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Space-Efficient Quantum Computer Simulators

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Abstract of Talk (for reference)

A widespread misconception about quantum computing is that simulating a quantum computer on a classical one requires exponential memory resources. In fact, it has long been known that quantum simulation requires only polynomial space, due to general space-time complexity tradeoffs discovered in the early days of computing. The basic approach essentially amounts to the numerical evaluation of a discretized path integral. Furthermore, amplitudes calculated in this way can be used to stochastically evolve a single computational basis state forwards in time in accordance with the precise flow of probability mass through configuration space that is dictated by quantum statistics, in a manner reminiscent of Bohm's "pilot wave" interpretation of quantum mechanics. In this way, we can properly account for interference effects without ever having to compute and store a full state vector.

In this informal talk, we'll briefly review the history of this method, and then discuss some existing and planned future implementations of it. We have already made available the C++ source code for a simple space-efficient quantum computer simulator based on these ideas. A future version will offer a convenient "Qubit" class that automatically executes the space-efficient simulation method behind the scenes, to allow arbitrary quantum algorithms to be directly written in C++ and executed without concern for memory limitations. We also are planning to develop an FPGA-based implementation of the core simulator which could offer speedups of 100x or more over CPU-based implementations.

Talk Abstract

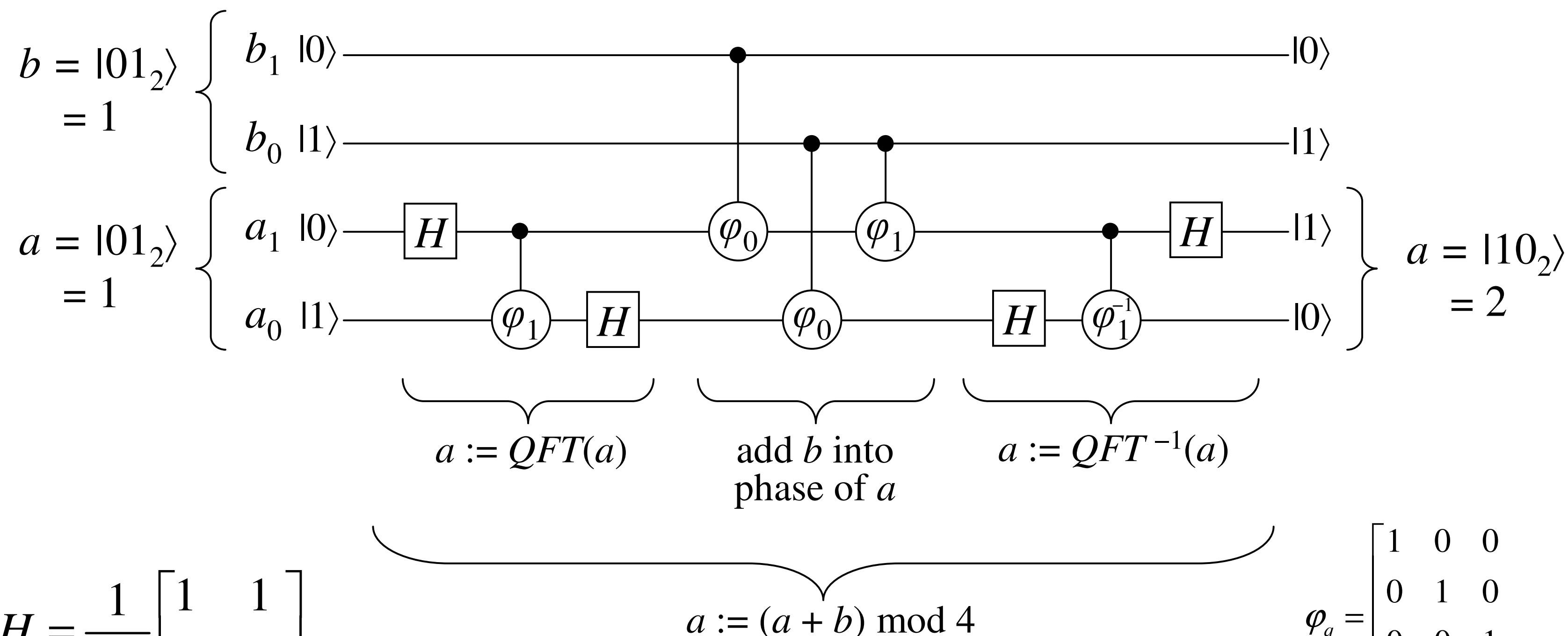
- A widespread misconception re: quantum computing:
  - "Simulating a quantum computer on a classical one takes exponential memory resources as a function of the number of qubits"
    - This is only true for a limited class of simulation techniques
- Computational complexity theorists have long known general ways to make space-intensive computations more space-efficient.
  - Applying this general method to quantum computer simulation yields a discrete analogue to numerically evaluating a path integral.
    - Can compute arb. amplitudes w/o ever storing a complete state vector!
- Computing amplitudes on-demand in this way lets us stochastically evolve just a single *classical* state over time in a way that exactly respects quantum statistics.
  - Method reminiscent of Bohm's "pilot wave" interpretation of QM.
- In this informal talk, we briefly review the history of this idea and discuss some existing & proposed implementations.

What is a Quantum Computer?

- A new, more powerful fundamental paradigm for computing within the laws of physics.
  - Apparently exponentially faster on some problems.
- Key differences btw. 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 $\mathbf{H} = \mathbf{B}^n \rightarrow \mathbf{C}$, mapping classical states to complex numbers ("amplitudes").
  - Logic operators ("gates"):
    - **Classical:** A function from several bits to one bit, $g:\mathbf{B}^k \rightarrow \mathbf{B}$
    - **Quantum:** A unitary (invertible, length-preserving) linear transformation $U:\mathbf{S} \rightarrow \mathbf{S}$, where $\mathbf{S} = \mathbf{B}^k \rightarrow \mathbf{C}$.
  - 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

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.



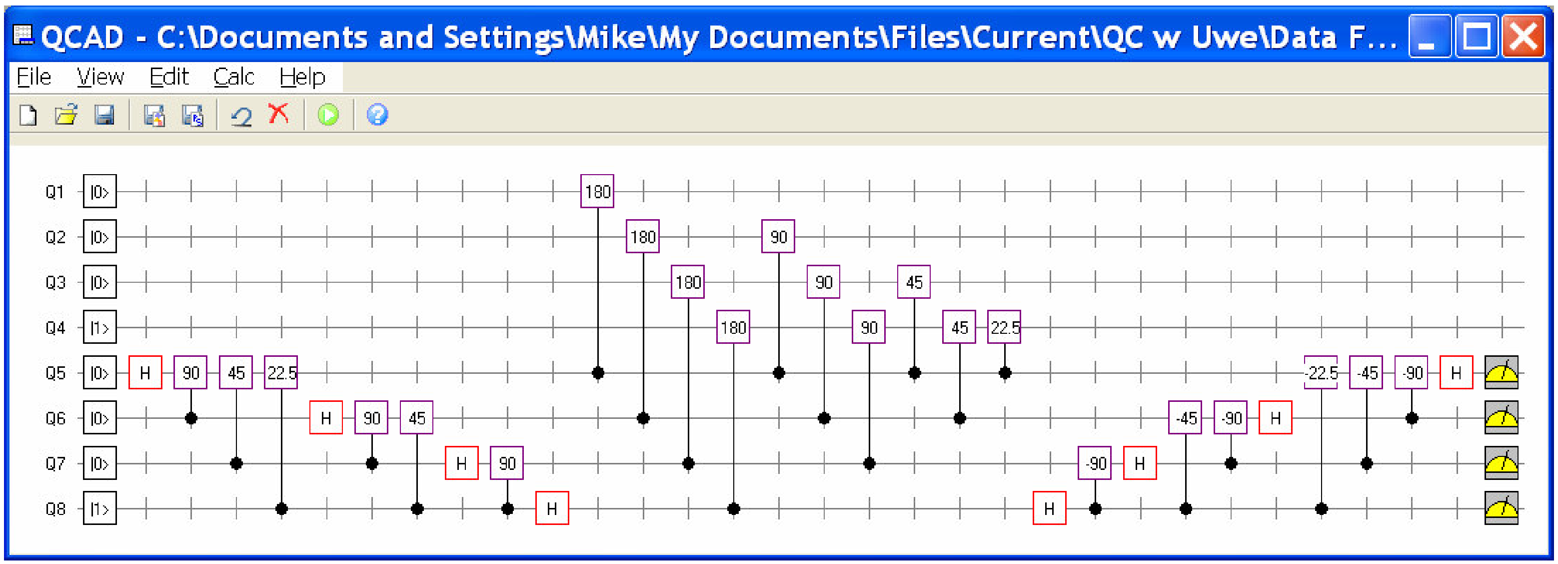
$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard gate

$$\varphi_q = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \exp(i\pi 2^{-q}) \end{bmatrix}$$

Controlled-phase gate

A Larger Draper Adder (2×4 bits)



QCAD design tool & simulator, 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, except when 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). (Shor's factoring algorithm.)
  - Polynomial-time simulations of quantum-mechanical physical systems. (Algorithms by Lloyd and others.)
  - Square-root speedups of simple unstructured searches of computed oracle functions. (Grover's search algorithm.)
  - And not a whole lot else, so far!
- A much wider variety of interesting & useful quantum algorithms is needed,
  - But new quantum algorithms are very difficult to develop.
    - Need flexible, capable simulation tools for design validation.

A Problem with Nearly All Existing Quantum Computer Simulators

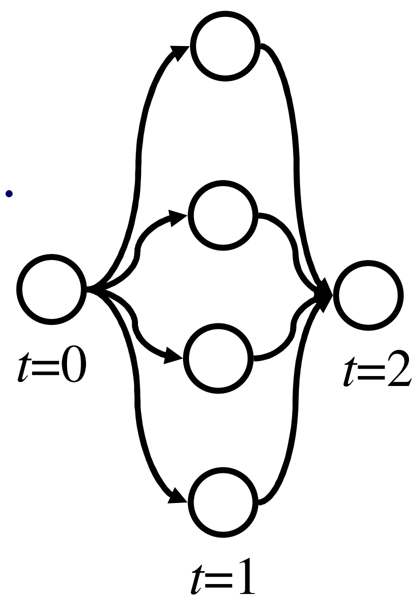
- They require *exponential space* as the number of bits in the simulated computer increases.
  - **Why:** They update a *state vector* explicitly representing the full wavefunction $\Psi: \mathbf{B}^n \rightarrow \mathbf{C}$.
    - Vector represented as a list of 2^n complex numbers
      - 1 for each 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 these large data sets
    - Relatively slow access to main memory (or even disk).

A Way to Solve This Problem

- We can reformulate quantum mechanics in an equivalent framework *without any state vectors*.
  - Feynman (1942): Any desired quantum amplitude (value of propagator between initial/final states) can be computed using a "path integral" expression summing over possible *classical* trajectories.
  - Bohm (1952): Can time-evolve a *classical* (i.e. position basis) state under the influence of only those amplitudes in its immediate neighborhood in configuration space.
- 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)
  - E.g. the graph at right uses 4 variables at time t=1, but only takes 2 time steps.



- We can make the algorithm more space-efficient by computing intermediate variables dynamically when required, instead of storing them.
- Bernstein & Vazirani, 1993: Can apply this generic tradeoff to simulating quantum computers.

$\therefore$ **BQP $\subseteq$ PSPACE**.

SEQCSim: The Space-Efficient Quantum Computer Simulator

- Core idea was conceived circa 2002 at UF.
  - Add 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 2008.
  - Future versions of the simulator will have a more expressive programming interface.
- A performance-optimized FPGA-based implementation is currently being developed.

Elements of the Approach

- Two basic categories of quantum gates:
  - *Trivial* gates are those that perform only a classical reversible transformation or phase rotation of a computational basis state.
    - *I.e.*, operation matrix is diagonalizable in the computational basis.
    - Examples: NOT, CNOT, CCNOT, φ_n, *etc.*
    - These gates can be executed immediately (& deterministically) w. no time or space penalty.
  - *Nontrivial* gates are those that combine amplitudes of multiple basis states.
    - Non-diagonalizable in comp. basis.
    - Examples: Hadamard gate, $\mathrm{NOT}^{1/2}$, *etc.*
    - Require computing amplitude(s) of neighboring predecessor state(s) (slow) & stochastically choosing a successor state.

SEQCSim Input Files for 2×2-Bit Draper Adder

```
qconfig.txt format version 1
bits: 4
named bitarray: a[2] @ 0
named bitarray: b[2] @ 2
```

Declare registers

```
qinput.txt format version 1
a = 1
b = 1
```

Input values to add

```
qoperators.txt format version 1
operators: 4
--------------------------------------------
operator #: 0
name: H
size: 1 bits
matrix:
(0.7071067812 + i*0)(0.7071067812 + i*0)
(0.7071067812 + i*0)(-0.7071067812 + i*0)
--------------------------------------------
operator #: 1
name: cZ
size: 2 bits
matrix:
(1 + i*0) (0 + i*0) (0 + i*0) (0 + i*0)
(0 + i*0) (1 + i*0) (0 + i*0) (0 + i*0)
(0 + i*0) (0 + i*0) (1 + i*0) (0 + i*0)
(0 + i*0) (0 + i*0) (0 + i*0) (-1 + i*0)
--------------------------------------------
```

... (*two additional operators elided for brevity*)

Gate definitions

Quantum circuit (sequence of gate applications)

```
qopseq.txt format version 1
operations: 9
operation #0: apply unary operator H to bit a[1]
operation #1: apply binary operator cPiOver2 to bits a[1], a[0]
operation #2: apply unary operator H to bit a[0]
operation #3: apply binary operator cZ to bits b[1], a[1]
operation #4: apply binary operator cZ to bits b[0], a[0]
operation #5: apply binary operator cPiOver2 to bits b[0], a[1]
operation #6: apply unary operator H to bit a[0]
operation #7: apply binary operator inv_cPiOver2 to bits a[1], a[0]
operation #8: apply unary operator H to bit a[1]
```

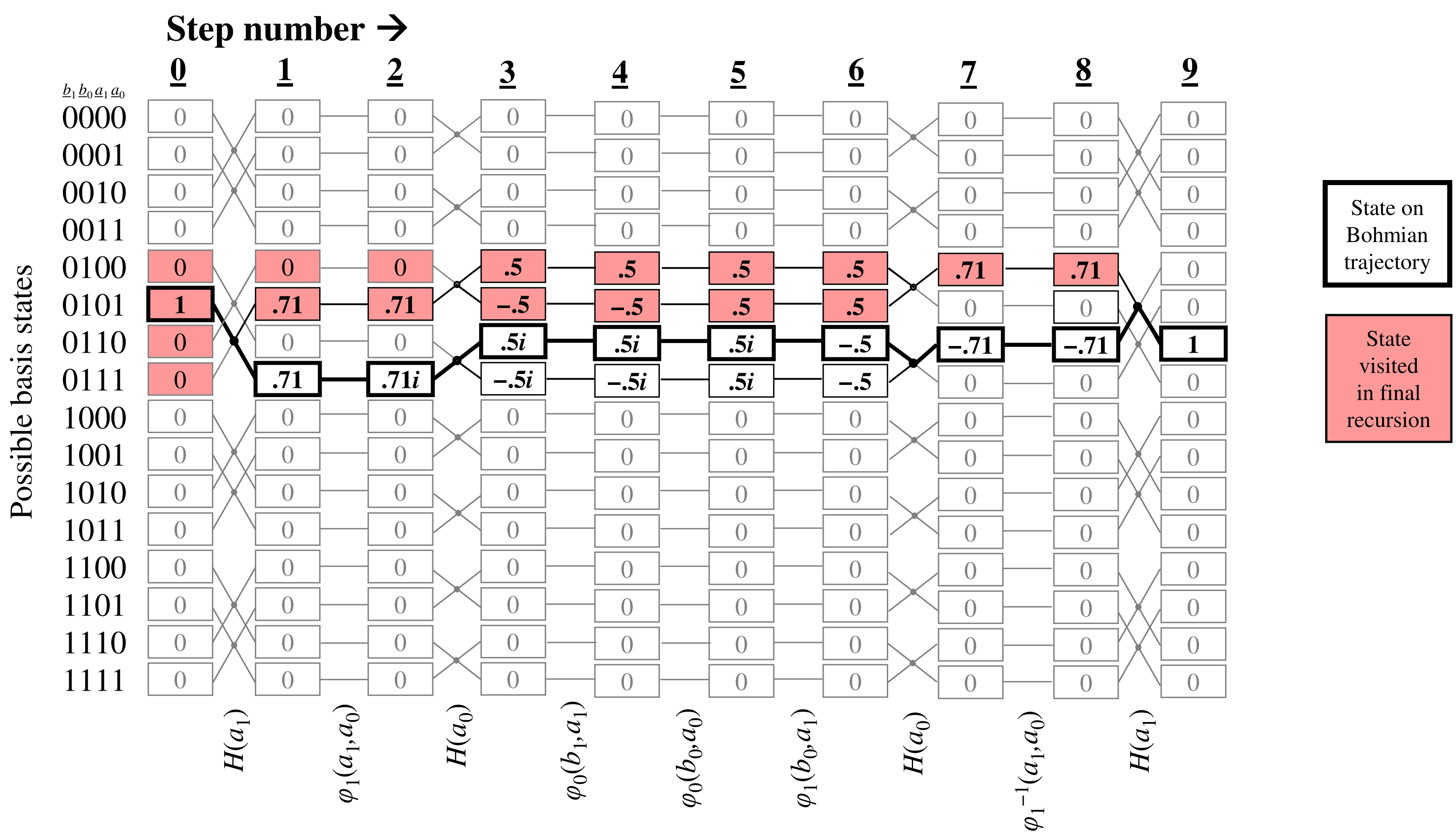
SEQCSim Core Algorithm

```
// Bohm-inspired iterative state updating.
procedure SEQCSim::run():
    curState := inputState;    // Current basis state
    curAmp := 1;               // Current amplitude
    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 gate operators
  - 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 straightforwardly-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.
```

$b=1$ $a=1$

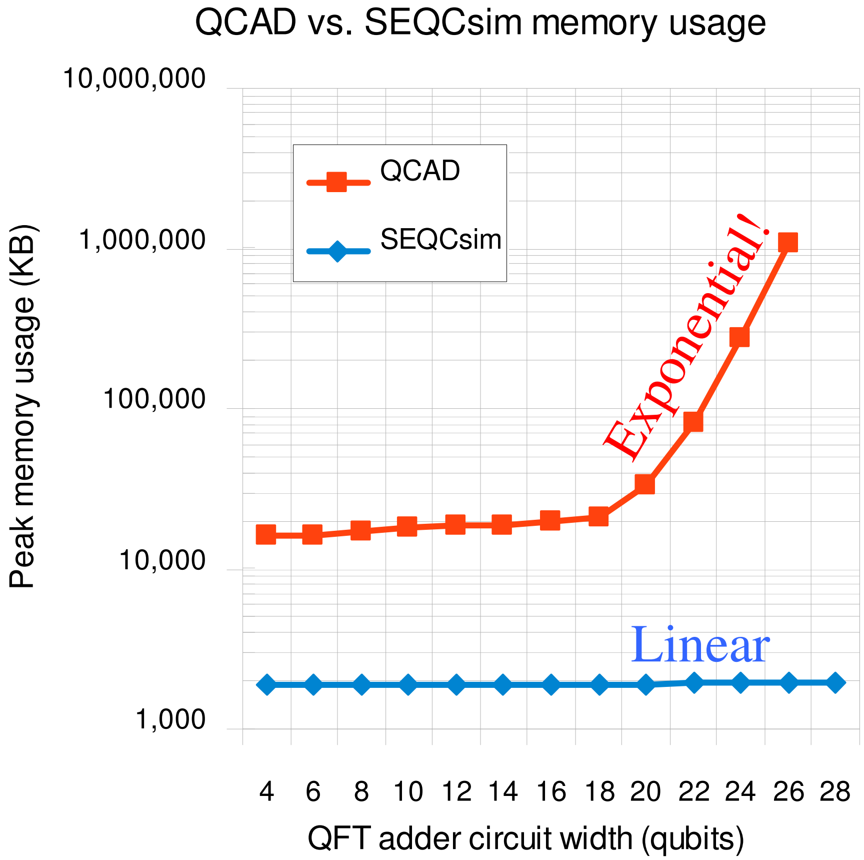
```
SEQCSim::run(): Initial state is 3->0101<-0 (4 bits) ==> (1 + i*0).
SEQCSim::Bohm_step_forwards(): (tPC=0)
   The new current state is 3->0111<-0 (4 bits) ==> (0.707107 + i*0).
SEQCSim::Bohm_step_forwards(): (tPC=1)
   The new current state is 3->0111<-0 (4 bits) ==> (0 + i*0.707107).
```

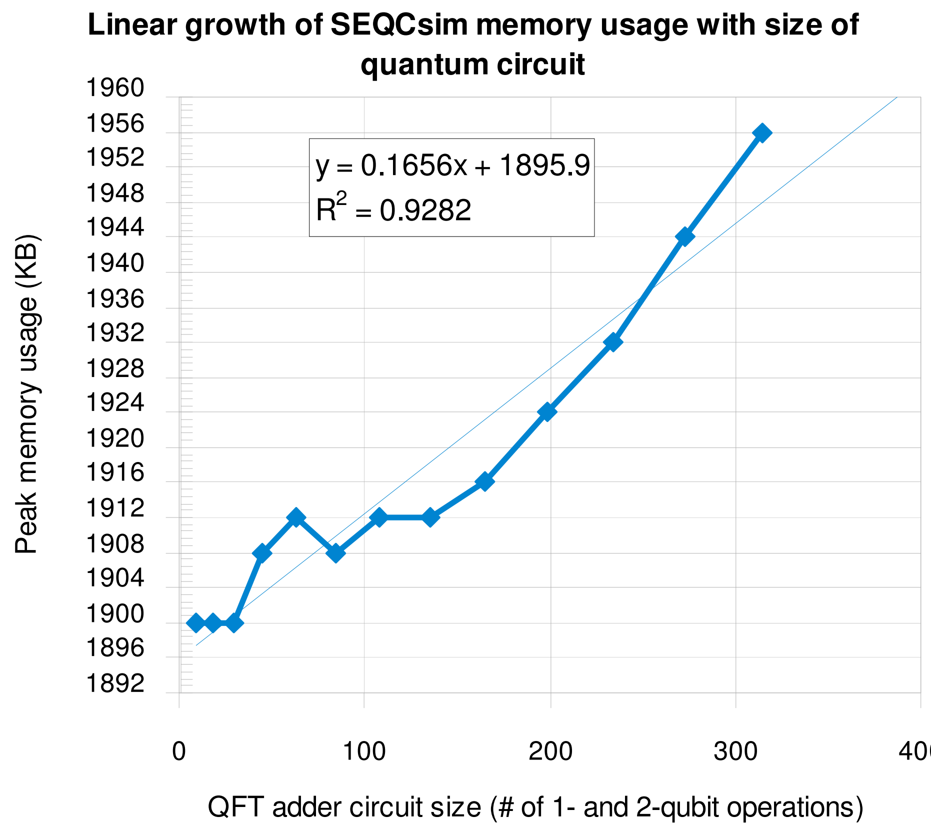
... (*5 intermediate steps elided for brevity*) ...

```
SEQCSim::Bohm_step_forwards(): (tPC=7)
   The new current state is 3->0110<-0 (4 bits) ==> (-0.707107 + i*0).
SEQCSim::Bohm_step_forwards(): (tPC=8)
   The new current state is 3->0110<-0 (4 bits) ==> (1 + i*0).
SEQCSim::done(): The PC value 9 is >= the number of operations 9.
     We are done!
```

$a = 1+1 = 2 = 10_2$

Empirical Measurements of Space Complexity

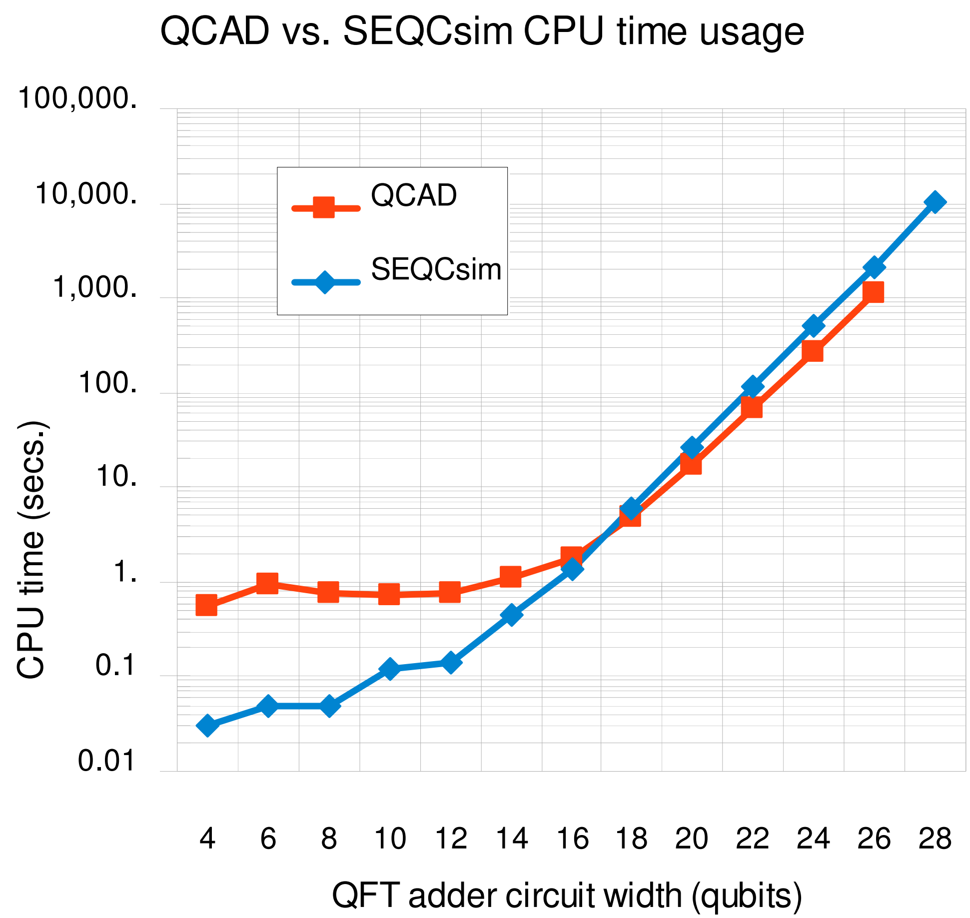




(**Note:** QCAD crashed on the 28-bit circuit, due to insufficient memory available on the test PC.)

Empirical Measurements of CPU Time Utilization

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

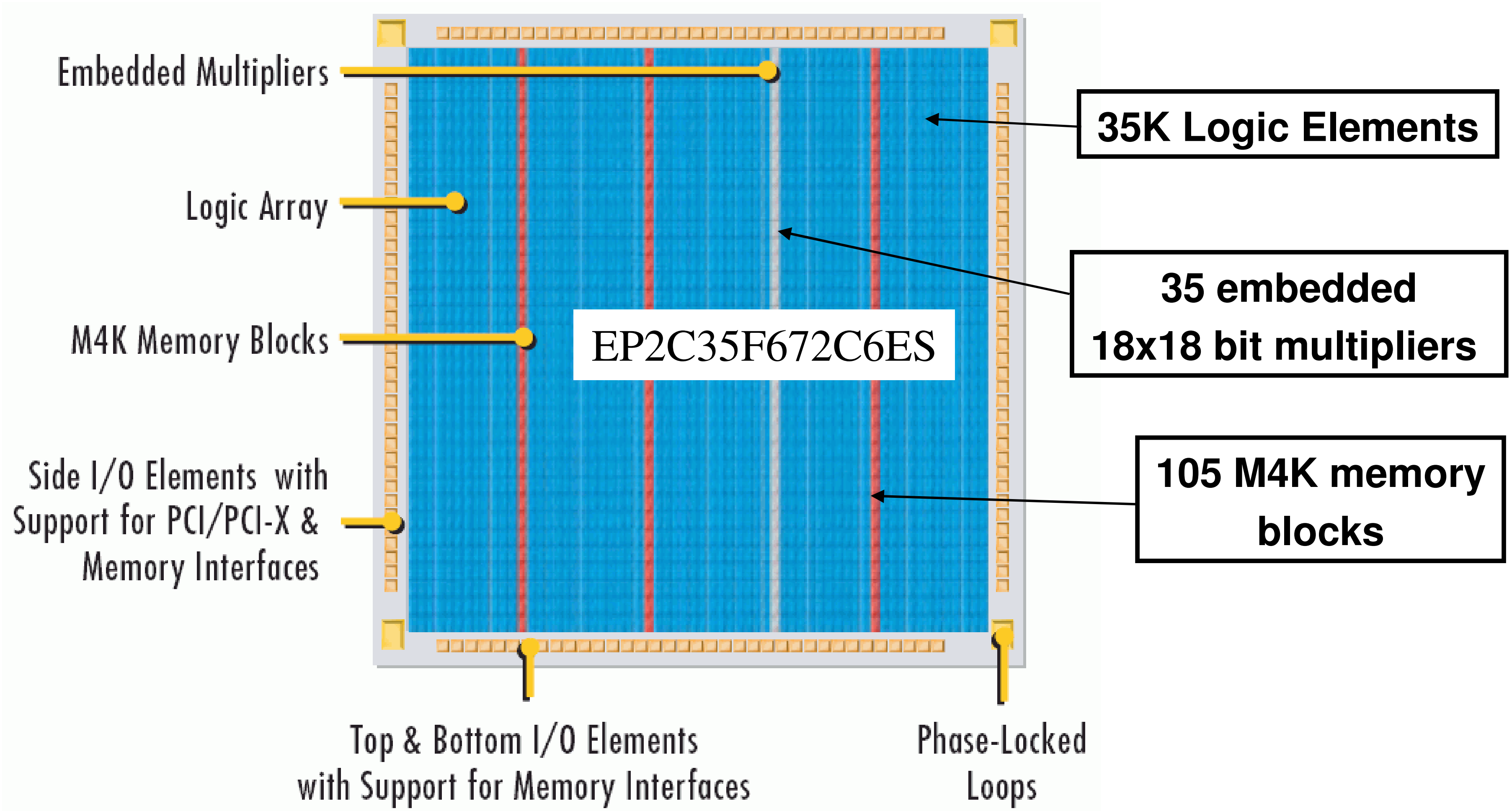


Next Steps

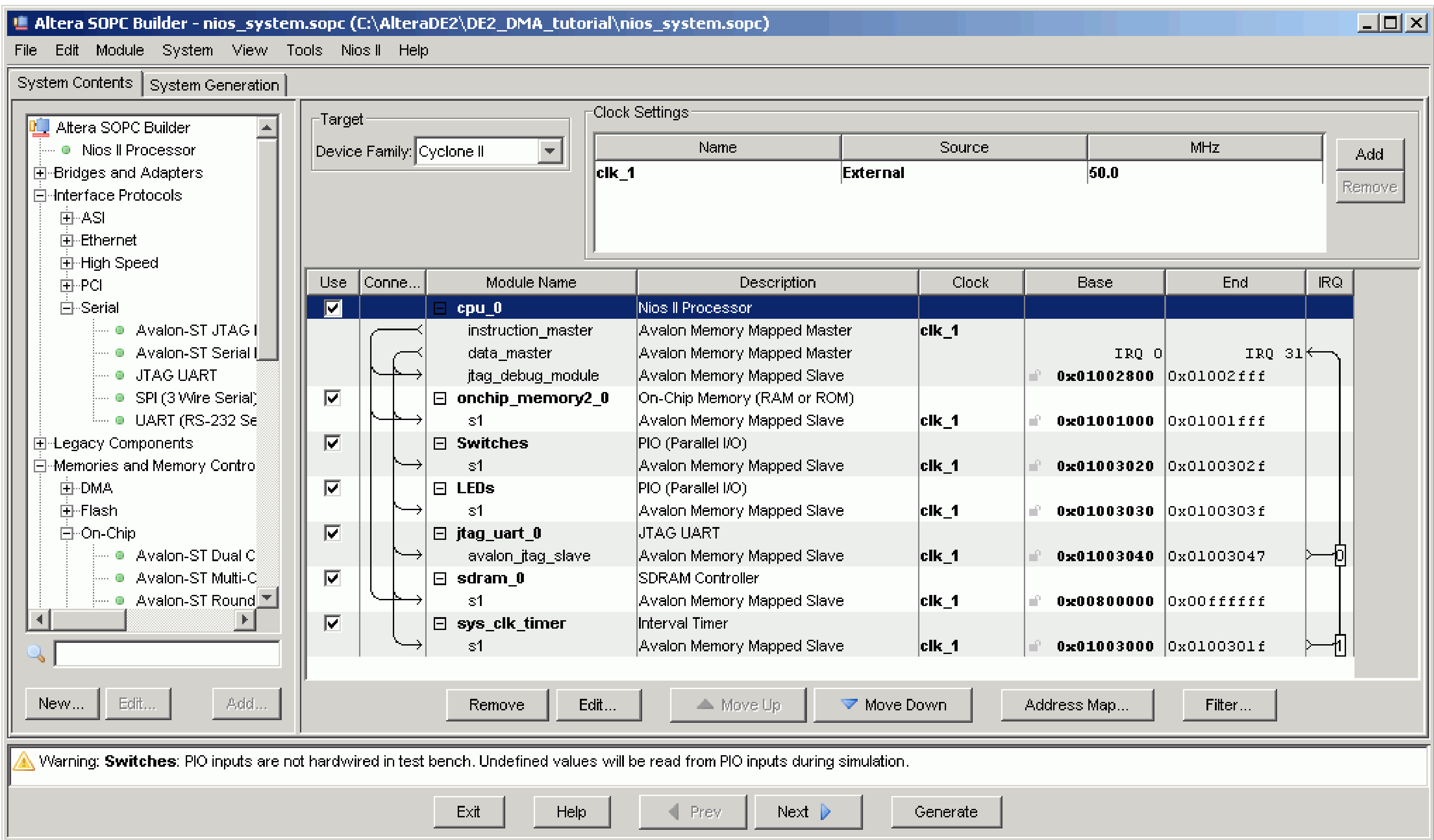
- Software implementation:
  - Implement a special cache for state amplitudes, to boost performance
  - Develop a new simulator API around a “Qubit” class that mimics the (ideal) real statistical behavior of quantum bits
    - Invokes SEQCSim engine “behind the scenes”
    - Allows coding quantum algorithms directly in C++
- FPGA-based hardware implementation:
  - Design custom register structures for faster bit-manipulation, and custom memory units for hardware caching of state amplitudes
  - Develop efficient adders/multipliers on FPGA platform for floating-point numbers in a simplified custom format
  - Use these as the basis for a custom parallel arithmetic datapath for quickly computing inner products of complex vectors
  - Design an optimized special-purpose iterative FSM for the graph traversal, to replace the recursive calcAmp() procedure

EXTRA SLIDES

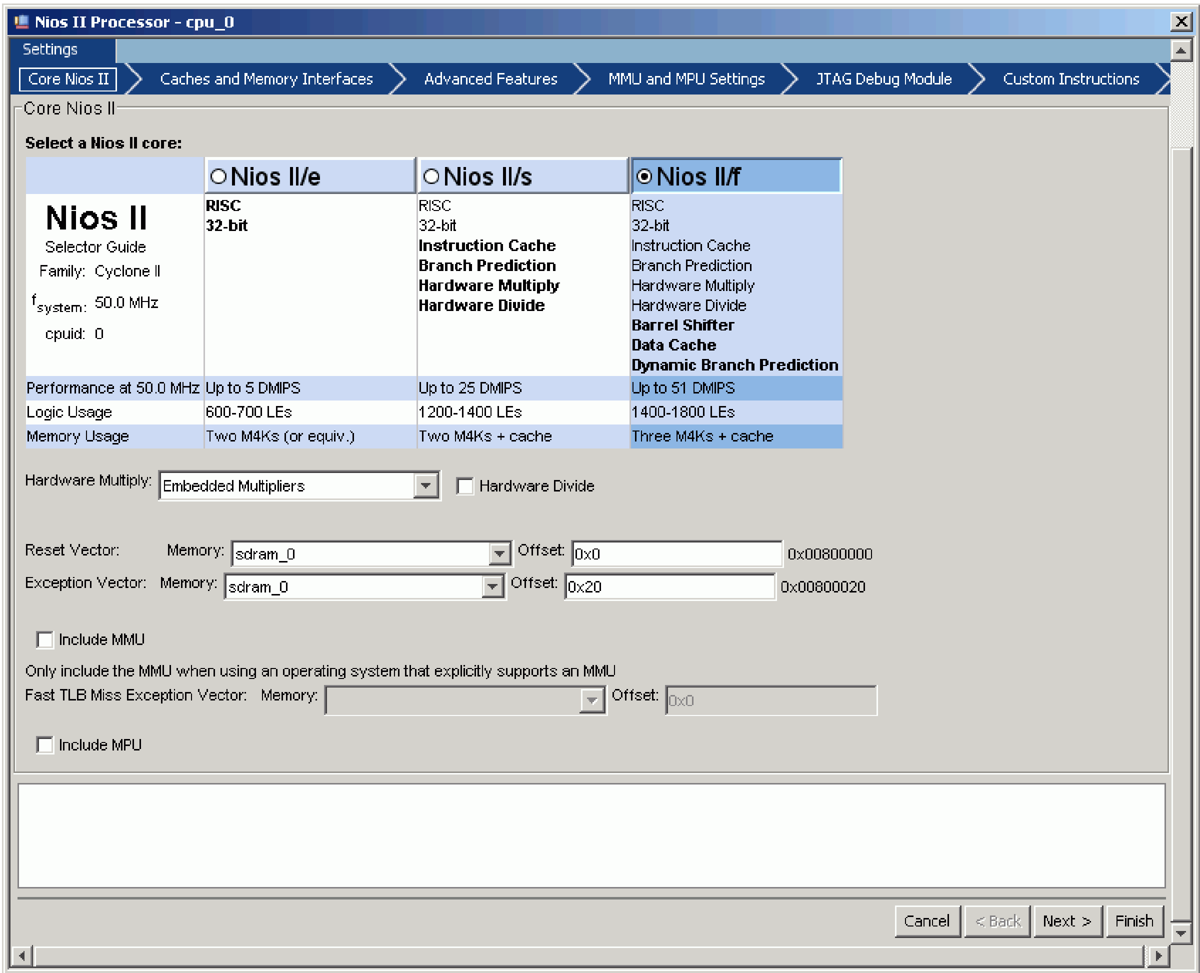
What is a FPGA?



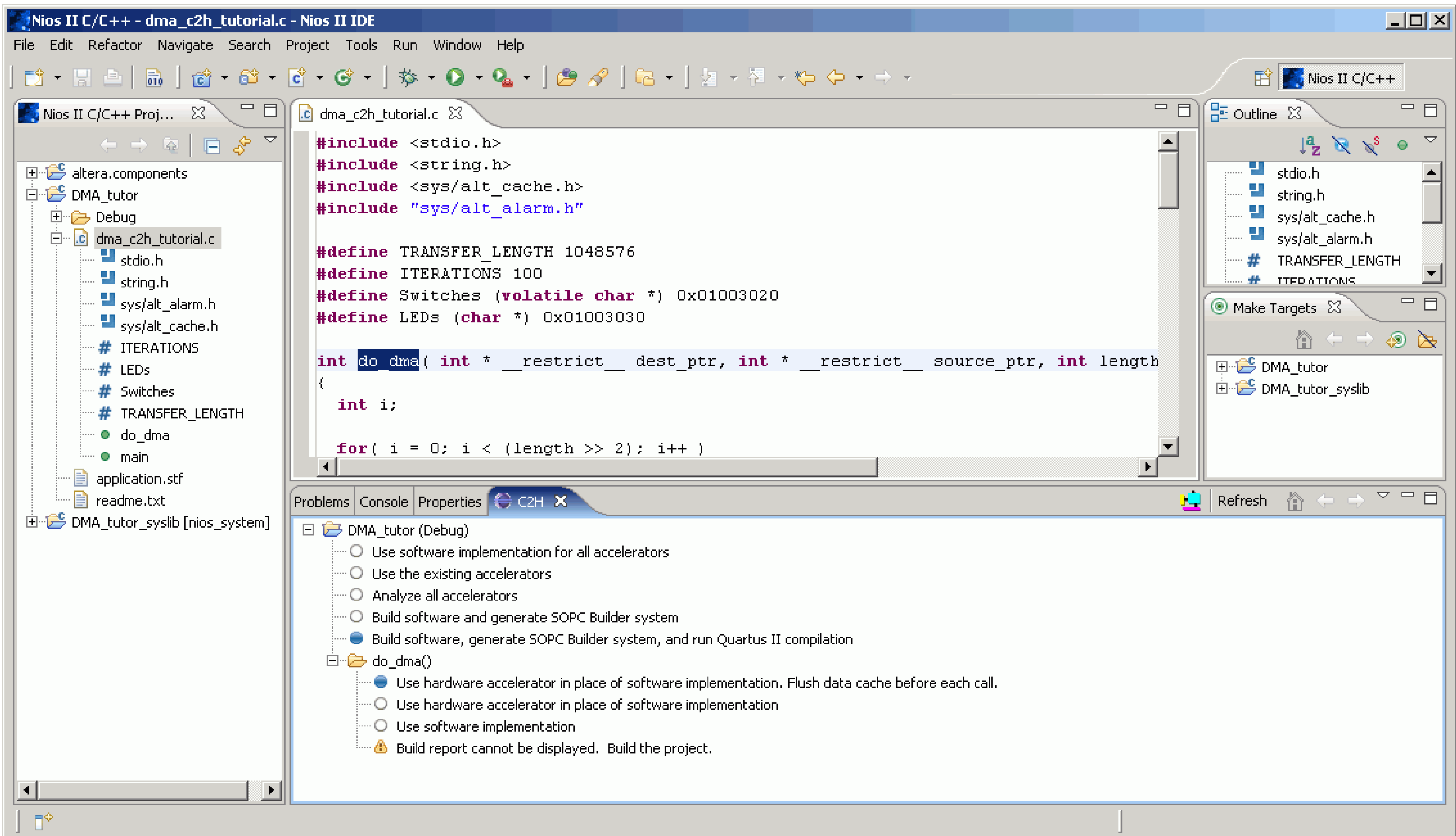
FPGA Tools (1 of 5): Altera SOPC Builder



FPGA Tools (2 of 5): NIOS II Soft-Core Configuration

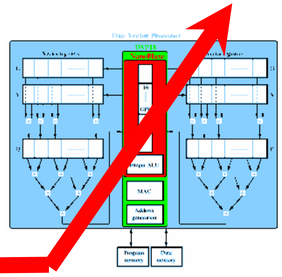


FPGA Tools (3 of 5): Custom Hardware Generation with C2H



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

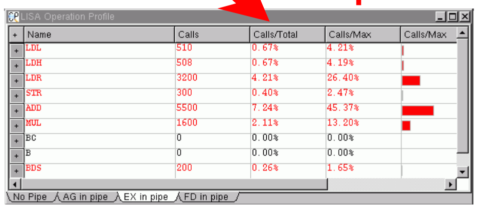
Architecture exploration



ISA, cache, Co-processor

Design tool generation

Assembler, linker, profiling, ISS, C-compiler

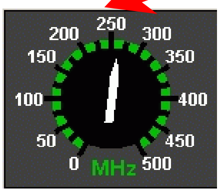


LISA Operation Profile

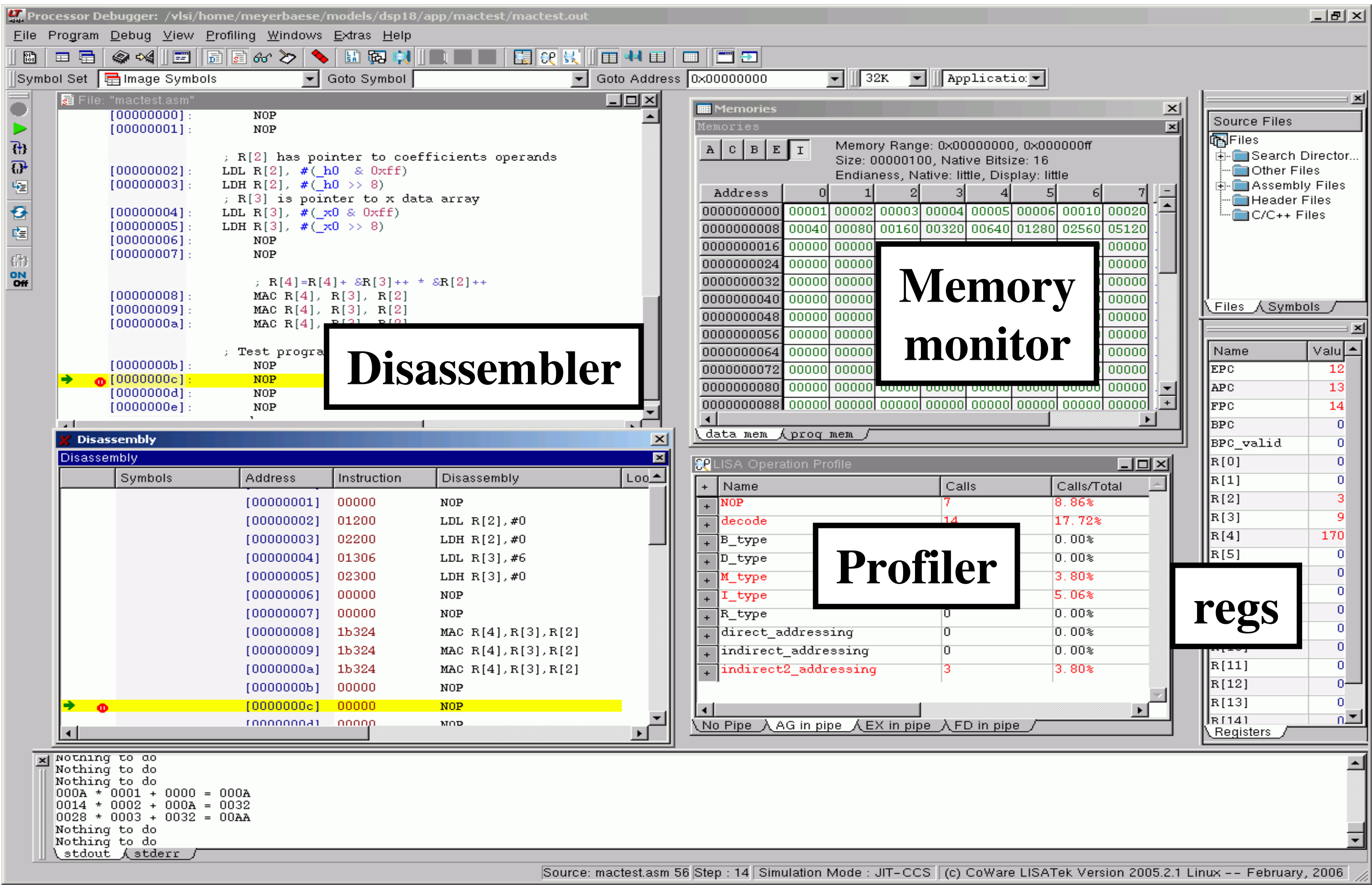
+	Name	Calls	Calls/Total	Calls/Max	Calls/Max
+	LDL	510	0.67%	4.21%	
+	LDH	508	0.67%	4.19%	
+	LDR	3200	4.21%	26.40%	
+	STR	300	0.40%	2.47%	
+	ADD	5500	7.24%	45.37%	
+	MUL	1600	2.11%	13.20%	
+	BC	0	0.00%	0.00%	
+	B	0	0.00%	0.00%	
+	BDS	200	0.26%	1.65%	

No Pipe / AG in pipe / EX in pipe / FD in pipe

FPGA Implementation
Size, speed, power



FPGA Tools (5 of 5): LISA Development Tools



Conclusion

- 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 http://www.eng.fsu.edu/~mpf/SEQCSim
    - Contact michael.patrick.frank@gmail.com with questions about 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.