# Quantum computing in geophysics: algorithms, computational costs and future applications

*Shahpoor Moradi[1], Daniel Trad[1], and Kristopher A. Innanen[1]*
*[1]University of Calgary, Department of Geoscience, Calgary, Canada*

## SUMMARY

Accurate modeling of seismic wave propagation in the subsurface of the earth is essential for understanding earthquake dynamics, characterizing seismic hazards on global scales and hydrocarbon reservoir exploration and monitoring on local scales. These are among the most challenging computational problems in geoscience. Despite algorithmic advances and the increasingly powerful computational resources currently available, including fast CPUs, GPUs and large volumes of computer memory, there are still daunting computational challenges in simulating 3D seismic wave propagation in complex earth environments. Recent advances in quantum computing are suggestive that geoscience may soon begin to benefit from this promising field. For example, Finite Difference (FD) modeling is the most widely used method to simulate seismic wave propagation. In the frequency domain, FD methods reduce solutions of the wave equation into systems of linear equations; such systems are just the type that quantum algorithms may be capable of solving with exponential speedup, in comparison with classical algorithms. For the computational geophysicist, to prepare to take advantage of these speed-ups, which could arrive in as few as 5-10 years, the tasks at hand are (1) to become familiar with the logic and concepts associated with quantum computing, and (2) to map our key computational algorithms (e.g., frequency domain FD) to this domain.

## CONCEPTS IN QUANTUM COMPUTATION

Unlike a classical bit, which exists either in 0 or 1 states, a quantum bit (qubit), the building block of quantum information, can exist in a coherent superposition of two distinct states. In the quantum regime, 0 and 1 are two orthonormal states represented by $|0\rangle = (1 \quad 0)^{\mathrm{T}}$ and $|1\rangle = (0 \quad 1)^{\mathrm{T}}$. A qubit is represented by $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha$ and $\beta$ are probability amplitudes. Measuring the qubit results in either $|0\rangle$ or $|1\rangle$, with respective probabilities $|\alpha|^2$ and $|\beta|^2$ satisfying $|\alpha|^2 + |\beta|^2 = 1$. In a quantum computer, a system of $n$ qubits can exist in $2^n$ states simultaneously, whereas in a classical computer, a system of $n$ bits can store and process only one of $2^n$ states at a given time. For example, a two-qubit system is capable of holding four two bits of information simultaneously; i.e. $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$. This coherent superposition is the essence of the supremacy that quantum computing offers over its classical counterpart. Quantum algorithms are unambiguous instructions, based on effects such as quantum coherence and entanglement, that are able to solve problems faster and with less computational complexity than their best classical algorithms (Nielsen and Chuang, 2000). In Figure 1 we show an illustration of a quantum search algorithm, which can locate a particular item in a database in very few passes, independently of the size of the dataset. In each iteration, without actually measuring the physical state of each sample, the amplitude of the desired answer is amplified until the correct answer is achieved with an optimal probability.

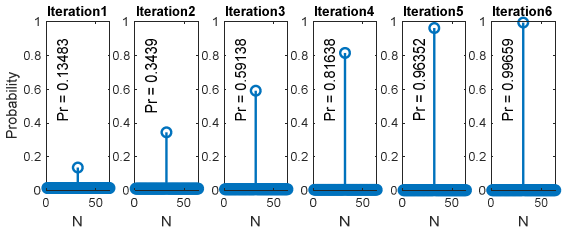


Figure 1. Illustration of amplitude amplification in the search algorithm. The size of the search space is 64 and the number of iterations to achieve the correct answer with high probability is 6.

On the other hand, there are significant obstacles in the application of quantum computers to numerical computations. Unlike classical computers, error correction is challenging for quantum computers. First, qubits are physical objects in nanoscale such as atoms, trapped ions or photons. Interactions of quantum computer with the environment affect the computation. Consequently, the first step to attain an error-free quantum computation is the isolation of physical qubits from any unwanted interactions. Second, direct measurement of numerical errors is problematic because the act of measuring the state of a qubit collapses it to a classical state, destroying the quantum correlation which is crucial for the desired speedup. Third, since qubits can exist as a superposition of multiple states, in addition to bit flip error, there is another non-classical source of error called phase error. As an example, a qubit $\alpha|0\rangle + \beta|1\rangle$ over time may change to $\alpha|0\rangle - \beta|1\rangle$. The standard way to recover a qubit from quantum errors is to utilize ancillary qubits called physical qubits. The idea is to transfer errors from logical qubits to physical qubits, and then discard them without measuring the logical qubits. Initially, the number of physical qubits to correct for arbitrary errors from a single qubit was nine (Shor, 1995) and later seven (Steane, 1996). The smallest number of physical qubits that physicists have yet proposed is five (Laflamme, 1996). Also, to allow a universal set of quantum gates to be used on the logical qubits, we need some extra resources called magic states. These states are

prepared using additional qubits and injected to the system (O'Gorman, and Campbell, 2017).
For example, implementation of factorization with Shor's algorithm for a 2000-bit number (600 decimal digits) requires approximately 4000 computational logical qubits. To successfully execute the algorithm with low error rate we need about 3600 physical qubits (including the magic qubits) per logical qubit. In total, to run the Shor algorithm to factorize the 2000-digit number we need approximately one million qubits (Fowler, 2012). Evaluation time for this task with 1MHz speed takes four days. So far, the largest number that can be factorized on the most powerful supercomputers is 768-bit number, and it took two years.

There are various schemes for physical implementation of quantum computation including, atoms, photons, trapped ions and electrons (Nakahara and Ohmi, 2008). Other potential candidates for qubits are superconducting circuits that behave as artificial atoms exhibiting a tunable energy. States '0' or '1' correspond to the absence or presence of microwave photons or the oscillating electrical current through a loop. One of the important requirements to implement a quantum computer is to have long relevant decoherence times, much longer than the gate operation time. In other words, the lifetime of a qubit should be much longer than the logic gate operation time. In this way, a quantum computer has enough time to execute gates before qubits' coherence is destroyed. For example, for ion traps decoherence time is 20s, which is much longer than gate operation times (0.01 ms). Electron spin qubits have the fastest gate times (~ns) with fastest decoherence time (~30μs). On the hardware side, many research groups and companies around the world are working on developing mini quantum computers for both commercial and research purposes. Among them, D-wave is the sole company that offers a quantum simulator capable to solve certain tasks known as optimization problems. Although D-wave is not a universal quantum computer, it has been utilized for certain quantum calculations. The regime in which D-wave operates is called quantum annealing.
Despite advances in the theoretical framework, the physical realization of quantum computing is still technologically daunting. Reliable quantum computers that actually demonstrate the exponential speed increase over their classical counterparts are not going to be immediately available. Well-known algorithms such as database search and prime factors of large integers have been demonstrated on few qubits in labs, and this represents serious progress in the field. The first genuine application of a quantum computer with 50 qubits (recently announced by IBM) under the assumption that the quantum computer operation is error-free, would allow for the simulation of a system with 50 particles, and this is a problem that is intractable with the current most powerful supercomputers.

To be able to investigate quantum algorithms in the absence of a scalable quantum computer, it is necessary to simulate their behavior on classical computers. This allows us to connect the theoretical advancement of quantum computation with its physical realizations. We emphasize that no speedup should be expected when we run a quantum algorithm on a classical computer; the exercise allows algorithms to be prepared for the introduction of a real quantum computer. The largest classical simulation so far was made in a 45-qubit circuit on the Cori II supercomputer using 8, 192 nodes and 0.5 petabytes of memory (Häner, T. and Steiger, 2017). To put things in perspective, the number of states that can be stored in 50 qubits is $2^{50}\sim10^{15}$=1 Petabyte.

Consequently, a 50-qubit simulation required over 1 Petabyte of main memory to store results.

## COMPUTATION CHALLENGES IN GEOSCIENCE

Is it possible that a scalable quantum computer capable of modeling 3D seismic wave propagation in a complex model of the earth could be developed in the next few years? To simulate seismic wave propagation in a 3D earth model, especially for resolving the high-frequency content of the data to capture small-scale features, we need a supercomputer with peta ($10^{15}$Flops) - or even exascale ($10^{18}$Flops) power. For example to simulate wave modeling with a $10^8$ grid cells and $10^{10}$ degrees of freedom we need a 1 PFlops supercomputer (Breuer, et al, 2014). As an example of the need for Tera-scale computational power, the simulation of an M8 earthquake in the Southern California fault up to 2 Hz for 360s requires 220 TFlops on NCCS Jaguar using 223,074 cores for 24 hours. The simulation volume is $3.2\times 10^5 km^2$ with a depth of 85 km meshed by 436 billion of 40 $m^3$ cubes (Cui et al. 2010). Analytical solution of wave propagation in the earth is possible with the assumption of spherical symmetry. However, a realistic model of the earth should include ellipticity as well as heterogeneous structures in the crust and mantle. For this reason, various numerical modeling schemes used to simulate wave propagation in realistic 3D earth models, such as the forward modeling for global and continental scales, are based on the Spectral Element Method (SEM). For local-scale exploration seismology, on the other hand, they are based on the finite-difference (FDM) or finite-element methods (FEM).

Finite difference modeling is a well-known technique to simulate seismic wave propagation in the subsurface of the earth. In this method, the medium is parameterized in a way that each node associates with a property of the earth. The finite difference thereafter is applied to each node to propagate the seismic wave from one time step to another. The problem of seismic modeling is challenging to solve

for complex earth models due to earth extremely large dimensions. For example, to define a cube of an anisotropic earth model with dimensions $10\times10\times 10$ km$^3$ and 10m grid spacing, $10^{10}$ parameters are required. With this model and $10^4$ time steps we need $10^{13}$ grid point time steps. Assuming an area of gridded sources with $10^3$ shots, we need roughly $10^{16}$ Flops (10 PFlops). This can be run on an IBM Blue Gene/Q which can carry out 20 PFlops. In contrast, quantum computers that achieve high performance by means of natural parallelism between entangled qubits, are capable of performing the aforementioned calculations with a small number of qubits. For the above example, $10^{16}\sim2^{53}$ Flops. Consequently, we can run such forward modeling only with 53 qubit quantum computer (assuming error free).

Let us next look in more detail at the computational complexity of 3D elastic wave modeling. Assume that the number of grid points in each direction is *N*, so the total size of the 3D model is $N^3$. The number of sources (receivers) would be $N^2$ as they are distributed on the 2D surface. In the time domain the number of time steps is proportional to *N,* so the computational complexity for 3D time domain elastic modeling is in order $N^6$(Li et al. 2015).

Seismic inversion needs more computational power than does simulation, as it requires the forward modeling of wave propagation to be carried out several times. Compared to conventional inversion methods, full waveform inversion (FWI) attempts to exploit the information content of the entire seismic waveform in a limited frequency band (Fichtner, 2010). In this technique, the inverse problem is solved through the minimization of a misfit (objective) function between the observed data and modeled (synthetic) data. The inversion is based on iterative local optimization methods such as steepest descent and conjugate gradients. A key step in FWI is to calculate the gradient of the misfit function with respect to the model parameters so-called Born or Fréchet kernel. For a one-parameter model, for example, an acoustic medium with constant density, the gradient of the misfit function respect to velocity is proportional to $\mathbb{F}^T\Delta u$, where $\Delta u$ is the wavefield residual. In addition, $\mathbb{F}$ is the $m \times n$ Fréchet kernel matrix, each element of which, $\mathbb{F}_{ij}$ , is the derivative of the *i*th data value with respect to the *j*th model parameter. Using the matrix $\mathbb{F}$ we can calculate the Hessian matrix $\mathbb{H} = \mathbb{F}^T\mathbb{F}$. This matrix consists of the second-order partial derivatives of the misfit function. The steepest-descent direction is proportional to $\mathbb{F}^T\Delta u$, and the Newton direction is proportional to $(\mathbb{F}^T\mathbb{F})^{-1}\,\mathbb{F}^T\Delta u$. For the Gauss-Newton method, the computational time is the summation of the cost for forward modeling, steepest-descent and Newton directions calculations. Assuming that the dimension of the model is *N,* the computational time for a frequency domain solver for a single forward modeling in 2D is $N^3$. Since the number of shots (receivers) is proportional to *N*, the complexity for the total forward modeling is $N^4$. In 2D, the velocity field has $n = N^2$ components and the dimension of the data is $m = n_{source} \times n_{receiver}\sim N^2$. Consequently the computational complexity of the steepest-descent and Newton directions is $m \times n\sim N^4$, the same as the total computational cost for forward modeling. In 3D, the number of shots (receivers) is proportional to $N^2$ and for each shot the computational cost reaches $N^6$. Together, the computational complexity for FWI in 3D reaches $N^8$(Table 1). Let us assume that the dimension of the problem is $N\sim O(10^3)$, therefore the number of operations that we need to execute for the 2D acoustic FWI with constant density is $10^{12}$ Flops=1 TFlops. Therefore, FWI for 2D acoustic acquisition is still practical (Butzer et al. 2013), but not for 3D acquisition, since we approximately need $10^{24}$ Flops=1 YFlops. This is far beyond the power of current supercomputers. Now, let us see how many qubits in a scalable quantum computer can solve these problems. We can run a 2D acoustic FWI with a quantum computer with $\log_2 10^{12}\sim40$ qubits. This is the kind of universal quantum computer that is presently available. However, the 3D FWI problem is intractable even for current quantum computers: to solve this problem we need an error-free quantum computer with $\log_2 10^{24}\sim80$ qubits (the largest available quantum computer at this moment has 50 qubits).

To estimate the number of required physical qubits to correct errors for this problem, we need to design and analyze the quantum algorithm in detail. Let us calculate the computational cost of 3D FWI for an ideal case with full spatial coverage of sources and receivers every 30 m in each direction for a surface domain 3km×3km. In each lateral direction, we have $10^2$ sources (receivers) and in total the acquisition consists of $10^4$ sources (receivers). If a time sampling of 2ms is used and each receiver measures 1000ms of data, this is equivalent to 500 data points per receiver. If we use high-resolution cube grid cells of size 27m$^3$ for the acoustic case, we need to recover $10^9$ velocity values. To apply the conjugate gradient method for FWI, we must model a Fréchet kernel of size $(10^4 \times 10^4 \times 500 \times 10^9)\sim5 \times 10^7$ TB. Ideally, this amount of data should be saved on memory to be used during each conjugate gradient iteration. The largest computer memory built by HPE, is 160TB. It is evident that there is no physical memory available to handle such a huge amount of data, as result a perfect 3D FWI even for acoustic media with current supercomputer capabilities is not practical. However, even a small quantum computer can solve this expensive problem with only $\log_2(5 \times 10^{19})\sim65$ qubits. Frequency domain forward modeling has advantages over time domain modeling if the number of iterations times the

number of frequencies is much less than the number of time.

| Modeling | Time domain | Frequency domain |
|---|---|---|
| 2D | $\boldsymbol{n_s n_t O(N^2)}$ | $\boldsymbol{n_s n_\omega\, O(N^3)}$ |
| 3D | $\boldsymbol{n_s n_t O(N^3)}$ | $\boldsymbol{n_s n_\omega\, O(N^6)}$ |

Table 1. Computational cost of the forward modeling in time and frequency domain.

| Method | Complexity |
|---|---|
| Gauss elimination | $O(\boldsymbol{N^2})$ |
| Jacobi/Gauss-Seidel iteration | $O(\boldsymbol{N^2 \log \epsilon})$ |
| Conjugate gradient | $O(\boldsymbol{N^{3/2} \log \epsilon})$ |
| Nested dissection | $O(\boldsymbol{N^{3/2}})$ |
| Alternating-direction iteration | $O(\boldsymbol{N \log N \log \epsilon})$ |
| Multigrid (iterative) | $O(\boldsymbol{N \log \epsilon})$ |

Table 2. Computational complexity of the classical solvers for Helmholtz equation in terms of size of dimension of model *N* and error $\boldsymbol{\epsilon}$.

## QUANTUM FORWARD MODELING ALGORITHMS

Recent developments in quantum algorithms promise efficient quantum solvers for high dimensional linear systems of equations with potential applications in diverse fields such as machine learning, signal processing, and others which are important for the geosciences. The most recent algorithm called HHL (Harrow et al. 2009) demonstrates the inversion of $N \times N$ matrix $A$ in run time $O\left(\frac{1}{\epsilon} s^2 \kappa^2 \log N\right)$ to solve $\mathbf{x} = A^{-1}\mathbf{b}$, where $\kappa$ is the condition number of matrix $A$, i.e. the ratio between the largest and smallest eigenvalues of $A$; $s$ is the number of nonzero entries per row and $\epsilon$ is the acceptable error for the output, i.e. the maximum allowed distance between the solution and the true result. The best general purpose classical matrix-inversion algorithm, the conjugate-gradient, has a run time of $O\left(Ns\kappa \log\frac{1}{\epsilon}\right)$. Therefore, the HHL algorithm offers an exponential speed up in terms of the size of the linear system. However, there is a restriction on the condition number $\kappa$ that must be scaled poly-logarithmically with the size of the matrix ($\kappa \sim \text{polylog}(N)$) (Childs et al. 2017). Although the HHL algorithm is faster than classical algorithms in terms of $N$, it is linearly slower in sparsity $s$ and condition number $\kappa$, and exponentially slower in precision number $\epsilon$. Recently it has been shown that for dense matrices with $s \sim N$ the running time to invert a matrix is $O\left(\frac{1}{\epsilon}\kappa^2\sqrt{N}\log N\right)$ (Wossnig e al. 2018). Several HHL experiments have been proposed to solve small-size matrix inversion problems using the currently-available technology Optical (Barz et al. 2014) and Superconducting Quantum Processors (Zheng et al. 2017). The HHL algorithm has also been implemented to solve the Poisson equation in $N$-dimensions. Other related work has been done for solving finite element problems by means of quantum algorithms. In addition, based on the HHL algorithm, several proposals introduced machine learning methods to solve such problems (Ciliberto et al, 2018), e.g., implementation of quantum linear regression for pattern recognition (Wang, 2017).

## Conclusions

While future scientific applications of quantum computing have been considered quite widely, its potential in geoscience has so far been largely unstudied. A basic question regarding any kind of quantum algorithm is how much faster it can be compared to the most efficient classical algorithms. Quantum computers do not offer exponential speed up for every classical problem. For example, a quadratic speed-up in search space size is predicted for a database search problem. However, for integer factorization in prime factors quantum algorithm runs exponentially faster on a quantum computer. Recently, a quantum algorithm to solve a linear system of equations with a running time exponentially faster than the best classical algorithm has been formulated. This algorithm suggests the same speedup for seismic wave modeling. With the recent breakthroughs in the construction of the universal quantum computer (IBM) and quantum simulator (D-wave), we anticipate quantum computation to expand, and be realized in computational methods in geoscience, including, e.g., 3D wave modeling and full waveform inversion.


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