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Quantum Dot Cellular Automata (QDCA)
Strategic Partnership: Extending Moore's Law: Part 2, Computer Sciences Issues

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(¹Sandia, ²Notre Dame, ³U. Virginia)

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Moore’s Law for Logic Switching Power

A 100 $k_B T$ “thermal device limit” closely related to $k_B T \ln(2)$ “Landauer Limit” creates a floor of Joules/logic operation that will halt evolutionary progress. This is an immediate concern evidenced by growing $\mu P$ heat.

Energy per operation = \frac{1}{Performance @ 100Watts}

Lower is Better

100 $k_B T$ Power Limit (to be discussed)

Today 2020 End of Roadmap 2030+
Emerging Research Devices (notes 2005)

- Table shows drop in replacements for CMOS transistors that defeat limit in previous slide
- Color code: OK, marginal, unacceptable
- CNFET on table only for political reasons
Obeying Moore’s Law and Beating CMOS

Energy per operation = \frac{1}{Performance @ 100Watts}

100 k_B T Power Limit (to be discussed)

Today 2020 End of Roadmap 2030+

Many proposed devices are subject to the same limits as CMOS

This project addresses approaches that can decisively beat CMOS at the end of the roadmap: Principal concepts: Reversible Logic and Quantum Computing
Tie Between Information and Device Physics

• We use Boolean logic today, based on AND-OR-NOT
• AND and OR gates “destroy” information, which creates heat irrespective of physical implementation (to be described later)
• This limit can be circumvented by a different form of logic that does not “destroy” information
• However, this will also require different devices…
Quantum-dot cellular automata

Represent binary information by charge configuration of cell.

**QCA cell**
- Dots localize charge
- Two mobile charges
- Tunneling between dots
- Clock signal varies relative energies of “active” and “null” dots

Clock need not separately contact each cell.
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.

“1”

“null”
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.

This is the COPY operation.
Majority Gate

“0”

“1”

“null”

“1”
Majority Gate

```
1
```

```
0
```

```
1
```

```
1
```

```
1
```

```
1
```

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1
```

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1
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1
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1
```

```
1
```
Majority Gate

Three input majority gate can function as programmable 2-input AND/OR gate.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
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</tr>
</tbody>
</table>
QCA single-bit full adder

Hierarchical layout and design are possible.

Simple-12 microprocessor (Kogge & Niemier)
Computational wave: adder back-end
Characteristic energy

We would like “kink energy” $E_k > k_B T$. 
Molecular Wire

\[ E_k = 0.8 \text{ eV} \]

ONIOM/STO-3G (Gaussian 03)
Power Gain in QCA Cells

- Power gain is crucial for practical devices because some energy is always lost between stages.

- Lost energy must be replaced.
  - Conventional devices – current from power supply
  - QCA devices – from the clock

- Unity power gain means replacing exactly as much energy as is lost to environment.

Power gain > 3 has been measured in metal-dot QCA.
Landauer Clocking
Energy dissipation in Landauer-clocked circuit

\[ \text{Dissipated Energy} / k_B = k_B T \ln(2) \]

A \oplus B

11       10

shift register   “OR” gate
Test circuit: OR gate

Landauer clocking with echo of inputs to outputs
Energy dissipation in the OR gate

Energy dissipation greatly reduced with inputs echoed to outputs

\[ \frac{\text{Dissipated energy}}{E_k} \]

\[ k_B T \ln(2) \]
Bennett clocking of QCA

Output is used to erase intermediate results.
Test circuit: OR gate

Bennett clocked OR gate
Bennett clocking of QCA

For QCA no change in layout is required.
Bennett-style computation may be practical in QCA

Direct time-dependent calculations show: Logically reversible circuit can dissipate much less than $k_B T \ln(2)$. 

\[ \text{Dissipated Energy}/E_k \]

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \]

\[ \begin{array}{c} L \quad B \\ \\ L \quad L \quad L \quad B \quad B \end{array} \]

\[ k_B T \ln(2) \]

\[ 11 \quad 10 \quad 11 \quad 10 \quad 11 \quad 10 \]
QCA implementations

- Semiconductor-dot QCA
  - SiGe quantum fortresses
  - Silicon P-doping
  - GaAs
  - Silicon dot SET’s
- Magnetic QCA
- Metal-dot QCA
- Molecular QCA
- CMOS analogue
Quantum Fortress Growth

$h \text{ nm } Ge_{0.3}Si_{0.7}/Si(100), 550^\circ C, 0.09 \text{ nm/s}$
Quantum Fortress QCA

FIB are used to deposit Pt contacts to ease the alignment requirements of the E-beam lithography.
Architecture Summary

1. Irreversible
2. Fully Reversible: Landauer Clocking
   - Reversible Components
3. Fully Reversible: Bennett Clocking
   - Possibly Irreversible Components
4. Fully Reversible: Collapsed Bennett
   - General purpose floorplan
   - Size of computation limited only by stack size
5. Partially Reversible: Pipelined Bennett
   - Advantages of reversible combined with higher throughput
Architecture Summary

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   • General purpose floorplan
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5. Partially Reversible: Pipelined Bennett
   • Advantages of reversible combined with higher throughput
QDCA Reversible Toffoli
Bennett’s Algorithm (1982)

- Original input saved throughout computation
- Intermediate state decomputed when possible
- Intermediate stage can be decomputed only if previous stage is computed
- Final state consists of original input and final output
- For 8 segments, at most 4 checkpoints need to be stored at any given time
Collapsed Bennett Layout: Regions of QCA Circuit
Collapsed Bennett Layout: Disable Regions

Logic Disable

Shift Disable
Collapsed Bennett Layout
Collapsed Bennett Layout

Compute

Uncompute

Shift Right

Shift Left

Logic Enabled
Shifter Disabled

Logic Disabled
Shifter Enabled

S.E. Murphy
Bennett Pipelined: Architecture (Top view)

**n clock phases:**
\[ \phi_n = \text{phased signals for Bennett clocking} \]
\[ V_{\text{min}} : \text{cell released} \]
\[ V_{\text{max}} : \text{cell locked} \]

**M stages:**
Bennett zones + Registers
Data pipelining

- **Computation:** A → B → C
- **Decomputation:** C ← B ← A

**M Stages**
- Initial latency: $M \times (T/2)$
- Throughput: $1/T$
Case study: XOR Tree

M stages parity checker

Partition in stages:
Lower limit: stage size = 2 QCA cell
Middle solution: stage size = 1 XOR GATE
Upper Limit: stage size = M XOR gates
• Landauer scheme shows higher throughput and the gap between the performances increases with the increase of c (c=14 only one Bennett stage). (note: c=1 not same as Landauer due to the size of the basic stage)
The improvement in terms of power consumption becomes better with the increase of $c$ (note: the power dissipated also with a pure Bennett scheme $c=14$ does not become zero as the inputs to the whole circuit are still deleted every $T$).
• “Given a second of time and a Joule of energy, what is the amount of operations (output bits) obtained?”
• The result shows an intersection of the two curves:
  – c<3 Landauer clocking has better performances
  – c>3 Bennett clocking behaves better
Silicon P-dot QCA cell

Demonstration of a silicon-based quantum cellular automata cell

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Centre for Quantum Computer Technology, School of Physics, University of Melbourne, Victoria 3010, Australia

(Received 8 March 2006; accepted 18 May 2006; published online 5 July 2006)

We report on the demonstration of a silicon-based quantum cellular automata (QCA) unit cell incorporating two pairs of metallically doped ($n^+$) phosphorus-implanted nanoscale dots, separated from source and drain reservoirs by nominally undoped tunnel barriers. Metallic cell control gates, together with Al–AlO$_x$ single electron transistors for noninvasive cell-state readout, are located on the device surface and capacitatively coupled to the buried QCA cell. Operation at subkelvin temperatures was demonstrated by switching of a single electron between output dots, induced by a driven single-electron transfer in the input dots. The stability limits of the QCA cell operation were also determined. © 2006 American Institute of Physics. [DOI: 10.1063/1.2219128]

• Dots defined by implanted phosphorus
• Single-donor creation foreseen
• Direct measurement of cell switching

FIG. 1. (Color online) (a) Simplified circuit equivalent of the QCA cell, (b) SEM image of phosphorus-implanted $n^+$ regions (dark in image), and (c) SEM image of completed device. The buried $n^+$ dots and leads are marked using dashed lines.
QDCA Logic Directly Attached to QC

Advantages:
- Integration on one substrate
- Low power dissipation reduces load on cooling system

Base diagram from Physical Review B 74, 045311 2006,
Two-dimensional architectures for donor-based quantum computing
Self-Contained Classical+Quantum Logic

Steane 5-bit QEC Measure-Classical Syndrome-Correct with no external connection except clock

Base diagram from Physical Review B 74, 045311 2006, Two-dimensional architectures for donor-based quantum computing
Large QC and QCA Arrays
Advantages

• QCA logic “lives” in the single electron world, thus avoiding the need to amplify single electron signals to CMOS levels.

• QCA logic would be used to execute the classical part of QEC recovery mechanisms, which is most (e.g. 99%) of the activity in a projected QC.

• Each QCA “island” would consume less resources than SET, amplifier, bonding pad, and cable to controller through cryostat it replaces.

• QCA would allow the classical circuitry to be implemented on-chip without over-heating the dilution refrigerator.
System + Application Architectures

Grounded in device physics & simulation

Incorporate clock driven dataflow

Device architecture maps well to many system architectures…

Reconfigurable

AND Plane

OR Plane

BC

AB

AC

AB + BC + AC

Systolic

Good for FIR, FT, Matrix multiply, graph algorithms, etc.

General Purpose
Simulations

New devices
New circuits
New architectures ↔ New simulators
Simulation levels

1) Quantum chemistry
   Ab initio, all-electron, and approx.
2) Density matrix (coherence vector)
   Quantum, dynamic, thermal effects, dissipation
3) Time-independent Schrod. Eq.
4) Semiclassical thermodynamic
5) Logic level
6) Architecture level
QCA design tools

QCADesigner

Konrad Walus
U. British Columbia

*QCADesigner* screenshot showing a simple 4-bit processor layout.
QCA design tools

QCATS
QCA
Thermodynamic Simulator
Semiclassical

Under development
M-AQUINAS
Molecular version of A QUantum Interconnected Network Array Simulator

- GUI allows point-and-click and drag-and-drop editing of QCA circuits.
- Schrödinger solver coupled to local clocking field.

Authors: Enrique Blair
Amy DeCelles
Simulation hierarchies

Architectural-level

+ Logic-level…

+ device-level…

Application-level performance metrics
Conclusions

• Power is a problem for logic today, and it is related to an approach to thermodynamic limits on computing
• However, these limits are due in part to historical choices that can be circumvented
  – Requires new basis for logic
  – Requires new devices, notably devices that handle information and heat differently

• Also: A tie in to coherent quantum computing
Partnership Opportunity

• This is a project under NINE and SBET
  – We are advocating research in
    • Computing beyond the limits of CMOS
    • Physics of information processing
  – The overall project’s deliverables to Sandia are to bootstrap multiple projects in
    • Physical science
    • Information science
    • Simulation
  – We’ve tried to outline opportunity and expose Sandia to willing partners
Applications and $100M Supercomputers

System Performance

Applications

Technology

No schedule provided by source

Quantum Computing Requires Rescaled Graph (see later slide)

④

③ Nanotech + Reversible Logic

μP

(best-case logic (green)

↑

μP

(red) →

② Architecture: IBM Cyclops, FPGA, PIM

↑

① Red Storm/Cluster

↓

100× ↑1000× [SCaLeS 03]

[SCaLeS 03] Workshop on the Science Case for Large-scale Simulation, June 24-25, proceedings on Internet a h t t p : / / w w w . p n l . g o v / s c a l e s / .

Experiments Under Discussion

- Continuation of Quantum Fortress work 1100
- Molecular QCA 1800
- Quantum Computing Tie-In
  - Architecture
  - Quantum Dot Measurements
  - Quantum Dot Manufacturing classical/quantum
- Computer Architecture beyond limits of Moore’s Law
- Simulation of information+Physics