Nanoscale Simulation by Quantum Computation

(NSF Nanoscale Modeling and Simulation Grant 0085557)

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Project Summary: As devices become smaller and smaller, they approach the scale at which their dynamics must be described by quantum mechanics. The quantum-mechanical nature of nanoscale systems brings both problems in the form of quantum noise and fluctuations, and opportunities in the form of novel methods for control and information processing. This proposal focuses on one of the most promising of opportunities for nanoscale modeling and simulation: quantum simulation by quantum computers.

Quantum computers are devices that process information in a way that preserves quantum coherence. Prototype quantum computers have been realized experimentally and larger `second-generation' quantum computers are currently being constructed. Quantum computers are uniquely suited for performing nanoscale simulations.

Nanoscale systems, though small, consist of many parts. The interaction between those parts is governed by quantum mechanics. The difficulty of simulating such systems on a classical computer increases exponentially with the number of parts. In 1982, however, Feynman noted that a quantum computer might be able to perform quantum simulations much more efficiently, so that the difficulty of simulation increases only linearly with the number of parts. In 1996, the PI of this proposal showed how Feynman's proposal could be put into practice. In 1998, the co-PI demonstrated the power of quantum simulation experimentally by using nuclear magnetic resonance (NMR) to construct a special-purpose quantum simulator capable of performing simulations far too difficult for any classical computer.

The proposed NSF research program will construct, program, and operate quantum simulators. Quantum simulators are essentially `analog' quantum computers that are programmed to mimic the behavior of another quantum system. In the first stage of the research program, quantum simulations will be performed on existing liquid-state NMR quantum computers and on special purpose solid-state devices. In the second stage, general-purpose, large-scale simulations will

be performed on the large-scale, solid-state, NMR quantum computers being constructed at MIT with separate (non-NSF) funding. These simulations will investigate the properties of chemical and physical systems, ranging from molecules to bulk spin systems, concentrating on issues of information propagation and processing, including examining quantum mechanisms for entropy production, decoherence, and chaos. In addition to generating algorithms for simulating such phenomena, the program will develop methods for using dynamic quantum models to manipulate and control nanoscale quantum systems.

Program Description: Modeling nanoscale systems is hard. In part, this difficulty arises because nanoscale systems are small. As a result, they are hard to measure; they are subject to large fluctuations; they frequently consist of too few parts to apply conventional statistical mechanical techniques. In addition, nanoscale systems are sufficiently small that their dynamics
must be described at least in part by quantum mechanics. In another sense, however, nanoscale systems are hard to model because they are big. Nanoscale systems consist of many atomic scale parts. The interaction between these parts is a complex quantum many-body problem which is hard to model on classical computers.

It is straightforward to understand why many-body quantum systems are hard to model on a classical computer. Consider a quantum system made up of N subsystems, such as spins. If each spin has two distinct quantum states, the system as a whole has 2^N distinct quantum states. The state of such a quantum system is described by a vector in a 2^N dimensional complex vector
space. Accordingly, just to write down the state of such a system requires 2^N numbers, and to evolve the state forward in time one needs to exponentiate a 2^N by2^N matrix. This is a hard problem. For N=10, it's not so bad: the system lives in a 10^{24} dimensional space, and the time evolution requires the exponentiation of a 10^{24} by 10^{24} matrix. For N=20, however, the system lives in a million dimensional space; for N=30, the system lives in a billion dimensional space; etc. For N=300, the system lives in a space with more dimensions than there are elementary particles in the universe. Clearly, simulating such a system on a classical computer is a hard problem: one cannot even write down the state of a many-body quantum system, let alone determine its dynamics.

Of course, classical simulations of many-body quantum systems can been often be done by making educated guesses to simplify the state description and dynamics. For simulation of nanosystems at the large end of the nanoscale (100nm), for example, semiclassical techniques often suffice. As nanosystems become smaller and smaller, however, quantum effects become more and more important. At the small end of the nanoscale, and for complex quantum systems in general, however, it is often not possible to perform direct simulations on a classical computer.

Simulating complex quantum systems at the nanoscale using classical computers is hard. But what happens when the computers used to perform the system are themselves quantum mechanical systems? The idea of quantum simulation was first proposed by Richard Feynman in 1982 (1). Feynman noted that simulating quantum dynamics on classical computers was intrinsically hard, as above: the memory space and processing time required to perform the simulation grows exponentially with the size of the quantum system to be simulated. He went on to suggest that this difficulty might be overcome by performing quantum simulations on devices --quantum simulators -- that required resources of memory space and processing time that grew only as a small polynomial in the size of the quantum system to be simulated. Essentially a quantum simulator operates as an analog computer: it is a quantum system whose dynamics can be programmed to mimic the dynamics of the quantum system of interest.

In the year 2000, the problem of quantum simulation is of even greater interest than in 1982. Now, as then, large amounts of classical supercomputing time are spent on simulating quantum
systems. Now, however, the range of quantum systems that are targets for simulation is vastly expanded. As Moore's law tests the quantum scale for large-scale device production, the problems of understanding

the dynamics of multi-part quantum systems have attained greater urgency. Although a considerable scientific industry for creating algorithms for simulating quantum systems on classical computers exists, Feynman's basic problem remains: classical simulation of quantum systems is exponentially hard.

In the last few years, the development of prototype quantum computers suggests the possibility of constructing useful versions of Feynman's quantum simulators. In 1996, the PI (S.L.) showed that digital quantum computers were examples of universal quantum simulators, and constructed the first algorithms for quantum computers to perform quantum simulations (2). This was followed by work showing that quantum simulations were the most straightforward type of computation that could be performed by a quantum computer: only a few tens of quantum bits are required to outdo even the most powerful classical supercomputer (3). In 1997, the co-PI (D.C.) carried out the first large-scale quantum simulations using solid state NMR (4). These simulations remain the only experimentally demonstrated example of a quantum computation whose result is too difficult to replicate on any existing classical supercomputer. These special-purpose simulations were followed by universal small-scale simulations in liquid state NMR (5). The PI's research on quantum simulation has been accompanied by research into the use of quantum modeling as a key component in the process of controlling systems at the nanoscale (6).

The goal of the proposed research is to extend the scope of nanoscale simulation by quantum computation to investigate a wide range of nanoscale phenomena and structures. In general, the research program will carry out a multi-scale investigation of the way in which quantum information propagates up from the atomic scale through the nanoscale, focusing on issues of quantum coherence, noise and decoherence. Small-scale, general-purpose NMR quantum simulators will be used to address problems in quantum dynamics of few-body systems. Large-scale, special-purpose quantum simulators consisting of solid-state NMR devices will be used to investigate phenomena associated with the propagation of quantum information over different scales, including many-body quantum coherence, quantum chaos, and decoherence.

Industrial Collaboration: The proposed research will be carried out in collaboration with researchers at IBM TJ Watson Research Laboratory. Dr. David Divincenzo and his co-workers at IBM have worked actively on the field of quantum simulation. Researchers at IBM will be able to carry out quantum simulations of nanoscale systems in collaboration with researchers at MIT, while students funded by the program will benefit from interaction with IBM's strong group in the physics of computation.

References:

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