

A Medical Informatics View of Quantum Computation

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Abstract

Many medical centers lack access to the parallel-computing capability that is now needed for large-scale, genetic diagnostic information. Such enhanced computer resources are also needed for recent diagnostic physiological model simulations, and for enhancements in medical imaging. Increases in classical parallel processing capability are incremental and expensive. Quantum computing is the only new computing method that promises a very-large increase in parallel-processing capability. The reason is that the classical-computing unit of information, the 0-bit, or the 1-bit, is replaced by the quantum qubit unit which can be superposed as multiple strings of 0's and 1's. Medical-center research units may also need enhanced parallel computing ability for genome research, protein structure prediction, and the use of new simulations of physiological models. It is suggested that health-research funding and collaboration needs to be directed towards the final development of large-scale quantum computing.

Key Words: medical computing, medical informatics, high-performance computing, quantum computation

NeuroQuantology 2011; 1: 202-205

Introduction

Successful completion of the development of large-scale Quantum Computers (QCs) is important for some domains of medical informatics, medicine, and biomedicine which now need more powerful parallel-computing resources. In biomedicine, the advances in rapid sequencing of DNA (ten Bosch and Grody, 2008; Tucker, Marra and Friedman, 2009) are restricted by inadequate access to powerful, parallel-processing, capability. The same is true for computer processing of the three-dimensional structure of the folding, and the active-sites, of proteins from the amino-acid sequences (Freed, Sosnick and Wilde, 2010; Raman *et al.*, 2008).

The US National Institutes of Health (National Institute of General Medical

Sciences) is already giving some support to QC, and to a few quantum-information projects. The main purpose of the present paper is to indicate how integrated research projects, in medicine and quantum computing, might enhance and accelerate the development of both general-purpose, and specialized, large-scale QCs.

The unique importance of QC lies in the superposition properties of its processing units, the entangled 'qubits', while the classical computer units, the '0-bit' and '1-bit', do not entangle or superpose. Consequently, the QC has very much greater parallel-processing capability than the classical computer. There is now a world-wide effort, by physicists, to build large-scale QCs. This is a difficult task, but there have been more than enough successes with QCs using 7 qubits, or less, to ensure that, generally programmable, and specialized large-scale QC can be built (Ladd *et al.*, 2010; Knill, 2010; Wilczek 2000). This is also the conclusion of detailed evaluations of

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Received 0000, 2011. Revised 0000, 2011. Accepted 0000, 2011.

the earlier QC research in USA (QIST v2.0, 2004) and in Europe (QIPC v2.0, 2004). The highly developed theory of QC continues to play an important role in development. Early successes include Shor's, (1996) quantum algorithm for factorization of large numbers, which runs successfully on several different kinds of small-scale QCs. This success, stimulated further the development of larger-scale QCs. Quantum large-number factorization is already in use in some commercial quantum-cryptographic communication systems (Poppe, Peev and Maurhart, 2008). Two other early quantum-search algorithms (Deutsch and Jozsa, 1992; Grover, 1997) run exponentially faster than any possible deterministic algorithm on classical computers.

The Physical and Programming Requirements of a Quantum Computer

Five basic physical requirements for quantum computers, and two more for quantum networking, were summarized by DiVincenzo (2000). The early 2-way reversible ("circuit" or "network") QC acts on the data by passing the qubit information through a sequence of logic-gate operations. A more recent measurement (also called "one-way") QC method proceeds differently (Briegel *et al.*, 2009a, b). A small classical computer provides the data and the program to a previously-prepared 2-D cluster state of highly entangled qubits. A sequence of single-qubit measurements are then started on selected qubits of the cluster. Each measurement is modified by the results of the preceding step. Finally, the outputs of each branch of the computation are sorted and aggregated. Even though the steps of the measurements occur randomly, the final computation result is determined correctly by the program.

A recent promising approach is to use photons as the qubits in the Linear Optics Quantum Computation (LOQC) method, described in the following section. This approach is based on the simplified "one-way" quantum-computer cluster state (Raussendorf and Briegel, 2001).

Linear Optics Quantum Computation and Communication

It has been shown that a QC can be built using only the components of linear optics, single-photon sources, and single-photon detectors (Kok *et al.*, 2006; QIPC, 2008). It was found that the lack of direct photon-photon interactions does not prohibit QC scalability as was previously *thought* (Knill, Laflamme and Milburn = 'KLM', 2001). Additional photons are used to operate the logic gates, but they are not part of the computation. One advantage of photon qubits is that they are almost entirely free from the loss of their information by decoherence. The LOQC methods further exploit measurement-based, quantum computing methods. Linear optics devices, such as mirrors or polarizer's, can be described by simple Hamiltonians, which allow the equations of motion to be linear. A considerable simplification is achieved by interacting with the photonic qubits of the cluster by the measurement procedure itself. LOQC uses the KLM architecture as described in the US Quantum Computation Roadmap (QIST, 2004), in Section 6.5 (Optical Approaches).

Such single-photon approaches as LOQC will benefit in scalability from the development of entangled, light-emitting diodes (Salter, *et al.*, 2010). A quantum dot which emits single pairs of entangled photons, is embedded in a semiconductor light-emitting diode (LED).

Optical Quantum Network and Quantum Memory

High-performance computer clusters are sometimes used to download the rapidly growing genome data from the Internet archives. The Cloud has been suggested for intermediate storage (Stein, 2010), however, as far as possible, it is desirable to hold the current genomic data locally rather than to totally rely on Cloud storage. The Cloud may partially, or completely, lose the data, if, for any reason, the storage service becomes unavailable. The Cloud may also have insufficient privacy, security, and robustness to install patient medical data, or identifiable genomic data, even if the data is encrypted by the usual classical-computer methods. Quantum computing can potentially store very large amounts of data using superposed qubits. The local storage can remain

completely secure by limiting the access to it by using a local quantum network.

Most problems of both optical quantum networking and quantum memory have been worked out in the use of QC for perfectly-secure networking (Poppe, Peev and Maurhart, 2008). Such long distance quantum communication requires quantum-repeater memory units. Current quantum-memory units are beginning to show good fidelity and lifetime of the data, by using atoms trapped in an optical lattice, or in a photonic chip (Devitt, Munro and Nemoto, 2008; Lvovsky, Sanders and Tittel, 2010; Nunn *et al.*, 2010).

Discussion

Reliance on Moore's Law (the number of transistors on a chip doubles every two years or so) to predict the computational power of petascale, and future, classical computers is coming to an end. The very-reduced, molecular size of current transistors now requires the use of probabilistic-quantum mechanical physics, rather than deterministic-classical physics. Error correcting QCs need thorough investigation as an alternative approach for meeting the current medical/biomedical needs for increased parallel-computing power. Consequently, leaders in medicine and biology could assist in QC development by organizing more grant support for both general and project-specific QCs, both nationally and internationally. At the very least, a new medical roadmap needs to be formulated that updates and evaluates the US (QIST, 2004) and the EU (QIPC, 2004) roadmaps.

An example of the need, as already mentioned, is the new massively-parallel sequencing of DNA. The same section of DNA is multiply scanned in a parallel manner. The sequence data must then be assembled using the most powerful parallel-computer machine available. International collaborations of large-scale sequencing centers are now generating terabytes of sequenced data, at high speed, and with low-cost per sequence (Feero, Guttmacher and Collins, 2010). The medical benefits of the dramatic increases in scale and scope of DNA sequencing, include recognition of the large number of genes involved in common,

multi-factorial diseases, such as hypertension and atherosclerosis. The detection of mutant breast-cancer BRCA genes can be life saving (ten Bosch and Grody, 2008). Other medical benefits include enhanced Grover (1997) type quantum algorithm searches of the very-large medical databases that are now used by national health services.

As also mentioned, structure prediction of proteins from amino-acid sequences also has to rely on petascale, or other high-performance computing. Often, functionally important proteins are insoluble in their natural state (e.g., membrane receptors), or if they are soluble, cannot be crystallized. Hence structure determination by X-ray diffraction or NMR analysis is excluded. Membrane receptor structure is needed in the search and development of new pharmaceuticals, and they play important roles in many physiological and pathological mechanisms (Shrivastava, Pardasani and Malik, 2010). Computational structure determination of proteins is needed using the basic amino-acid sequence, assisted by the incorporation of similar portions of previously determined protein structures.

Correct folding into the intended shape is needed for each specific protein function. Without it the protein is either inactive, the cause of an allergy, or a degenerative disease. The complex configuration of large proteins requires more powerful parallel, atomic-level computing than is readily available. Without it, calculation of the minimum free energy of each conformation cannot be made to validate the correct structure, for a given function, or for binding to one of its receptors. As of December 2008, 47,132 protein structures had been solved by X-ray crystallography, 7,627 by Nuclear Magnetic Resonance (NMR), and none by computation alone. Currently, computed structures of average-to-large molecular weight proteins are not credible unless there is additional wet-structure information (X-ray or NMR) (Li, 2010).

QC is suggested as a possible solution to this problem since classical computing is only improving incrementally, and X-ray diffraction requires the protein to be

available in a crystalline form (Harris and Kendon, 2010).

Conclusions

It has been proved that several different approaches to building large-scale quantum computers (QC) are possible but the technical problems are severe. Some important medical and biomedical advances

are being held back by a lack of ready access to more powerful classical-computer resources. A boost is recommended in funding and collaboration to realize programmable QCs as soon as possible. This objective will also be facilitated by new evaluation and roadmaps for the more recent QC developments.

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