Parallel **Si**mulation of **Q**uantum **Co**mputation by **P**ractically **A**diabatic **T**ime-dependent **H**amiltonians (PSiQCoPATH)

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March 17, 2005

1. Intro: Quantum vs Classical Computation

   1.1 Classical Information

   a) The fundamental unit of classical information is the bit $b \in \mathbb{Z}_2$
   b) We can store larger amounts of information by bringing N bits together to form an N-bit register
   c) The state space of such a register is an N-dimensional vector space over the field $\mathbb{Z}_2$, called ${\mathbb{Z}_2}^N$
   d) Data is stored as a particular state of the register, called an N-bit word or "bit string"
      i) e.g. $x = 1010001101110010 \in {\mathbb{Z}_2}^{16}$
      ii) An N-bit register can be set to represent any one of the 2^N possible states of ${\mathbb{Z}_2}^N$

   1.2 Quantum Information

   a) The state of a quantum system is a vector $|\,\psi\,\rangle$ in a vector space $\mathcal{H}$ over the field $\mathbb{C}$
   b) Fundamental unit of quantum information is the qubit $|\,\psi\,\rangle \in \mathcal{H}_2$
      i) $\mathcal{H}_2$ is a two (complex) dimensional vector space spanned by the basis states $|\,0\,\rangle$ and $|\,1\,\rangle$
      ii) e.g. A two-level system such as that of spin-1/2 particle
      iii) Basis vectors are $|\,0\,\rangle$ and $|\,1\,\rangle$, but qubit $|\,\psi\,\rangle$ can be *any* vector $\alpha|\,0\,\rangle + \beta|\,1\,\rangle;\ \alpha, \beta \in C$
   c) Larger amounts of quantum information stored by bringing N such systems $\{\mathcal{H}_2^{(1)}, \mathcal{H}_2^{(2)}, \ldots \mathcal{H}_2^{(N)}\}$ together
   d) The total 2^N dimensional state space ${\mathcal{H}_2}^N = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)} \otimes \cdots \otimes \mathcal{H}_2^{(N)}$
      i) Basis States: $|\,1\,\rangle \otimes |\,0\,\rangle \otimes |\,1\,\rangle \otimes \cdots \otimes |\,0\,\rangle \equiv |\,101\cdots0\,\rangle$
      ii) Thus any classical bit string x can be mapped to a basis state $|\,x\,\rangle \in {\mathcal{H}_2}^N$

   1.3 Classical Computation

   a) Perform an operation $f : {Z_2}^N \to {Z_2}^N$ such that $f(x) = y$

   1.4 Quantum Computation

   a) Operations on quantum systems are accomplished by the action of *linear* operators on $\mathcal{H}$
   b) Analogous operation $\hat{f} : {\mathcal{H}_2}^N \to {\mathcal{H}_2}^N$ such that $\hat{f}|\,x\,\rangle = |\,y\,\rangle$
   c) Canonical basis states are mapped according to action of f on their classical counterparts
   d) Let $|\,\psi\,\rangle = \sum_{x\in\mathcal{H}} \alpha_x |\,x\,\rangle$, then

$$\hat{f}|\,\psi\,\rangle = \sum_{x\in\mathcal{H}} \alpha_x \hat{f}|\,x\,\rangle = \sum_{x\in\mathcal{H}} \alpha_x |\,y\,\rangle$$

      i) Natural perfect SIMD parallelization
      ii) Unfortunately, can only read out one of the answers

iii) Reaping the benefits of quantum power requires more cleverness

2. Adiabatic Model of Quantum Computation

2.1 Models of quantum computation

a) Several equivalent models of quantum computation have been proposed
b) Most natural for computer scientists is the Quantum Gate Array (QGA) model
c) Simulating a QGA is not particularly interesting in terms of gaining any new understanding of quantum physics

2.2 Quantum Computing by Adiabatic Evolution

a) Special operator $\hat{H}$ is the "energy" operator of quantum system
b) Eigenvectors/eigenvalues are the "energy levels" of the system
c) Suppose we can design a system whose Hamiltonian $\hat{H}_p$ encodes an instance of a particular problem
   i) e.g. traveling salesman — energy $\leftrightarrow$ "distance" of a path, eigenvectors $\leftrightarrow$ paths
d) Lowest energy level (ground state) is the solution to the problem
e) In general, we don't know how to prepare this state, but we do know how to prepare the system in the ground state of a simpler Hamiltonian $\hat{H}_0$
f) **Adiabatic Theorem**: Consider a system initially in the ground state $|\,\psi_0\,\rangle_0$ of $\hat{H}_0$. If by changing some external parameters, the system's Hamiltonian $\hat{H}(t)$ is *slowly* and smoothly transformed from $\hat{H}_0$ to $\hat{H}_p$, then the final state of the system will be the ground state $|\,\psi_0\,\rangle_p$, the ground state of $\hat{H}_p$.
   i) e.g. $\hat{H}(t) = (1-t)\hat{H}_0 + t\hat{H}_p,\ t \in [0,1]$
g) Idea: start the system in the ground state of a simple Hamiltonian, then slowly change some parameter to evolve the Hamiltonian into the particular problem Hamiltonian and read out the answer
h) Problem: How slow is "slow enough?"

3. Simulating Adiabatic Quantum Evolution

3.1 Interesting both for quantum computation and general study of quantum dynamics

3.2 Quantum evolution given by Shrodinger equation (SE)

$$i\hbar\frac{d}{dt}|\,\psi\,\rangle = \hat{H}(t)|\,\psi\,\rangle$$

3.3 Naive serial simulation: $|\,\psi(t+\varepsilon)\,\rangle = \left[\mathbb{1} - i\frac{\varepsilon}{\hbar}\hat{H}(t)\right]|\,\psi(t)\,\rangle$

3.4 We can do better with parallel!

4. Parallel Calculation of the Time Evolution Operator

4.1 For any Hamiltonian evolution of a quantum system, can define the Time Evolution Operator $\hat{U}(t,t_0)$ such that $|\,\psi(t)\,\rangle = \hat{U}(t,t_0)|\,\psi(t_0)\,\rangle$

4.2 For time independent $\hat{H}$, SE is solved by $\hat{U}(t,t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$

4.3 For $t_0 < t_1 < t$, $\hat{U}(t,t_0) = \hat{U}(t,t_1)\hat{U}(t_1,t_0)$

4.4 If $\hat{H}(t)$ varies slowly in time, break the interval up into pieces over which $\hat{H}$ is roughly constant.

4.5 Discretized version of complete information about state of the system given by

$$[\mathbb{1},\, U(t_0+\varepsilon,t_0),\, U(t_0+2\varepsilon,\, t_0+\varepsilon)U(t_0+\varepsilon,t_0),\ldots]$$

5. Advantages of Parallel Algorithm

5.1 By re-ordering the calculation (not going on sequence), we can recast it into a variation on parallel prefix

5.2 By focusing on the time evolution operator itself rather than evolving a particular state, we

a) get complete information about dynamical behavior for all possible initial states

b) can take advantage of BLAS-3 matrix-matrix operations

c) would need 2^N runs of serial BLAS-2 code to get same dynamical information

5.3 Hope to simulate up to 9 or 10 qubits

5.4 Can learn about "how slow" is slow enough for quantum adiabatic computation

5.5 Try to integrate recently developed efficient algorithms for systems with low-entanglement