Basics of Quantum Physics

Possible Medical and Biomedical Uses of Quantum Computing

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Abstract

There is now abundant experimental evidence available to indicate that large-scale Quantum Computing (QC) is feasible. QC uses entirely different physical principles to those used by the classical computer. It depends on several characteristic quantum properties. These properties include quantum bit ("qubit") and entanglement where the states of two or more atomic particles influence one another. The information about these states can overlap and provide the very large parallel-computing power of the QC. The objective of the present report is to summarize the status of the development of QC, and to suggest medical domains that will most benefit by the substitution of QC for classical high-performance computing.

Key Words: quantum computing, quantum mechanics, medical computing, computer science

NeuroQuantology 2011; 3: 596-600

Introduction

In the last few years, several kinds of biomedical and medical data have greatly increased in volume and scope. DNA sequencing improvements have reduced the cost, and increased the throughput, of genome sequencing by more than three orders of magnitude (Tucker, 2009). Also, the challenge of obtaining the atomic-level, 3-dimensional structure of proteins from their amino-acid sequences remains largely unfulfilled (Raman, 2008). There is now an urgent need for access to large-scale, parallel computing in order to bring this new information into clinical use. I focus on quantum computing (QC) because it is based on entirely different (wave mechanical) principles from the classical (conventional) computer. In particular, the quantum bits (qubits) can be overlaid (superposed) and the information on many qubits can be simultaneously processed, thus providing a large increase in parallel computing capability over that of the classical computer. No other new- computer approach is known to intrinsically possess this level of parallel-processing capability.

In the following sections I first review advances in parallel computing with classical (conventional) computers, then the status of the realization of practical quantum computers (QCs), then the simulation of QCs on classical computers, followed by the simulation of complex quantum systems on QCs, and, finally, in the Discussion, I review the biomedical domains most urgently in need of the massively-parallel capabilities of the QC.

Advances in the parallel-computing of classical computers

Nowadays, supercomputers may use hundreds of thousands of core processors. Programs must be modified to obtain full benefit from the processors. Multiple Instruction Multiple Data (MIMD) algorithms are included in order to send load-balanced data streams to all local, or grid-distributed, processors. In load

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Received June 23, 2011. Revised June 30, 2011. Sept 9, 2011.

balancing, data streams are adjusted in size so that the concurrency of processing is optimal (Barney, 2010). As of May 2010, the fastest supercomputer, world-wide, is the AMD Opteron-based CRAY, XT5 Jaguar. This is a massively-parallel computer cluster at the US Oak Ridge National Laboratory (Barney, 2010). Leaving aside the limited access and the expense, such supercomputers have not solved the Technical problems of providing atomistic models of proteins from the amino acid sequence. The number of computer processes increases exponentially, with the number of atoms in the molecule. Only the smallest molecules can be modeled at the atomic level (Li, 2010). The atomic level is necessary in order to compute the minimum energy of different, possible natural conformations.

Quantum computing (QC)

QC offers a much larger increase in parallel computing capability over that of supercomputers. The bits of all classical computers take either '0', or '1', but not both. The bits of the QC (called "qubits"), can superpose (overlay) whole groups of '0', and '1', and can process all of these groups simultaneously. The operation of a QC involves first, initialization of qubits in the register (a portion of memory directly linked to the core processor) and then routing the qubits to arrays of quantum-logic gates. The quantum logic gates are analogous to the logic gates of classical computers. They produce single binary outputs from the net logic value of each group of qubits in the register, as selected by the quantum algorithm (or software). There have been a number of successful realizations of QCs with a limited number of qubits (2 to 5). Some very successful quantum algorithms have been written that solve certain problems that cannot be solved on the classical computer. Foremost of these is the Shor algorithm for factoring of large numbers (Shor, 1994). Also, the Grover algorithm searches for objects in very large unstructured collections of data (Grover, 1997). The success of these, and other quantum algorithms on the newly-developed small-scale QC gave a large stimulus to the world-wide development of QCs and quantum algorithms.

Up to recently, the superposition capability of qubits was entirely attributed to the quantum process of entanglement. Entanglement occurs when atomic particles which are local (close together) experience a quantum change in state (e.g., in energy or spin). For a limited time (the coherence time), the particles remain interdependent, even if they separate. A reversal of spin of one entangled qubit immediately flips the spin of the other. However this local interference is now being reexamined. Quantum information processing, including the speedup of quantum computing, involves a second factor called "Quantum Discord (QD)" which can operate even if entanglement is not present (Fanchini, 2010).

Successes in practical realization of small-scale QC covers a wide-range of different experimental physical approaches. Ladd, and coworkers, classified them in the following way: (1) using photons as the qubits; (2) using trapped atoms as the qubits; (3) using nuclear magnetic resonance with nuclear spin as the qubits; (4) using 'quantum dots' (microscopic semiconductors with characteristic shapes and trapped-electron behaviors) and various dopants in solids (usually elements trapped in silicon lattices); (5) using free electrons in superconductors as qubits; and (6) using other technologies. They conclude that, at present, there is no single approach that is obviously ahead of the others (Ladd, 2010).

As an example of the above 'class (1)', using photons as qubits (Devitt, 2009), designed a QC with arrays of uniquely designed photonic silicon chips which operate at room temperature. When inexpensive photonic qubits are used for the QC, they can be protected from several kinds of decoherence errors. It is believed that high-fidelity factory manufacture of these photonic chips will soon be possible. In related work, experimental success has already been obtained with an optical implementation of the Shor factoring algorithm, using five photon qubits (Politi, 2009). Some high-performing photonic QCs have used modified diamonds containing clusters of selected interstitial atoms or selected crystal-lattice defects. The use of other room-temperature solids, with trapped

atom-particle clusters, have been described (Naumann, 2010).

Super-conductive chip QC has been tested to pseudo-model the large, fast, neural networks of the brain. Several different types of fast-switching Josephson-Effect chips are giving promising results. In nature, the brain appears to have already solved the qubit decoherence problem since its warm, hydrated environment is always present. The mechanism of this is not yet understood. The Josephson Effect refers to the current flow between two superconducting layers which are separated by a thin insulating barrier. These artificial-neuron models show simulations of action potentials, refractory periods, and firing thresholds that are characteristic of live neurons (Crotty, 2010).

Simulating QC on classical computers Ouantum algorithms

While awaiting the final development of large-scale QC, we can simulate QC on classical computers. Richard Feynman pointed out that computers would be far more efficient if they made use of the properties of quantum bits (qubits) instead of classical bits (Feynman, 1982). Some portion of this improvement may be recoverable using simulations of QC on classical supercomputers but possibly due to QD (Quantum Discord), not entanglement. Many QC simulator programs have been developed and also high-level quantum programming languages (Quintiki, 2010). The QCL programmable simulator (Hunting, 2001), allows a choice of the number of simulated qubits. However, the required memory increases exponentially with the number of qubits used. The program also provides choices for the sequence of functions of selected logic gates. A simulated QC is useful for development of quantum algorithms. Many quantum algorithms involve the quantum version of the Fourier Transform – QFT, as used in the Shor algorithm (Griffiths, 2007; Browne, 2007), or derive from Grover's search algorithm (Grover, 1997). More recently, many new quantum algorithms depend on quantum random walks which relate to the classical random walks used in statistics (Random walk, 2010).

Quantum chemistry requires precise information about the electronic structure of atoms and molecules. The quantum chemistry can be explored using a simulated quantum computer (Kassal, 2010). The processing time for computing the energy of atoms and molecules scales exponentially with system size on a classical computer but polynomially if quantum algorithms are used (Aspuru-Guzik, 2005). Simulation of QC on classical computers is limited by the exponential scaling of the Hilbert (extended Euclidian) space of a QC with the number of qubits used. The computer memory is quickly used up. De Raedt and collaborators (De Raedt, 2007), have developed Fortran 90 QC simulation packages that run on a series of supercomputers, using up to 36 qubits (depending on the available memory), and with up to 4096 processors in particular supercomputers It is much more efficient to simulate complex quantum systems on a QC.

Simulation of complex quantum systems and quantum chemistry on a QC

The examination of quantum chemistry or a quantum physics phenomenon requires detailed description in 2-dimensional or 3-dimensional Hilbert (extended Euclidean) space. As mentioned, this description step often requires excessive classical-computer memory. Feynman pointed out that if the quantum system is simulated on a QC there is no such problem because the space description is included in the qubit information (Feynman, 1982). This has been tested for small molecules, using a QC simulation on a classical computer using 4 qubits. The accuracy obtained was barely sufficient. Precise results would require tens to hundreds of qubits (Aspuru-Guzik, 2005).

Discussion

Establishing the configuration of folded proteins from the amino-acid sequence depends on accurate calculation of the minimum energy for different possible conformations (Dill, 2008). In initial steps, QC graphics imaging should provide an approximation to the global optimum for the assignment of hydrophobic- and polar-amino acids in a cubic search space. At present, the search is limited to less than 30

residues. In a few ways, QC simulation is also proving useful (Perdomo, 2008). A current drug discovery project is being conducted on an IBM System BlueGene/L supercomputer. The project screens libraries of millions of compounds for their molecular docking with particular cell receptors (Peters, 2008). High-throughput validation for this drug-discovery project used the DOCK program, after optimizing for load balancing to the very large number of processors on this computer.

The present high-speed parallel-sequence methods usually involve fragmentation of the DNA to provide "short reads" of sequences of less than 100 base pairs each. To obtain the complete DNA sequence, parallel-processing algorithms are required to match, to insert spaces, and join the short sequences back together. An even larger parallel-processing computing load involves comparing thousands of genotypes and phenotypes to each other in order to learn the clinical significance of sequence variations (Venter, 2010).

Large-scale parallel computer processing is needed for evaluating some quantum-assisted applications of medical images (Tolxdoff, 2009). The medical imaging capabilities may include acquisition, registration and fusion, visualization and simulation, segmentation and validation, image-guided surgical intervention, and the use of physical phantoms. Content-based medical-mage retrieval often needs multi-core based parallel classical computing (Chen, 2010). The essential image details are identified, classified, and compared with other related images for diagnosis or grading of the condition. Often the image comparisons need to be carried out in vector space. A start has been made in processing images using QC methods. In classical computing, much descriptive information must be stored in memory. However, for QC, this information is included directly by the qubits (Chen, 2010; Venegas-Andraca, 2010). Other QC work on images has concentrated on developing a flexible representation of quantum images (FRQI) for use in medical image processing (Le, 2010).

The status of quantum-assisted bio-molecular modeling has been reviewed (Harris, 2010). The authors anticipate that the ability of the QC to compare several different promising molecular conformations simultaneously is the key advantage. This approach could apply, for example, to the protein-folding problem, or to the search for new drugs using docking algorithms (Harris, 2010).

Conclusions

Development of large-scale QC is underway worldwide (Parsons, 2011). Working small-scale QCs have been demonstrated using up to 5 qubits. Large-scale QCs need hundreds, or thousands of qubits. A review of classical supercomputing shows that the QC is the only approach able to provide massive parallel-computing capability. Without QCs, new DNA sequencing data, the learning of the specific activities of the folded conformations of proteins, and the search for new drugs by docking algorithms, are being held back from full clinical application.

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