Space-Efficient Simulation of Quantum Computers

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Abstract (for reference)

Traditional algorithms for simulating quantum computers on classical ones require an exponentially large amount of memory, and so typically cannot simulate general quantum circuits with more than about 30 or so qubits on a typical PC-scale platform with only a few gigabytes of main memory. However, more memory-efficient simulations are possible, requiring only polynomial or even linear space in the size of the quantum circuit being simulated. In this paper, we describe one such technique, which was recently implemented at FSU in the form of a C++ program called SEQCSim, which we releasing publicly. We also discuss the potential benefits of this simulation in quantum computing research and education, and outline some possible directions for further progress.



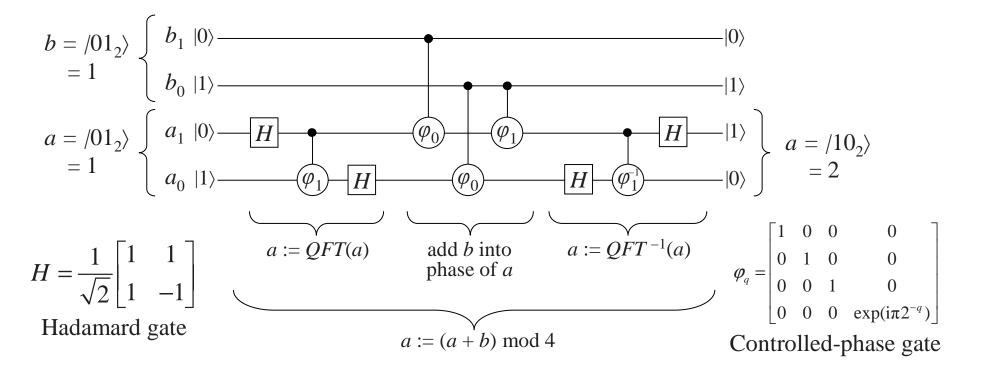
What is a Quantum Computer?

- □ A new, more powerful fundamental paradigm for computing within the laws of physics.
 - Apparently exponentially faster on some problems.
- Some key differences between Classical vs. Quantum Computation:
 - State representations:
 - **Classical:** A sequence of *n* bit values, $w \in \mathbf{B}^n$, where $\mathbf{B} = \{0,1\}$.
 - **Quantum:** A function $\Psi \in \mathbf{H}$, where $\mathbf{H} = \mathbf{B}^n \to \mathbf{C}$, mapping classical states to complex numbers ("amplitudes").
 - Logic operators ("gates"):
 - **Classical:** A function from several bits to one bit, $g: \mathbf{B}^k \to \mathbf{B}$
 - **Quantum:** A unitary (invertible, length-preserving) linear transformation $U: \mathbf{S} \to \mathbf{S}$, where $\mathbf{S} = \mathbf{B}^k \to \mathbf{C}$.
 - Measurement of computation results:
 - **Classical:** Measured value is exactly determined by machine state.
 - **Quantum:** Probability of measuring state as being *w* is $\propto |\Psi(w)|^2$.

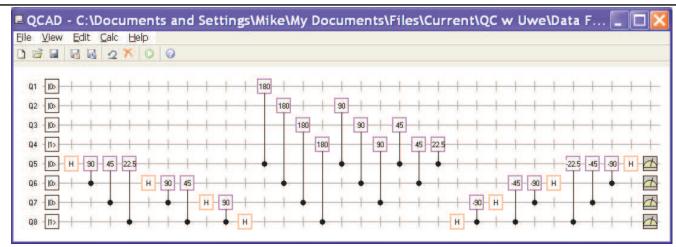
A Simple Quantum Circuit: Draper Adder

FAMU-FSU College of Engineering

Uses the quantum Fourier transform (QFT) and its inverse QFT⁻¹ to add two 2-bit input integers in a temporary phase-based representation. Here it is computing 1 + 1 = 2.



A Larger Draper Adder (2×4 bits)



QCAD tool, by Hiroshi Watanabe, University of Tokyo, available from http://apollon.cc.u-tokyo.ac.jp/~watanabe/qcad/index.html

- □ Some advantages of the Draper adder:
 - Minimal quantum space usage: Requires no ancilla bits for carries.
 - A good simple, but nontrivial example of a quantum algorithm.
- □ A disadvantage of the Draper adder:
 - Slow; requires $\Theta(n^2)$ gates for an *n*-bit add!
 - □ Unlikely to be used in practice, unless qubits are very expensive.



Some Potential Applications of Quantum Computers

- □ If quantum computers of substantial size are built, known quantum algorithms can be applied to obtain:
 - Polynomial-time cryptanalysis of popular public-key cryptosystems (*e.g.*, RSA).
 - Polynomial-time simulations of quantum-mechanical physical systems.
 - Square-root speedups of simple unstructured searches of computed oracle functions.
 - And not a whole lot else!
- A much wider variety of interesting & useful quantum algorithms is needed,
 - But new quantum algorithms are difficult to develop.
 - Need flexible, capabable simulation tools for design validation.



A Problem with Nearly All Existing Quantum Computer Simulators

- □ They require *exponential space* as the number of bits in the simulated computer increases.
 - Why: They update a *state vector* explicitly representing the full wavefunction $\Psi: \mathbf{B}^n \to \mathbf{C}$.
 - \Box This vector contains 2^n complex numbers
 - 1 for each possible configuration of the machine's *n* bits
 - If the available memory holds $1G(2^{30})$ numbers,
 - □ We can only simulate <30-bit quantum computers!
 - The large space usage also imposes a significant slowdown to access main memory or disk.

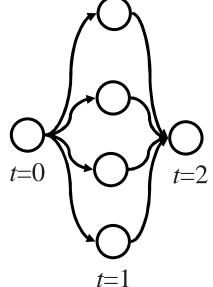


A Way to Solve This Problem

- □ We can reformulate quantum mechanics in an equivalent framework *without state vectors*.
 - Feynman (1942): Any desired amplitude can be computed using a *path integral* expression summing over possible *classical* trajectories.
 - Bohm (1952): Can maintain a *classical* state that evolves under the influence of only wavefunction amplitudes in the immediate neighborhood.
- □ The only real requirement is to obtain the right probability of arriving at each final state!

A Complexity Theorist's View of Feynman's Path Integral

- □ Consider any computation with a wide dataflow graph (uses more space than time)
 - The graph at right uses 4 variables at time *t*=1, but only takes 2 steps.
- We can make the algorithm more space-efficient by recomputing intermediate variables dynamically when needed, instead of storing them.



Bernstein & Vazirani, 1993: Can apply this generic tradeoff to simulating quantum computers (duh).



SEQCSim: The <u>Space-Efficient</u> <u>Quantum Computer Simulator</u>

- □ Core idea was conceived circa 2002 at UF.
 - Adding Bohm updates to Feynman recursion.
 Avoids having to enumerate all possible final states.
- □ A working C++ software prototype was developed and demonstrated at FSU in 2007.
 - Future versions of the simulator will have a more expressive programming interface.
- A performance-optimized FPGA-based implementation is currently being developed.



SEQCSim Input Files for 2×2-Bit Draper Adder

qconfi	ig.txt	form	nat v	ers	sion	1
bits:	4	Dec	lare 1	eg	giste	ſS
named	bitarı	ray:	a[2]	@	0	
named	bitarı	ray:	b[2]	@	2	

qinput.txt format version 1
a = 1
b = 1
Input values to add

qoperators.txt format version 1					
operators: 4					
operator #: 0	Quantum circuit (gate application sequence)				
name: H	Quantum circuit (gate application sequence)				
size: 1 bits qops	seq.txt format version 1				
matrix: open	rations: 9				
(0.7071067812 + i*0)(0.7071067812 + i*0) open	ration #0: apply unary operator H to bits a[1]				
(0.7071067812 + i*0)(-0.7071067812 + i*0) open	ration #1: apply binary operator cPiOver2 to bits a[1], a[0]				
operator #: 1 Operator	operation #2: apply unary operator H to bits a[0]				
name: cZ Gate open	ration #3: apply binary operator cZ to bits b[1], a[1]				
size: 2 bits definitions oper	ration #4: apply binary operator cZ to bits b[0], a[0]				
	ration #5: apply binary operator cPiOver2 to bits b[0], a[1]				
(1 + i*0) (0 + i*0) (0 + i*0) (0 + i*0) open	ration #6: apply unary operator H to bits a[0]				
(0 + i*0) (1 + i*0) (0 + i*0) (0 + i*0) open	ration #7: apply binary operator inv_cPiOver2 to bits a[1], a[0]				
(0 + i*0) (0 + i*0) (1 + i*0) (0 + i*0) open	ration #8: apply unary operator H to bits a[1]				
(0 + i*0) (0 + i*0) (0 + i*0) (-1 + i*0)					
(two additional operators elided for brevity)					



SEQCSim Core Algorithm

// Bohm-inspired iterative state updating.

procedure SEQCSim::run():

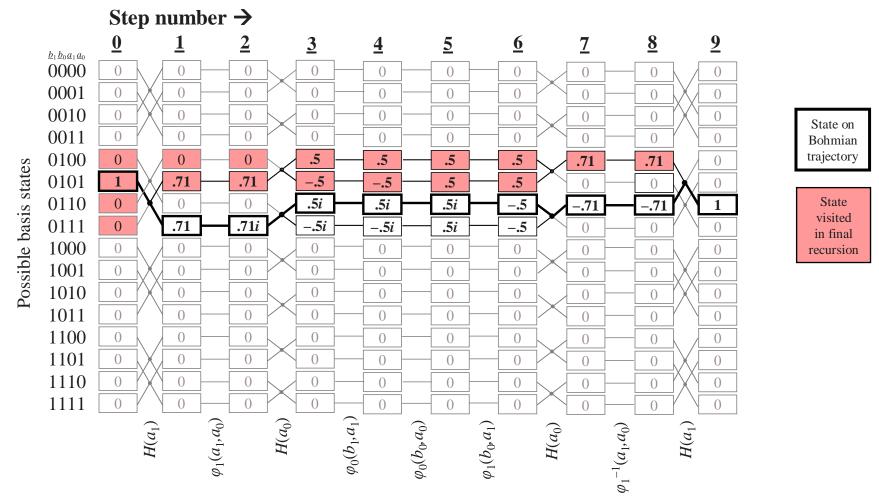
curState := inputState; // Current basis state // Current amplitude curAmp := 1;for PC =: 0 to #gates, // Current gate index (w.r.t. gate[*PC*] operator and its operands,) for each neighbor *nbri* of *curState*, if *nbri* = *curState*, *amp*[*nbri*] :=*curAmp*; else *amp*[*nbri*] := calcAmp(*nbri*); amp[] := opMatrix * amp[]; // Matrix prod. // Calculate probabilities as normalized // squares of amplitudes. prob[] := normSqr(amp[]); // Pick a successor of the current state. *i* := pickFromDist(*prob*[]); curState := nbri; curAmp := amp[nbri].

// Feynman-inspired recursive
// amplitude-calculation procedure.

function SEQCSim::calcAmp(Neighbor nbr): curState := nbr; if PC=0 return (curState = inputState) ? 1 : 0; (w.r.t. gate[PC-1] operator and its operands,) for each predecessor predi of curState, PC := PC - 1; amp[predi] = calcAmp(predi); PC := PC + 1; amp[] := opMatrix * amp[]; return amp[curState];

Complete C++ console app has 24 source files, total size 115 KB

Illustration of SEQCSim Operation on 2×2-Bit Draper Adder





Complexity Analysis

- □ Defining the following parameters:
 - a = const. = max. arity of quantum gates
 - s = width (# of qubits) in simulated circuit
 - t = time (# of operations) in simulated circuit
 - k(< t) = # of *nontrivial* operations in sim'd circ.
- □ For a moderately well-optimized implementation of SEQCSim, we can have
 - Space complexity: O(s + t)Time complexity: $O(s + t \cdot 2^{ak})$



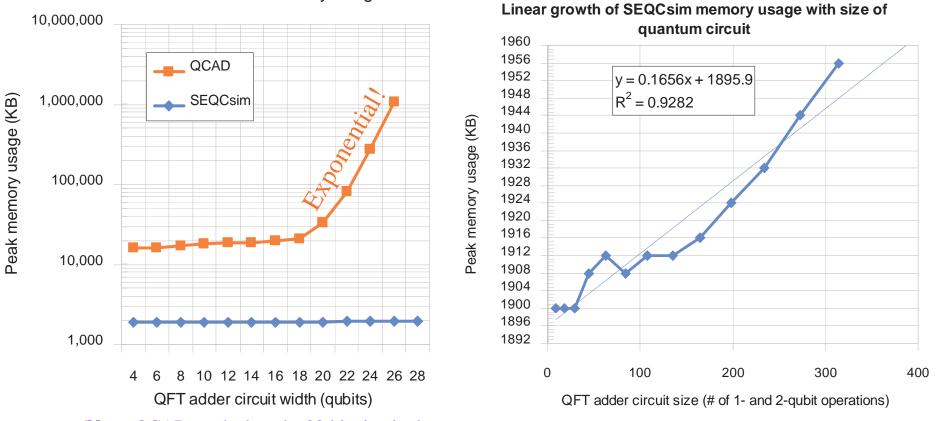
SEQCSim Output on 2×2-Bit Draper Adder

```
Welcome to SEQCSIM, the Space-Efficient Quantum Computer SIMulator.
    (C++ console version)
By Michael P. Frank, Uwe Meyer-Baese, Irinel Chiorescu, and Liviu Oniciuc.
Copyright (C) 2008 Florida State University Board of Trustees.
    All rights reserved.
SEQCSim::run(): Initial state is 3->0101<-0 (4 bits) ==> (1 + i*0).
SEQCSim::Bohm_step_forwards(): (tPC=0)
   The new current state is 3 - 0111 < 0 (4 bits) ==> (0.707107 + i*0).
SEQCSim::Bohm step forwards(): (tPC=1)
   The new current state is 3 \rightarrow 0111 < 0 (4 bits) ==> (0 + i*0.707107).
... (5 intermediate steps elided for brevity) ...
SEQCSim::Bohm_step_forwards(): (tPC=7)
   The new current state is 3 \rightarrow 0110 < -0 (4 bits) ==> (-0.707107 + i*0).
SEQCSim::Bohm step forwards(): (tPC=8)
   The new current state is 3 \rightarrow 0110 < 0 (4 bits) ==> (1 + i*0).
SEQCSim::done(): The PC value 9 is >= the number of operations 9.
                                               -1+1 = 2 = 10_{2}
    We are done!
```



Empirical Measurements of Space Complexity

QCAD vs. SEQCsim memory usage

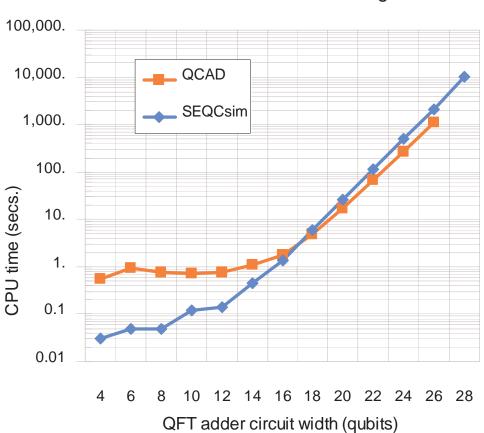


(Note: QCAD crashed on the 28-bit circuit, due to insufficient memory available on the test PC.)



Empirical Measurements of CPU Time Utilization

- SEQCSim is 10× faster than QCAD on small circuits
 - This is probably largely because QCAD has a GUI and SEQCSim doesn't.
- SEQCSim is ~2× slower than QCAD on large circuits.
 - But there is much room for improvement.
 - □ Take better advantage of available memory.
 - Reimplement in specialpurpose hardware



QCAD vs. SEQCsim CPU time usage



FPGA Tools (1 of 5): Altera SOPC Builder

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····· JTAG UART		$ \searrow $	jtag_debug_module	Avalon Memory Mapped Slave		■ 0x01002800	0x01002fff	
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IUART (RS-232 Se		$ \rightarrow $	s1	Avalon Memory Mapped Slave	cik_1	■ 0x01001000	0x01001fff	
Legacy Components			Switches	PIO (Parallel I/O)				
-Memories and Memory Contro		$ \rightarrow$	s1	Avalon Memory Mapped Slave	cik_1		0x0100302f	
⊕ ··DMA			🗆 LEDs	PIO (Parallel I/O)				
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FPGA Tools (2 of 5): NIOS II Soft-Core Configuration

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Core Nios II	í		í	
Select a Nios II core:				
	○Nios II/e	○Nios II/s	⊙Nios II/f	
Nios II Selector Guide Family: Cyclone II f _{system:} 50.0 MHz cpuid: 0	RISC 32-bit	RISC 32-bit Instruction Cache Branch Prediction Hardware Multiply Hardware Divide	RISC 32-bit Instruction Cache Branch Prediction Hardware Multiply Hardware Divide Barrel Shifter Data Cache Dynamic Branch Prediction	
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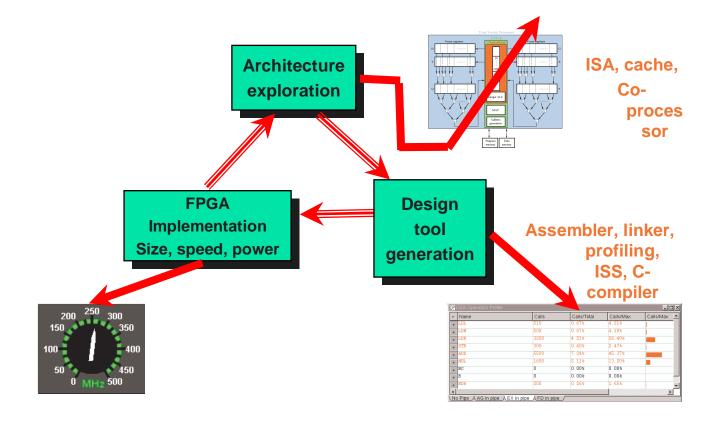
FPGA Tools (3 of 5):

Custom Hardware Generation with C2H

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FPGA Tools (4 of 5): LISA Processor Design Cycle





FPGA Tools (5 of 5): LISA Development Tools

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Conclusion & Future Work

- We have implemented in C++ and validated a working prototype of a quantum computer simulator that uses only linear space.
 - This tool can be useful to help students & researchers validate quantum algorithms.
 - □ Online resources at <u>http://www.eng.fsu.edu/~mpf/SEQCSim</u>
 - □ Contact <u>michael.patrick.frank@gmail.com</u> for source code
 - A future version will provide a more expressive quantum programming language based on C++.
- □ We are also designing an FPGA-based hardware implementation to boost simulator performance.
 - This approach is made much more feasible by the extreme memory-efficiency of our algorithm.