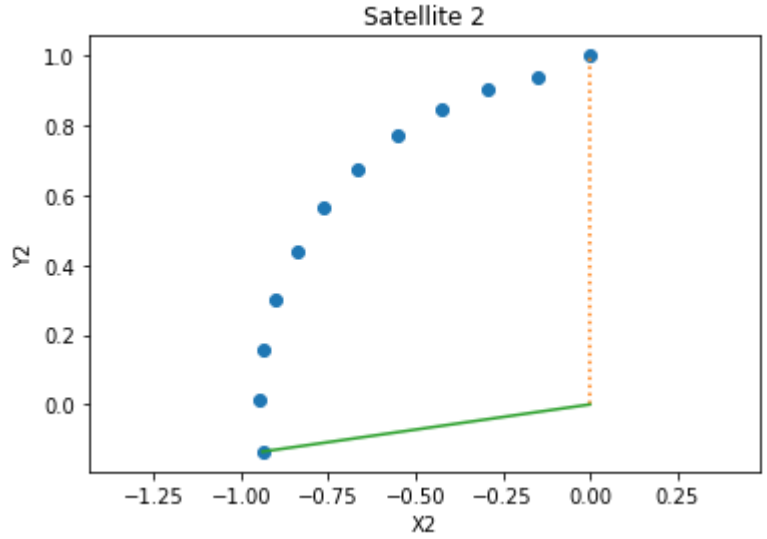
@ NASA

HHL Algorithm

Simulation of 2 satellites

$$\Delta t = \frac{1}{40}\ ; t_{End} = \frac{1}{4};\ \begin{cases} T_1 = 3 \\ r_1 = 2 \end{cases} And \begin{cases} T_2 = 1 \\ r_2 = 1 \end{cases}$$





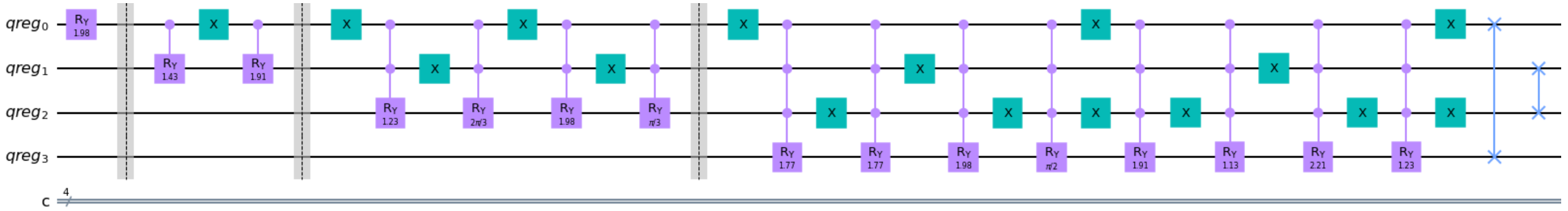
Amplitude Encoding of the input

Given N satellites whose initial position are $(x_1, y_1, x_2, y_2, \dots, x_N, y_N)$

We use $n = [Log_2(2N)]$

Apply uniformly controlled rotation described in [1] and [2]

Example of 8 satellites position encoding



References

- [1] Transformation of quantum states using uniformly controlled rotations, Mikko M¨ott¨onen, Juha J. Vartiainen, Ville Bergholm, and Martti M. Salomaa
- [2] A divide-and-conquer algorithm for quantum state preparation,Israel F. Araujo1, Daniel K. Park, Francesco Petruccione & Adenilton J. da Silva

Amplitude Encoding of the input

	Classical	Quantum		
		HHL	Amplitude encoding	Quantum
Complexity	$O(N)$	$O(log(N))$	$O(N)$	$O(log(N)) + O(N) = O(N)$

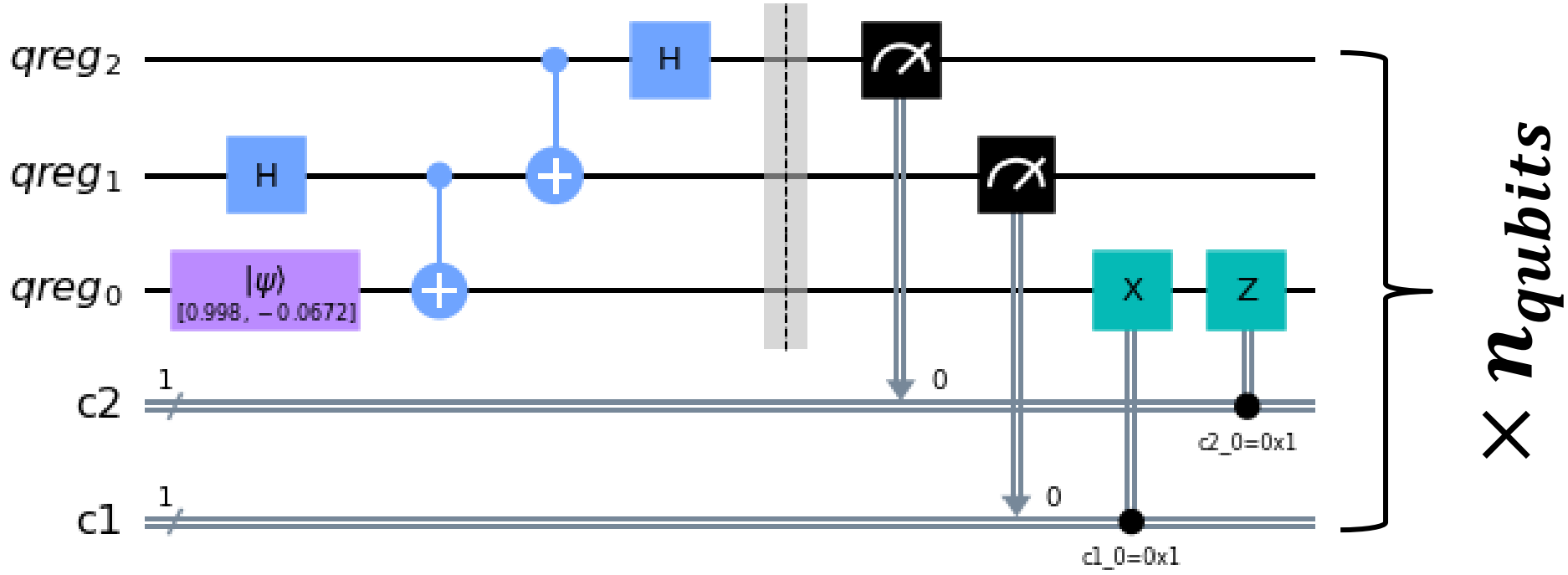
Size of the system	Classical	Quantum
10 x 10	1s	1s
	$t_c = C \times n \rightarrow C = 0.1$	$t_q = C \times \log_{10}(n) \rightarrow C = 1$
10^{12} x 10^{12}	10^{11}s ≈ 3169 years	12s

The encoding step is slowing down the quantum algorithm which makes it lose its advantage!

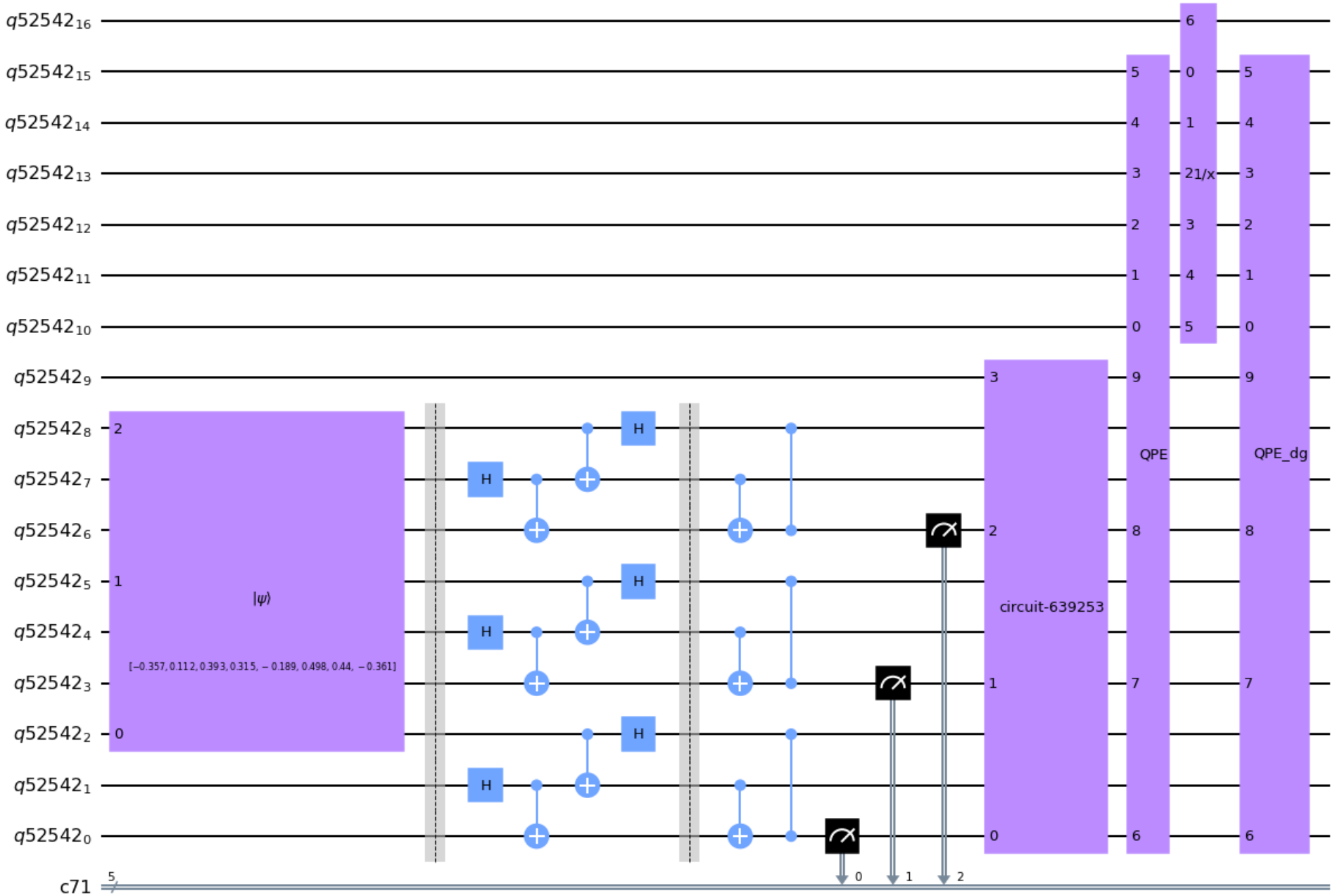
Quantum teleportation

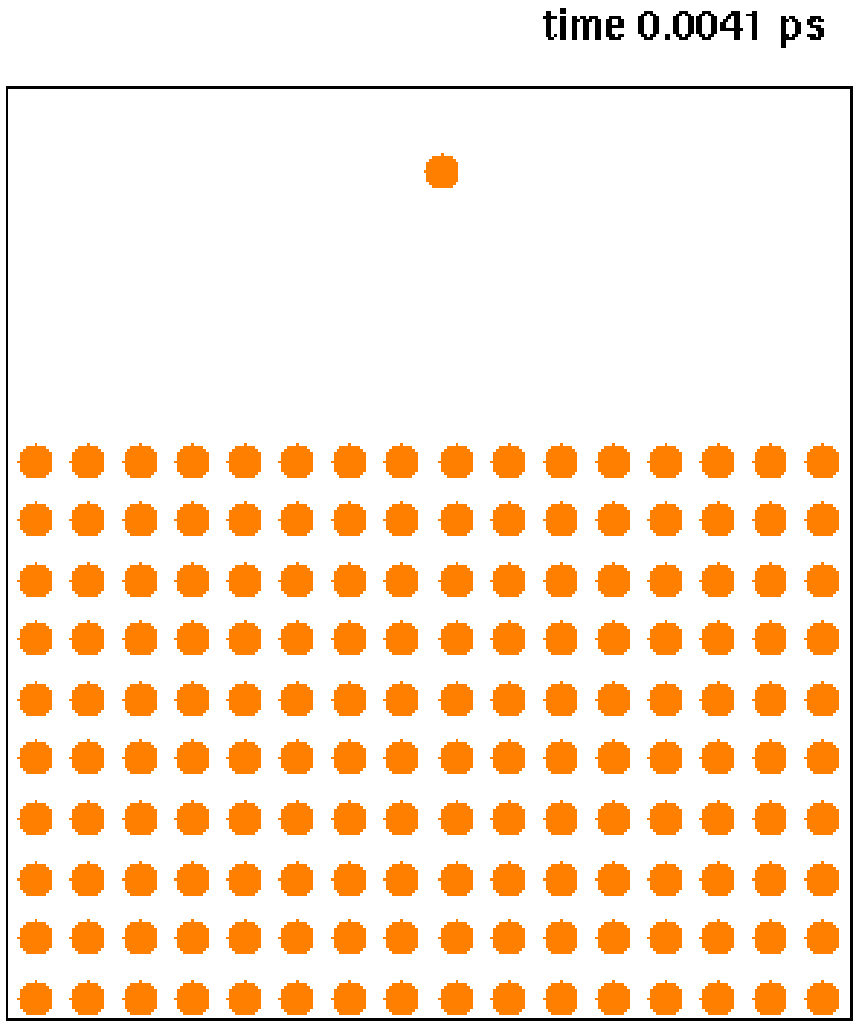
Imagine that a quantum sensor prepares the states,

→ all we have to do is teleport them to the quantum computer



4 satellites positions
($size = 8 = 2^3$)





@Wikipedia

Molecular dynamics Synthesis of 2D materials

Goal

Molecular dynamics aims to predict atoms position time evolution using classical approximation to quantum equations governing the movement

Approximations

- DeBroglie wavelength is very small with regards to interatomic distances
- The possibility to dissociate electron motion from that of nuclei according to Born–Oppenheimer approximation.

Applications

- Production of new material with high performances adapted to usage in future Qubits and Quantum computers

Molecular dynamics

Input preparation

Given a set of N atoms composed of n substrate atoms and N-n deposited atoms

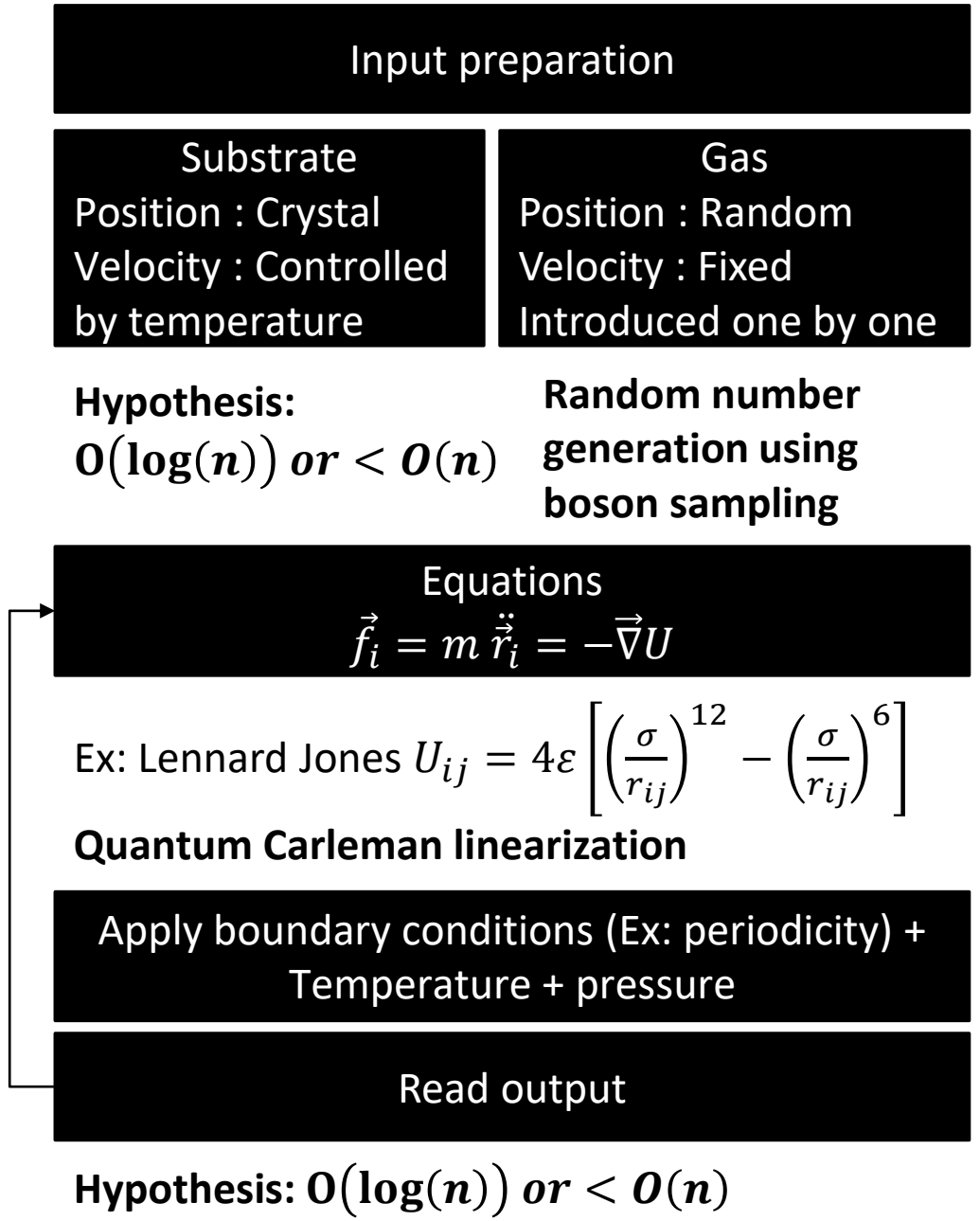
We consider crystalline substrates and gas deposition

Substrate

- - The substrate atoms follow a certain pattern thus we can hope there exists an algorithms that can prepare it in Log(n) or at least poly log(n) time
- - Initial speed 0

Gas

- Position and speed of the rest of atoms is arbitrary, thus it can be generated by algorithm profiting from the randomness related to quantum mechanics, maybe the result of this challenge **" Random number generation using boson sampling "**



Molecular dynamics

Equations

We solve 3N equations of motion describing the classical theory motion of N atoms

$$\vec{f}_i = m\,\ddot{\vec{r}}_i = -\vec{\nabla}U \; and \; E = \frac{1}{2}\sum \frac{p_i^2}{m_i} + U(r_i)$$

The simulation requires the implementation of the adequate potentials in order to describe the state of the atoms with high fidelity

An example of the potential is:

Lennard-Jones $U_{ij} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$

The equations can be linearized, (nonlinear potentials), using **Quantum Carleman linearization** described here.

Input preparation

Substrate	Gas
Position : Crystal Velocity : Controlled by temperature	Position : Random Velocity : Fixed Introduced one by one

Hypothesis: $\mathbf{O}\left(\log(n)\right)$ or $< O(n)$

Random number generation using boson sampling

Equations

$$\vec{f}_i = m\,\ddot{\vec{r}}_i = -\vec{\nabla}U$$

Ex: Lennard Jones $U_{ij} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$

Quantum Carleman linearization

Apply boundary conditions (Ex: periodicity) + Temperature + pressure

Read output

Hypothesis: $\mathbf{O}\left(\log(n)\right)$ or $< O(n)$

Future perspectives

Solving the general case where:

- all particles have predefined positions
- all initial speeds are arbitrary or predefined

Developing fast algorithms to read the output $< O(n)$

Extending use to other applications:

- Interaction between solids liquids and gases
- Drug and biomolecules simulation

Thanks