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Space-Efficient Simulation of Quantum Computers

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Abstract of Paper (for reference)

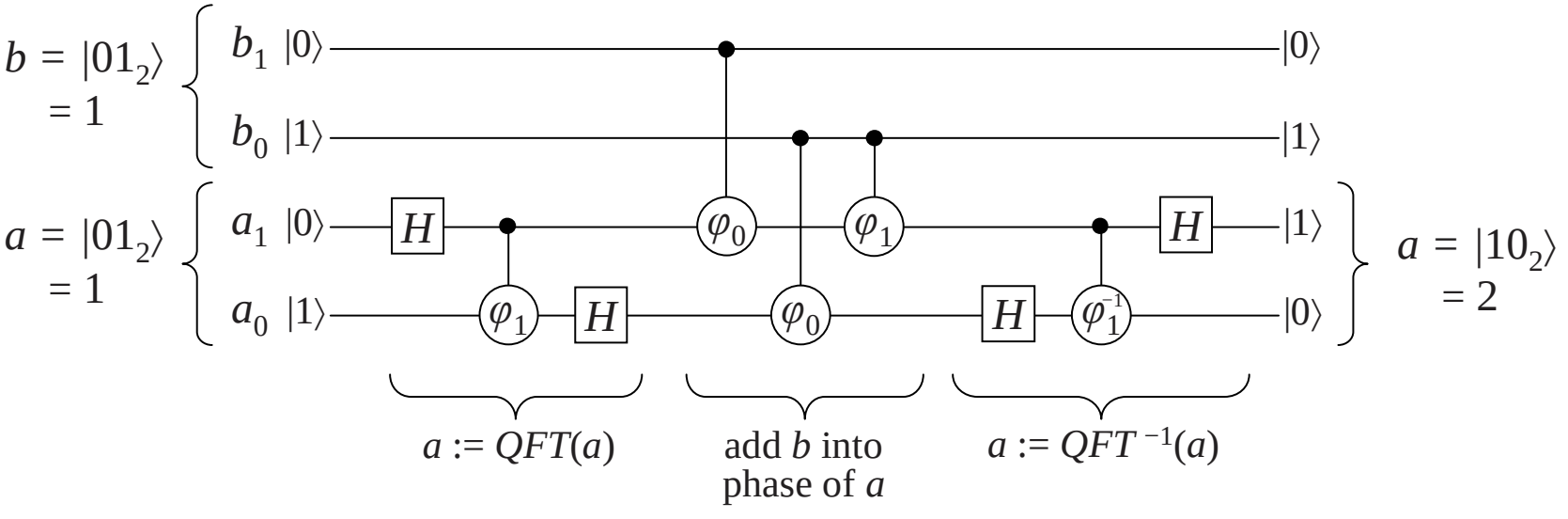
- Traditional algorithms for simulating quantum computers on classical ones require an exponentially large amount of memory,
  - and so typically cannot simulate general quantum circuits with more than about 30 or so qubits on a typical PC-scale platform with only a few gigabytes of main memory.
- However, 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.
- 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.



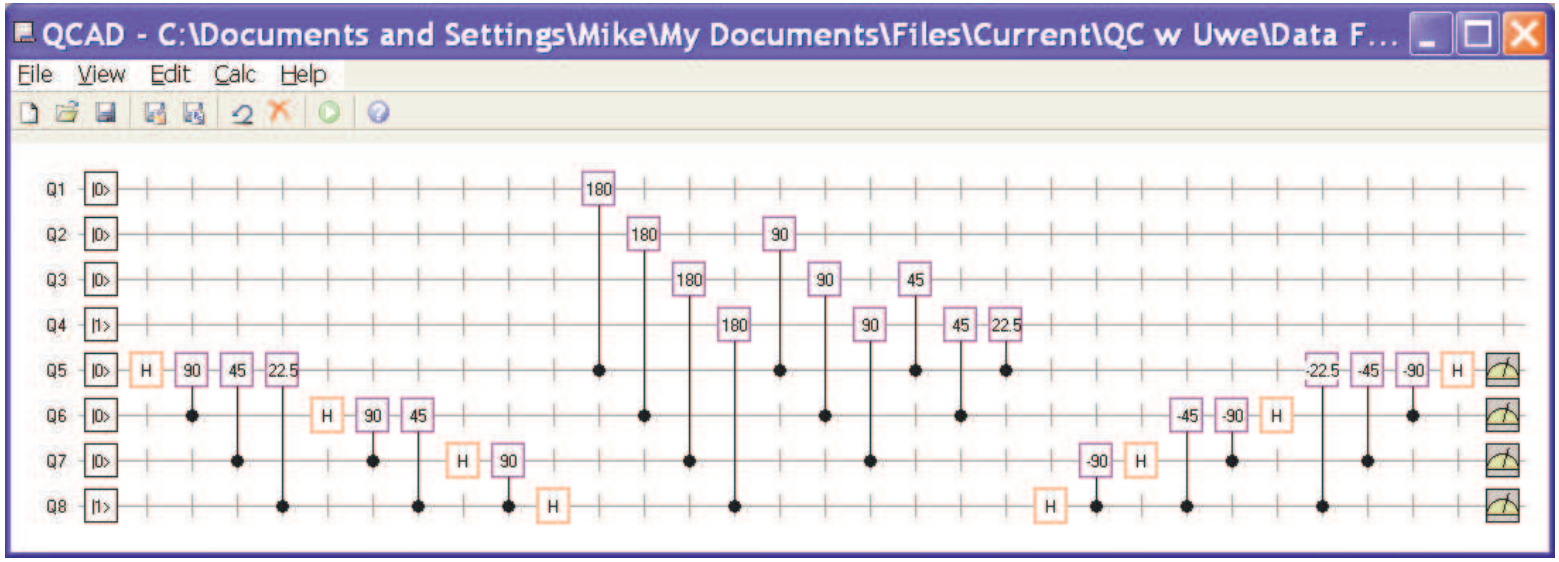
$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard gate

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

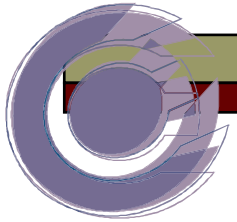
Controlled-phase gate

A Larger Draper Adder (2×4 bits)



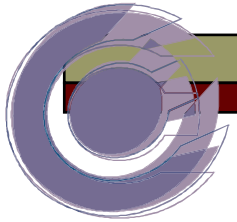
QCAD design tool & simulator, by Hiroshi Watanabe, University of Tokyo, available from http://apollon.cc.u-tokyo.ac.jp/~watanabe/qcad/index.html

- 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.



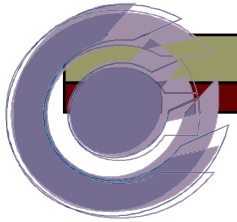
Some Potential Applications of Quantum Computers

- 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, 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 Ψ: $\mathbf{B}^n \rightarrow \mathbf{C}$.
    - 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).

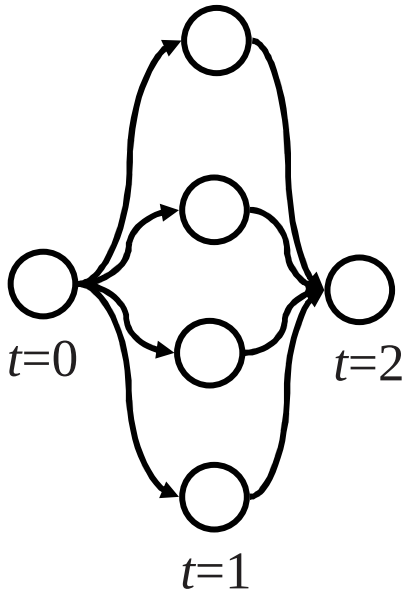


A Way to Solve This Problem

- We can reformulate quantum mechanics in an equivalent framework *without any state vectors*.
  - Feynman (1942): Any desired quantum amplitude can be computed using a "path integral" expression summing over possible *classical* trajectories.
  - Bohm (1952): Can time-evolve a *classical* 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 || 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.

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)

Gate definitions

... (two additional operators elided for brevity)

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]

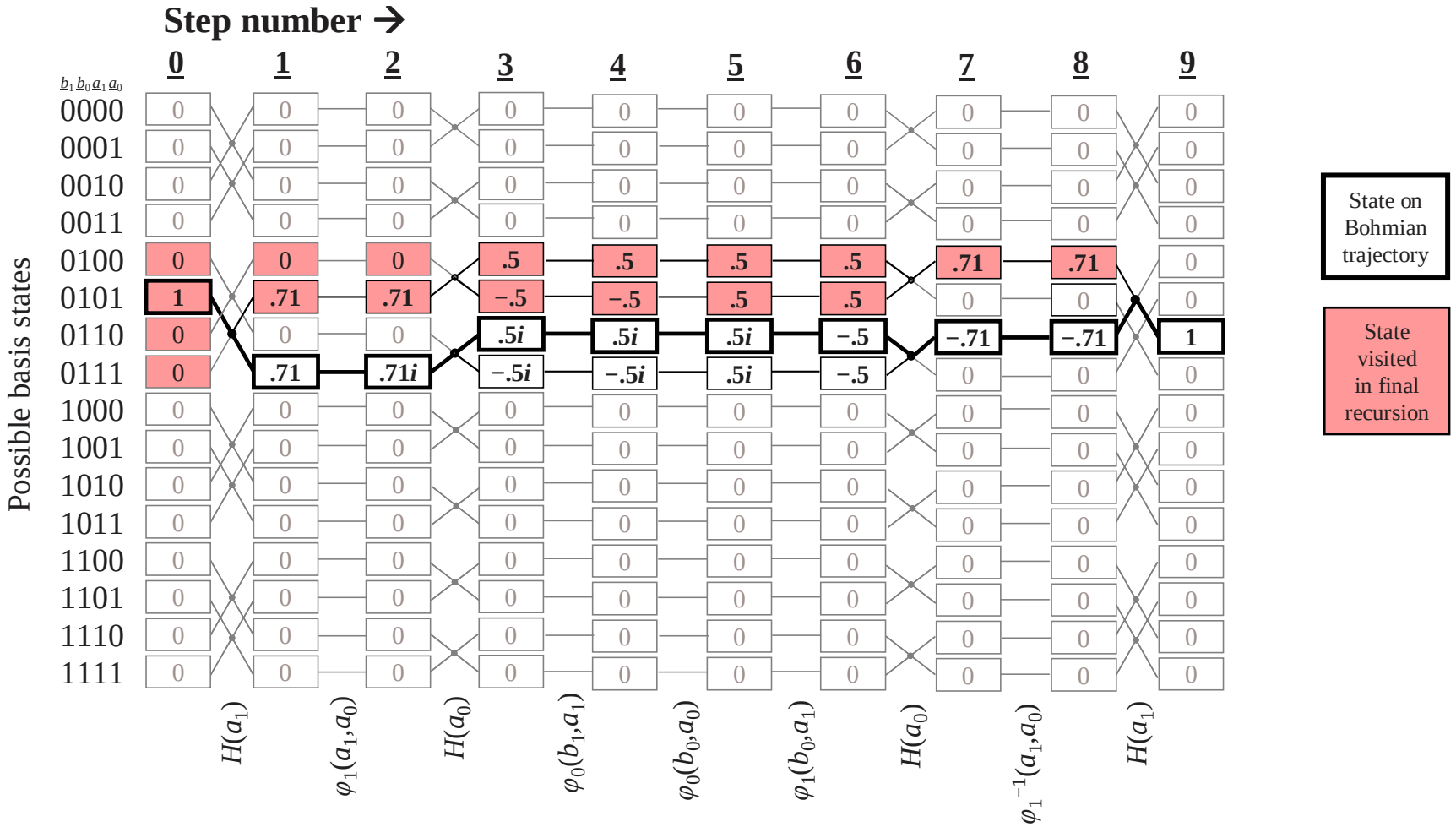
SEQCSim Core Algorithm

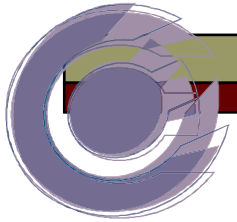
```
// Bohm-inspired iterative state updating.
procedure SEQCSim::run():
    curState := inputState;    // Current basis state
    curAmp := 1;               // Current amplitude
    for PC =: 0 to #gates,     // Current gate index
        (w.r.t. gate[PC] operator and its operands,)
        for each 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: $O(s + t \cdot 2^{ak})$

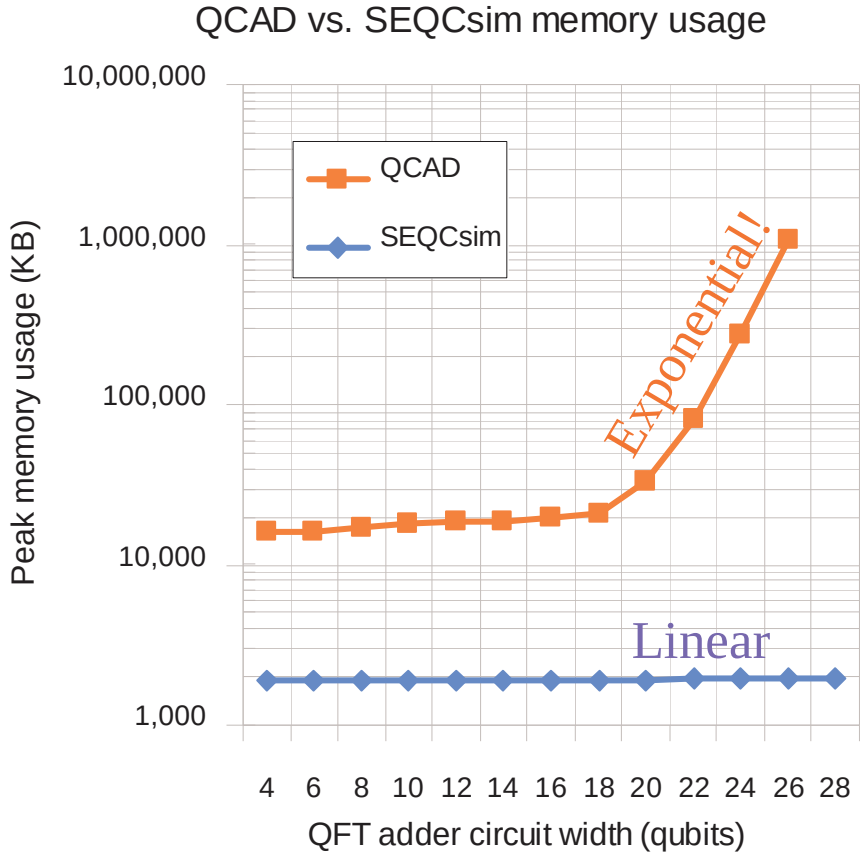
SEQCSim Output on 2×2-Bit Draper Adder

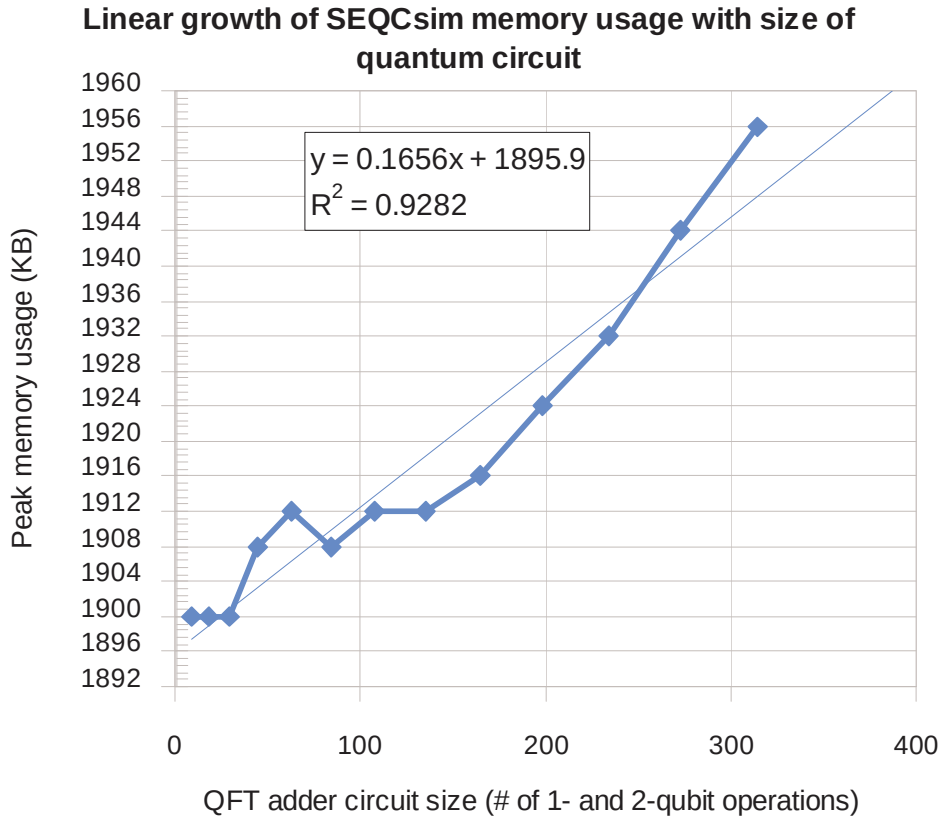
```
Welcome to SEQCSIM, the Space-Efficient Quantum Computer SIMulator.
    (C++ console version)
By Michael P. Frank, Uwe Meyer-Baese, Irinel Chiorescu, and Liviu Oniciuc.
Copyright (C) 2008 Florida State University Board of Trustees.
    All rights reserved.

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!
```

$b=1$ $a=1$

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

Empirical Measurements of Space Complexity

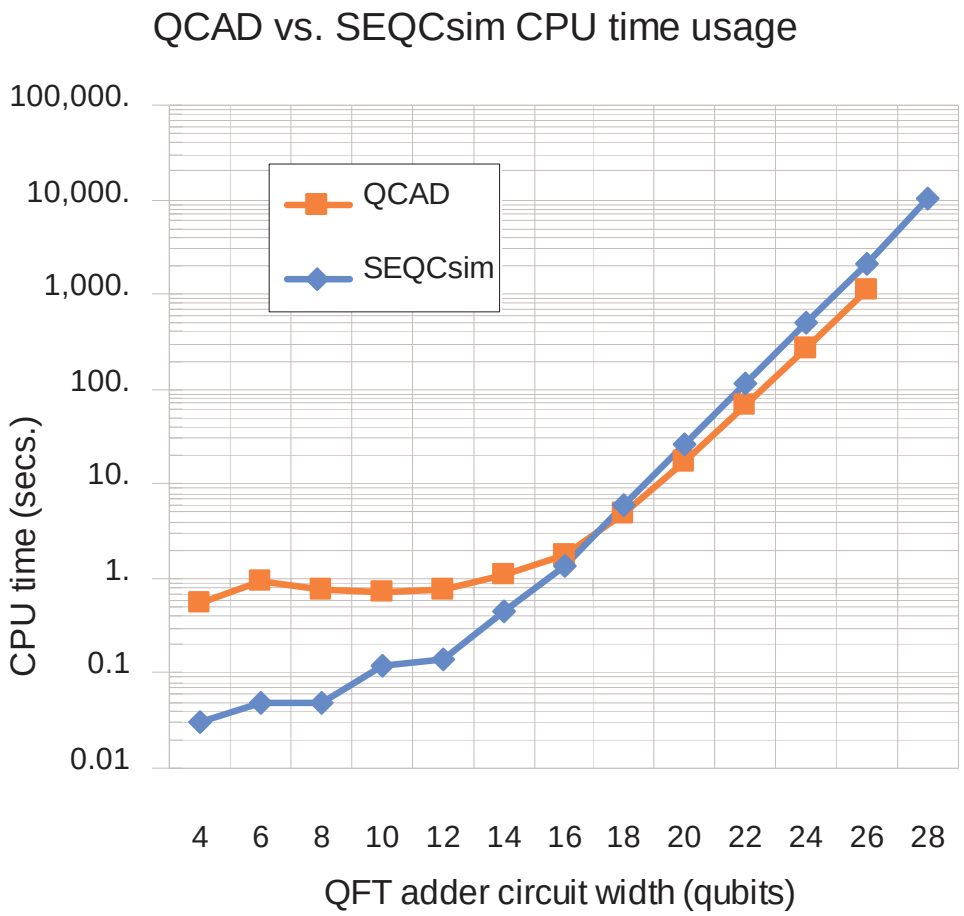


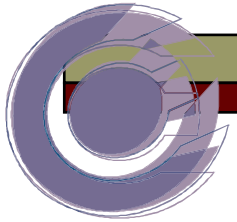


(Note: QCAD crashed on the 28-bit circuit, due to insufficient memory available on the test PC.)

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

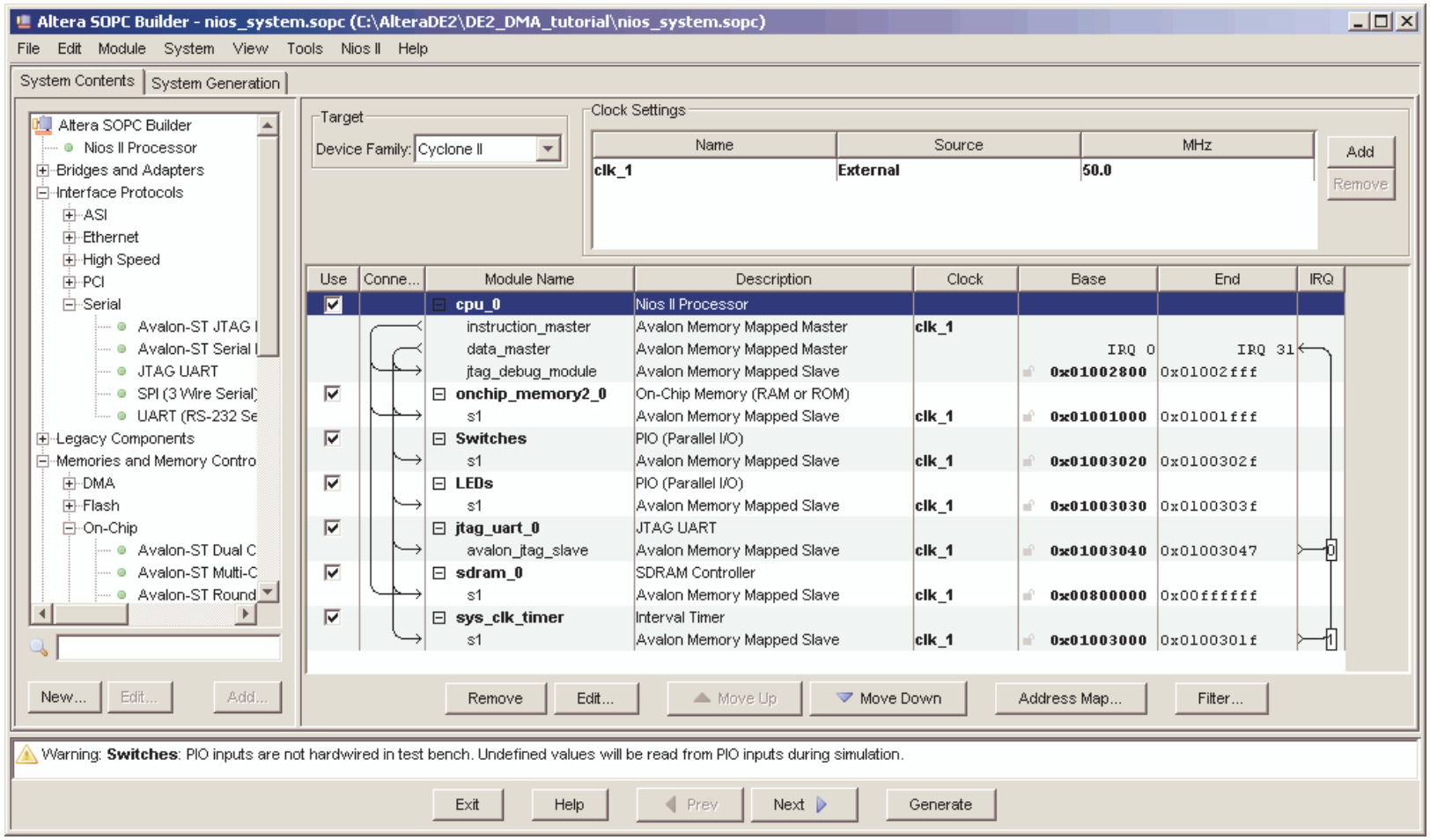




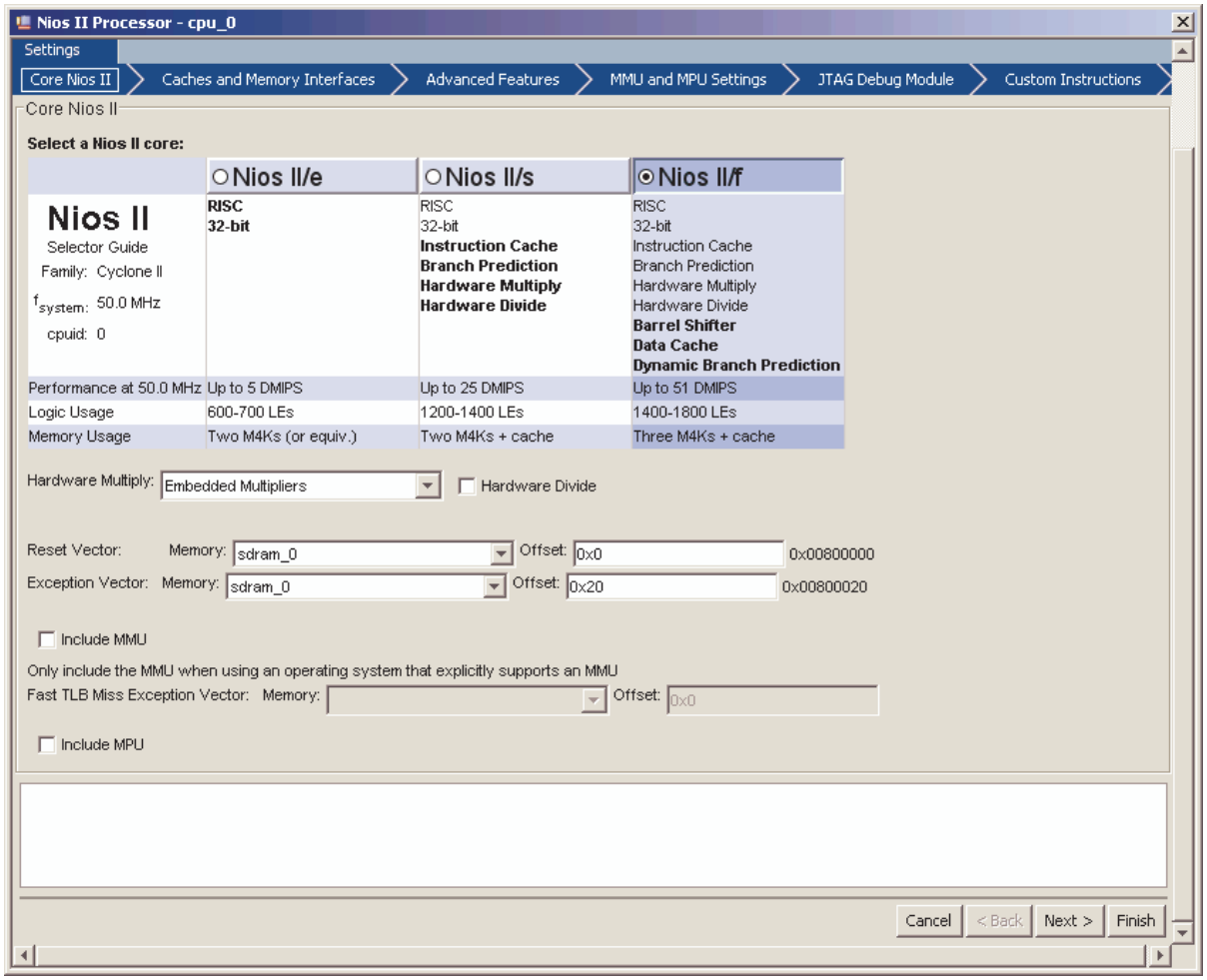
Next Steps

- 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

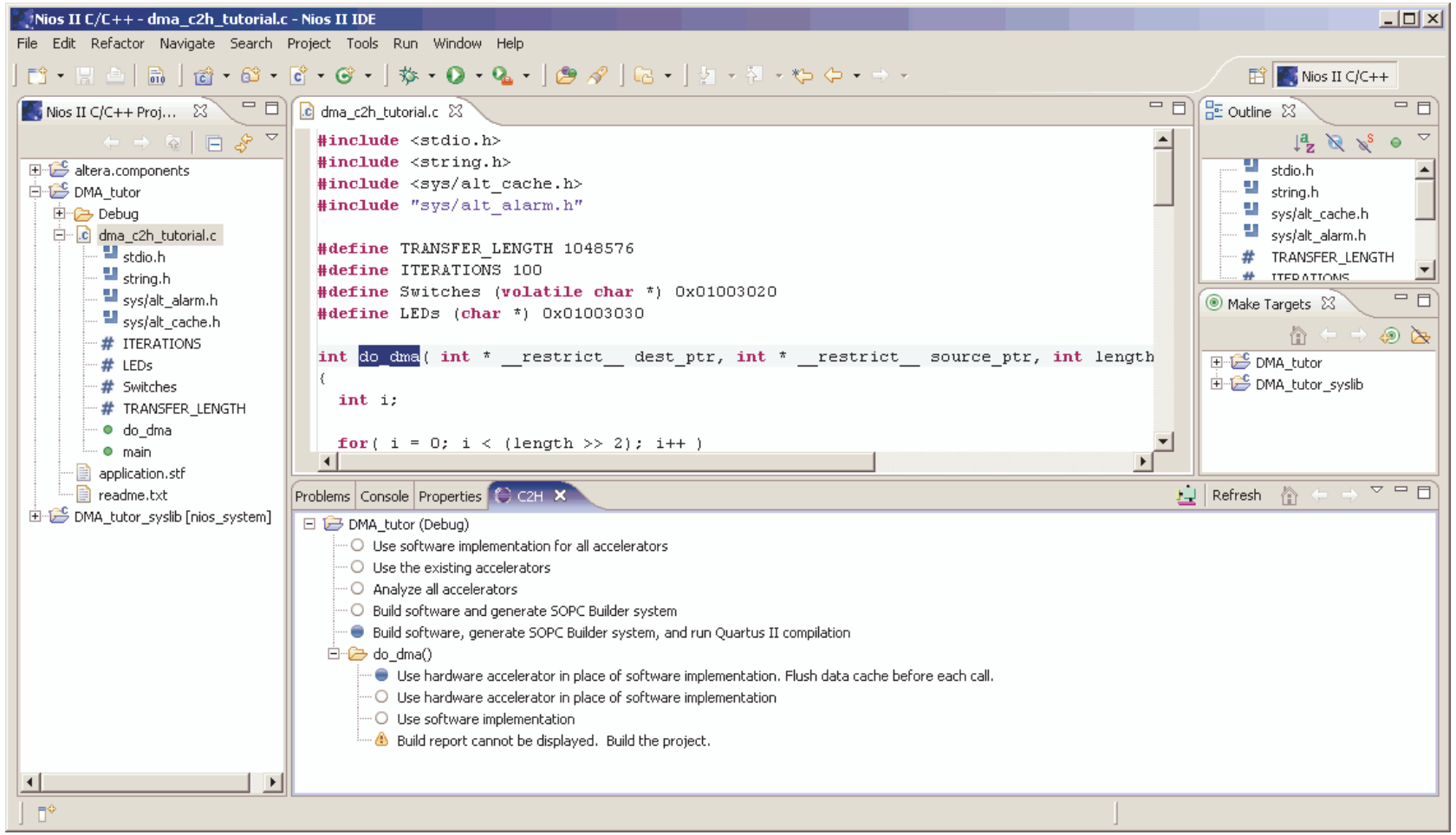
FPGA Tools (1 of 5): Altera SOPC Builder



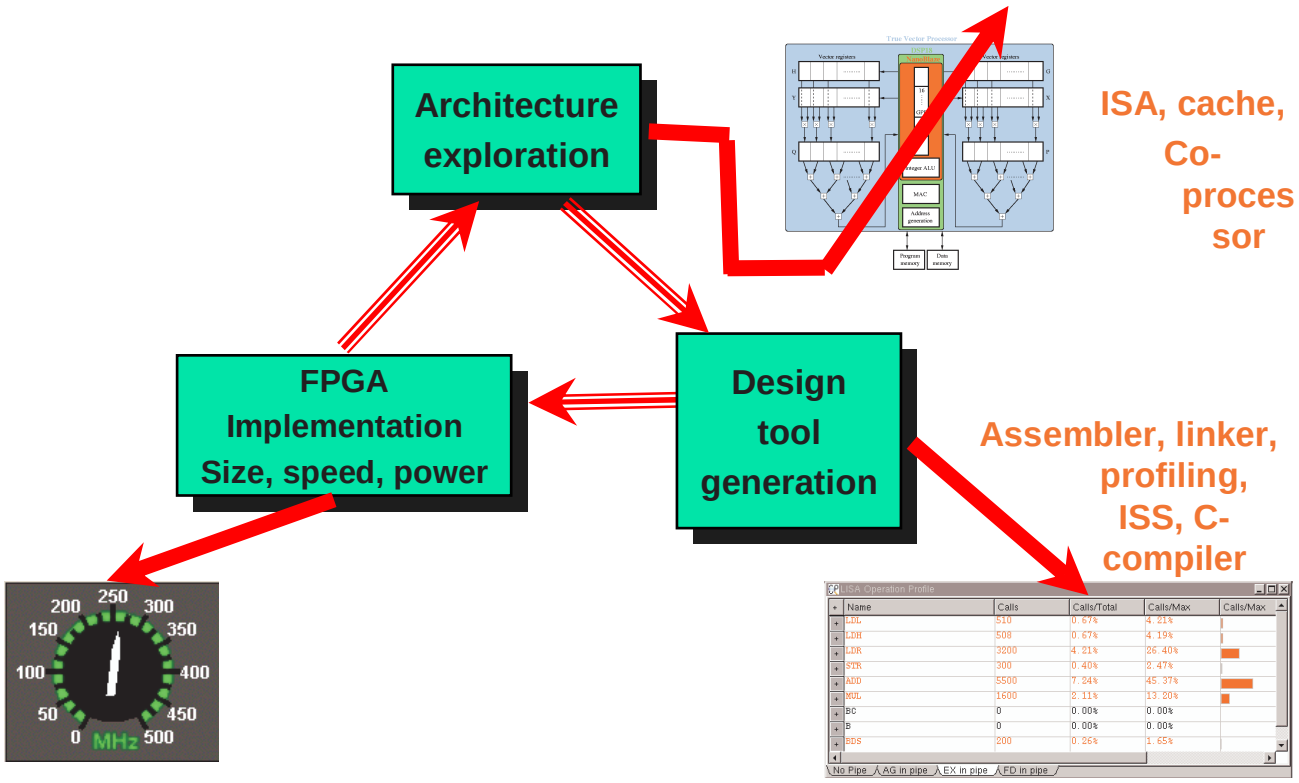
FPGA Tools (2 of 5): NIOS II Soft-Core Configuration



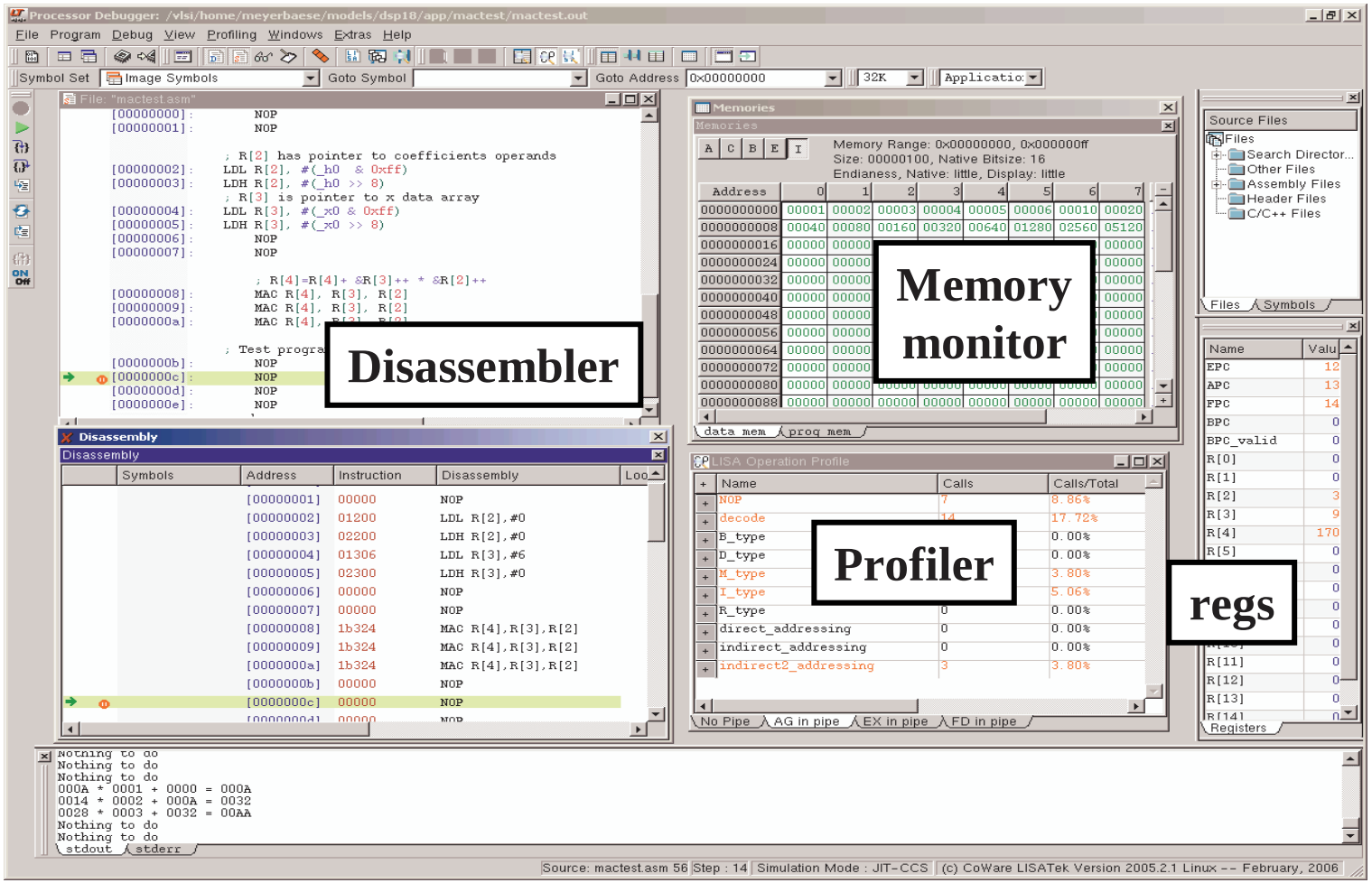
FPGA Tools (3 of 5): Custom Hardware Generation with C2H

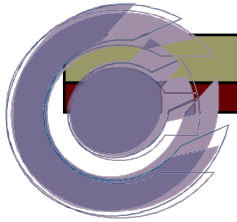


FPGA Tools (4 of 5): LISA Processor Design Cycle



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 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.