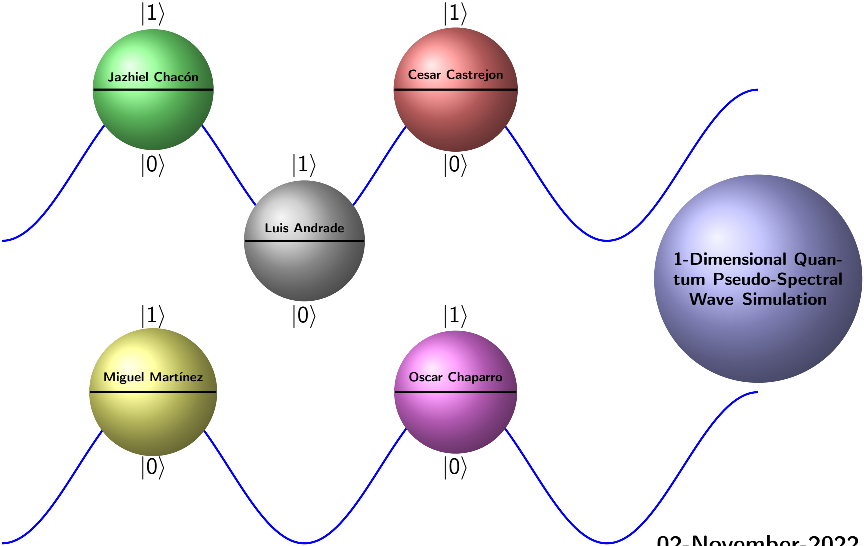
Qiskit Fall Fest 2022

Qiskit



02-November-2022

Contents

Objectives

- Develop a first approximation of Quantum Wave Simulation applied to seismic wave propagation.
- Analyze the usefulness of the Quantum Fourier Transform in the 1D acoustic wave simulation

Introduction to 1-Dimensional Quantum Pseudo-Spectral Wave Simulation

Wave propagation equations require the approximation of spatial derivatives. However, in the long-distance ranges (above 500 km) this approach leads to different issues that need to be addressed. In this regard, there have been different developments and alternative methods to compute these space derivatives, for example the finite-differences, finite-element and pseudo-spectral methods. (Moczo et al., 2011; Seriani and Oliveira, 2020).

Introduction to 1-Dimensional Quantum Pseudo-Spectral Wave Simulation

The wave equation is solved in physical space in the pseudo-spectral method, such as the finite-differences method. However, the space derivatives are calculated using functions like Fourier Integrals or Chebyshev polynomials. The derivatives could be evaluated using the Fast Fourier transform (FFT).

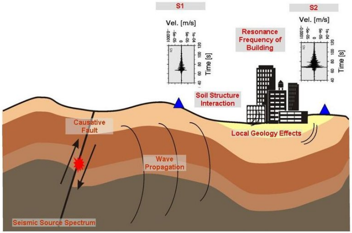


Figure: Seismic wave propagation after an earthquake.

Wave Simulation Applications

In Geophysics there are numerous applications of wave simulations, which could broadly be divided as:

- Earthquake Seismology
  - Study of the interior of the Earth,
  - Study of seismic wave behavior,
  - Development of earthquake scenarios;
- Seismic Exploration
  - Generation of synthetic (simulated) data,
  - Analysis of proposed geological structures (geophysical modeling and inversion).

Justification why Quantum approach

In recent years, due to the importance of the applications mentioned before, experts have worked on reducing the simulation time or even calculating them in real-time, without reducing the input sizes (where recent needs tend to increase them in order to improve the resolution). A cornerstone to do so is reducing the algorithms' complexity via code or mathematical optimization.

The difference between the classical and the Quantum Fourier transform complexity could help to reduce the simulation time using pseudo-spectral method, bringing the opportunity to explore new applications of Quantum Computing.

Fourier Spectrum in Seismology

From a sequence or vector of size N, with each entry x_n, the discrete classical FFT is defined as:

$$X_k = \sum_{k=0}^{N-1} x_n \cdot e^{-\frac{j2\pi kn}{N}} \quad (1)$$

which transforms the original vector in a new sequence X_k.

Likewise, the discrete classical inverse FFT^{-1} is defined as:

$$x_n = \frac{1}{N} \sum_{n=0}^{N-1} X_k \cdot e^{\frac{2j\pi kn}{N}} \quad (2)$$

Classical solution

The general case of the 1D acoustic wave equation (replacing the time derivatives by classical finite differences) is:

$$\frac{p(x,t+dt) - 2p(x,t) + p(x,t)}{dt^2} = c(x)^2 \frac{\partial^2 p(x,t)}{\partial x^2} + s(x,t) \quad (3)$$

where c^2 is the squared P-wave velocity, $p(x,t)$ is the pressure field in coordinate x at t time and s is the source term.(Igel, 2016)

In the general case, the pseudo-spectral method calculates the spatial derivative as follows:

$$p(x,t) \rightarrow FFT \rightarrow p(k,t) \rightarrow (ik)^2 p(k,t) \rightarrow FFT^{-1} \rightarrow \frac{\partial^2 p(x,t)}{\partial x^2} \quad (4)$$

Wave simulation and representation

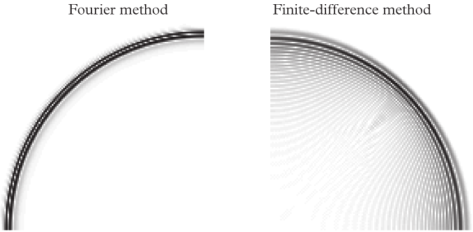


Figure: Comparison between the pseudo-spectral method, solved with Fourier transform (**right**) and the Finite-difference method (**left**). The gray waves in the FD snapshot could be interpreted as noise. That noise does not appear in the PS method.(Igel, 2016)

Ricker Wavelet Generator and Discrete Fourier Transform

We use a Python module called *Ricker Generator* in order to generate the Ricker wavelet amplitudes. This wavelet is defined as:

$$A = \left(1 - 2\pi^2 f^2 t^2\right) e^{-\pi^2 f^2 t^2} \tag{5}$$

where f is the peak frequency and t the time.

In seismic theory, the convolutional model states that any seismic signal is the result of *summing* (actually, convolving) a wavelet with the reflection coefficient (which is related to changes in rock properties such as density and velocity) of the medium. In simulation, it is common to use *zero-phase* wavelets, like the Ricker one, because they tend to provide sharper definitions and the distortion distortion between changes in rock properties.(Glossary, n.d.)

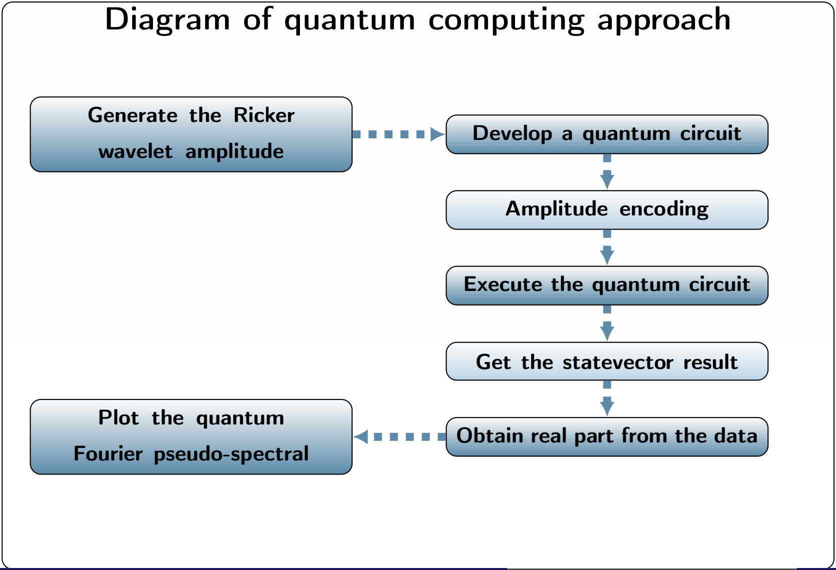


Diagram of quantum computing approach
Generate the Ricker wavelet amplitude
Develop a quantum circuit
Amplitude encoding
Execute the quantum circuit
Get the statevector result
Obtain real part from the data
Plot the quantum Fourier pseudo-spectral

Quantum Fourier Transform

As it was explained in (*Quantum Fourier Transform* n.d.), the Fourier transform occurs in many different versions throughout classical computing, in areas ranging from signal processing to data compression to complexity theory. The quantum Fourier transform (QFT) is the quantum implementation of the discrete Fourier transform over the amplitudes of a wave function. It is part of many quantum algorithms, most notably the Shor's factoring algorithm and quantum phase estimation (Nielsen and Chuang, 2010).

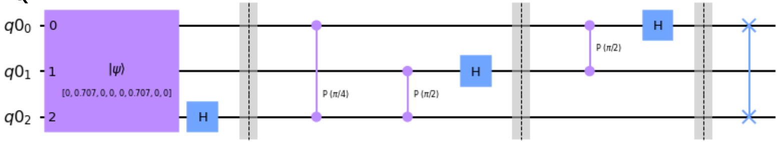
The Quantum Fourier Transform (QFT) on qubits is the operation:

$$|j\rangle \mapsto \frac{1}{2^{n/2}} \sum_{k=0}^{2^n-1} e^{2\pi ijk/2^n} |k\rangle \tag{6}$$

Quantum Fourier Transform Example

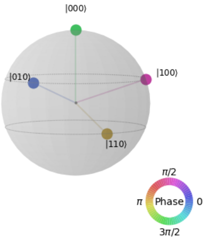
0	1	0	0	0	1	0	0	← Array input data

Quantum circuit:



Statevector result:

$$\frac{1}{2}|000\rangle + \frac{i}{2}|010\rangle - \frac{1}{2}|100\rangle - \frac{i}{2}|110\rangle$$



Encoding Classical data into Qubits

Amplitude encoding : the main reason to implement this encoding is the fact that is needed $n = log_2 M$ qubits to encode a dataset of M inputs. Promises of exponential speedups from qubit-efficient (Leymann and Barzen, 2020). For this particular experiment, a 1024 1-Dimentional signal is encoded in the following way:

$$n = log_2(1024) \tag{7}$$

$n = 10$, so 10 qubits are needed for each basis state of the system.

$$|\psi_{signal}\rangle = M_0 |0000000000\rangle + M_1 |0000000001\rangle + \cdots + M_{1024} |1111111111\rangle \tag{8}$$

Encoding Classical data into Qubits

Since $|\psi_{signal}\rangle$ in Ec.(8) is a quantum state, therefore the sum of the amplitudes must be equal to 1.

This means that each amplitude must be normalized. For this normalization the Frobenius norm is applied (Golub and Van Loan, 2013):

$$||A||_F = \left[\sum_{ij} abs(ij)^2 \right]^{\frac{1}{2}}, \tag{9}$$

The nuclear norm is the sum of the singular values.

Quantum Solution

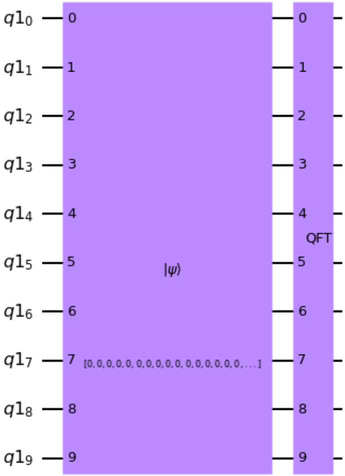


Figure: Quantum circuit with input data encoding and applying quantum Fourier transform.

Quantum Solution

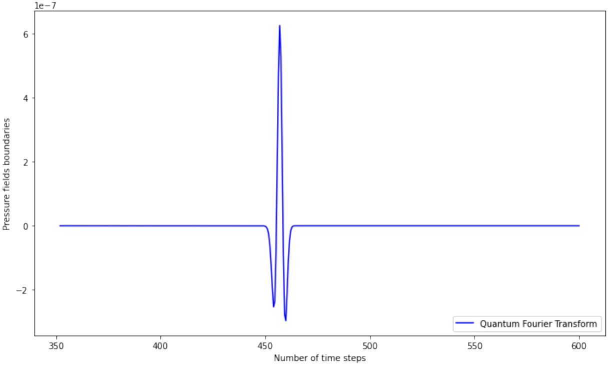


Figure: Plot of number of time steps vs pressure field boundaries.

Conclusions

- A first approximation of quantum wave simulation applied to seismic wave propagation was proposed and presented to map classical algorithms to the quantum approach and yield a quantum computing advantage.
- The quantum Fourier transform's complexity helps reduce time simulation using a pseudo-spectral method and brings the opportunity to explore new implementations of Quantum Computing in reals applications of Geophysics.

What is next?

- Develop more experiments with finite differences vs. Fourier transform for:
  - Gravitational Wave Collapse,
  - Numerical simulations of gravitational fields.
- In order to clean a signal, a quantum Hadamard transform could help as a filter.

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