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Quantum computation for physical modeling

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Foreword

One of the most famous American physicists of the twentieth century, Richard Feynman, in 1982 was the first to propose using a quantum mechanical computing device to efficiently simulate quantum mechanical many-body dynamics [1–3], a task that is exponentially complex in the number of particles treated and is completely intractable by any classical computing means for large systems of many particles. In the two decades following his work, remarkable progress has been made both theoretically and experimentally in the new field of quantum computation [4,5]. Ironically, however, most of the theoretical progress in quantum computing has developed within the purview of the computer scientist with the principle applications of efficient quantum information processing related to cryptography and secure quantum communication.¹ In an effort return to Feynman's original direction, the Air Force Research Laboratory and the Air Force Office of Scientific Research has established a multidisciplinary basic research theme called *Quantum Computation for Physical Modeling* to explore quantum algorithms to model dynamical physical systems. Our goal is to establish a practical and generic means by which the power of quantum mechanics (that is, quantum parallelism due to the superposition and entangle-

ment of states) can be used to speedup numerical simulations of interest to computational physicists.

Notwithstanding the veritable stampede towards computer science related applications by most researchers in the field of quantum computing, a few maverick physicists have developed some quantum algorithms to model quantum mechanical systems. A starting point for this development was a problem posed by Feynman himself to show that the one dimensional Dirac equation could be modeled by a single-speed particle traveling in a two-dimensional space-time as a sum over zigzag paths of straight line elements [6], with the amplitude of a particular path contributing to the kernel by the number of “collisions” or corners along that zigzag path. This *quantum lattice gas* representation of quantum mechanics is equivalent to the well known path integral representation.² A quantum lattice gas accounts for all contributing paths by simultaneously evolving many particles in a unitary fashion. Therefore, instead of summing (or integrating over) paths as individual entities, all contributing paths are effectively simulated in one fell swoop as a combined field quantity. In the end, the collisional interaction between particles in the quantum lattice representation can be described by an effective field theory (the Dirac equation in this particular case) at the large-scale called the *continuum limit*.

Beginning in the mid 1990's, a contemporaneous series of quantum lattice-gas algorithms to model the relativistic Dirac equation, equivalent to Feyn-

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¹ References to specific publications in these subjects are so ubiquitous in the quantum computing literature that we do not include any here. Comprehensive collections of quantum computing papers have been recently published [4,5].

² A solution to Feynman's “quantum lattice gas” problem was published in 1984 by Jacobson and Schulman [7].

man's original algorithm, were published by Succi [8, 9], Bialynicki-Birula [10], and Meyer [11–15]. Furthermore, a series of papers on modeling the non-relativistic Schrödinger equation were published by Boghosian and Taylor [16–18] and by Yepez and Boghosian [19], the latter article appearing in this issue. Our present goal in the Quantum Computation for Physical Modeling project is accelerate this algorithmic developmental effort that has occurred over the past decade.

In fact, we hope to go further in the application of this quantum algorithmic method. We have developed new efficient quantum lattice-gas algorithms to model classical dynamical systems [20–23]. Meyer also addresses this subject in his article on physical quantum algorithms contained in this issue [24]. In the past, we have considered quantum algorithms suited to globally phase-coherent quantum computers [25], however our focus is presently on those quantum algorithms suited to implementation on locally phase-coherent quantum computers that are technologically much simpler to experimentally implement [26]. This program to use one quantum mechanical system to model another quantum mechanical system or classical system can perhaps best be described as efficient analog computing, which in this context may be termed *analog quantum computing*.

The principle technological obstacle to globally phase-coherent quantum computation is the problem of the uncontrolled decoherence of the quantum computer's wave function. The quantum computing community at large, following the traditional computer scientist's mindset for correcting bit-flip errors using redundancy, has been investing much theoretical work in attempts to develop generalized methods for quantum error correction of bit-flip and phase-change errors [27–29]. As an expedient alternative to this cumbersome approach, as demonstrated by the advent of several nuclear magnetic resonance quantum computing experiments [30–33], it is possible to avoid bit-flip and phase-change errors altogether: *Keep the individual quantum computing elements small enough so that all computation occurs within a single spin-spin decoherence time where bit-flip and phase-change errors are irrelevant.*

Given this possibility of avoiding errors, it is natural to consider building a large-scale quantum computing system by connecting many small ones together

in an array interconnected by nearest-neighbor classical communication channels. We call this type of quantum mechanical device a *type-II quantum computer* [26]. This hybrid architecture, combining classical massively parallelism and quantum parallelism, is suited to modeling dynamical physical systems, such as turbulent Navier–Stokes fluids [21–23,25]. In collaboration with the Nuclear Engineering Department of MIT, we have developed a prototype type-II quantum computer based on spatial nuclear magnetic resonance spectroscopy. We use a gradient magnetic field to distinguish individual layers in a liquid sample so that each layer effectively becomes an individual quantum computing node comprising an ensemble of molecules. The first simulation of a quantum lattice-gas model for the one-dimensional diffusion equation [22] has been carried out on this quantum computer prototype using the atomic spin-state of Carbon-13 and Hydrogen nuclei within a linear array of chloroform molecules [34]. This milestone represents the first physical simulation to date on a quantum computer and is contained in this issue. A subsequent paper presenting an improved version of our type-II quantum computer prototype, that corrects for various implementation errors and uses better quantum control, is also in preparation [35].

The rather rapid proof-of-concept achieved by spatial nuclear magnetic resonance spectroscopy of a type-II quantum computer has led to interest in the subject by the Office of the Secretary of the Air Force and the House Appropriations Committee of the US Congress leading in turn to a strong commitment to the field of quantum computation for physical modeling by the Department of Defense. Our new quantum computing research theme is supported by several directorates of the Air Force Office of Scientific Research with about two dozen university research projects across the country to date. The design and construction of several new type-II quantum computer prototypes are now underway using various technologies including superconducting electronics and quantum optics for example.

We have established a new annual workshop series dedicated to this subject of quantum computation for physical modeling (see our web site at <http://qubit.plh.af.mil> for more details). The first workshop in this series was held in the fall of 2000 in North Falmouth in Cape Cod, Massachusetts and the fol-

lowing collections of articles contained in this issue were contributed from this workshop. Our goal for this workshop series is to annually publish a collection of such contributed articles, to review our progress, and to provide an open forum for new collaborators to join us in this activity.

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