Title: Quantum Dot Cellular Automata (QDCA) Strategic Partnership: Extending Moore's Law -- Part 1, Physical Sciences Issues

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Agreement: Sandia Contact has agreed to incorporate above listed conditions prior to release.

Comments:
1. The Title should spell out "- Part 1, Physical Sciences Issues" 2. This needs endorsement from a subject matter expert. Lyndon Pierson is being approached for the purpose.
Created by WebCo  Problems? Contact CCHD: by email or at 845-CCHD (2243).

For Review and Approval process questions please contact the Application Process Owner
Quantum Dot Cellular Automata (QDCA) Strategic Partnership: Extending Moore's Law: Part 1, Physical Sciences Issues

Erik DeBenedictis¹ (PI), Jerry Floro¹,³, Robert Hull³, Peter Kogge², Craig Lent², Sarah Murphy¹,², Mike Niemier², Marco Ottavi¹, Aaron Prager¹,², Greg Snider²

(¹Sandia, ²Notre Dame, ³U. Virginia)
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
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.

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

<table>
<thead>
<tr>
<th>Logic Device Technologies</th>
<th>Scalability</th>
<th>Performance</th>
<th>Energy Efficiency</th>
<th>Gain</th>
<th>Operational Reliability</th>
<th>Room Temp. Operation ***</th>
<th>CMOS Compatibility **</th>
<th>CMOS Architectural Compatibility *</th>
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<tbody>
<tr>
<td>1D Structures</td>
<td>2.4</td>
<td>2.4</td>
<td>2.1</td>
<td>24</td>
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<td>29</td>
<td>24</td>
<td>2.6</td>
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<td>1.7</td>
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<td>1.5</td>
<td>1.2</td>
<td>1.8</td>
<td>15</td>
<td>1.8</td>
<td>2.2</td>
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<td>2.2</td>
<td>15</td>
<td>2.0</td>
<td>2.2</td>
<td>1.7</td>
<td>1.8</td>
</tr>
</tbody>
</table>

For each Technology Entry (e.g. 1D Structures, sum horizontally over the 8 Criteria
Max Sum = 24
Min Sum = 8
Obeying Moore’s Law and Beating CMOS

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

100 k_B T Power Limit (to be discussed)

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

Lower is Better
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.
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

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<table>
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<tr>
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<th>0</th>
<th>1</th>
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</table>
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Three input majority gate can function as programmable 2-input AND/OR gate.
QCA single-bit full adder

Hierarchical layout and design are possible.

Simple-12 microprocessor (Kogge & Niemier)
Computational wave: adder back-end
We would like “kink energy” $E_k > k_B T$. 

Characteristic energy
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

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

shift register | 10
---|---
“OR” gate | A+B

A

B
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
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 shows: Logically reversible circuit can dissipate much less than $k_B T \ln(2)$
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
LDRD Status

• Current work underway at Sandia to find novel ways to create QCA cells
• SiGe identified as potential material system
• MBE growth of SiGe Quantum Fortresses underway
• FIB pattern designed and fabricated to allow electrical testing of Quantum Fortresses
• Electrical contact and testing will be undertaken this fall at University of Notre Dame
SiGe Quantum Fortresses

- Potential new way to create QCA cells
- Self-Assembled with 4 fold symmetry
- Fortress growth can be directed
SiGe Quantum Fortresses

- When grown at optimum conditions, Silicon Germanium alloys form “fortress-like” structure
- 4-fold symmetry of structure may allow it to be used as a QCA cell
- Growth can be directed by introducing defects to the crystal surface
3D Surface Sculpture
SiGe / Si (001)

Quasi-equilibrium
repulsion-driven
coarsening / phase transitions

Temperature
750°C

Ordered pyramidal dots

25 Å

Dot nucleation

100 Å

Dense dots

275 Å

Close-packed dome dots

550°C

Quantum ridges

Quantum wire/antiwire arrays

Discrete quantum molecules

HIGH SUPERSATURATION
kinetically-enforced cooperative nucleation

Anneal

300 Å

0.1 Å/s

Rate

0.9 Å/s

Thickness

50 Å

Irregular discrete dots

50 Å

Antidot nucleation

Anneal
SiGe Quantum Fortresses

- Silicon is patterned using a gallium FIB
- 7nm Si buffer is grown
- .6Å/s Si and .3Å/s Ge are grown, to a total thickness of 200Å.
Quantum Fortress Growth

$h_{nm} \text{ Ge}_{0.3} \text{Si}_{0.7}/\text{Si}(100)$, $550^\circ C$, $0.09 \text{ nm/s}$
SiGe Quantum Fortresses

• Quantum fortresses form around the gallium damage sites, roughly 220nm x 220nm.

• X-Ray Diffraction indicates that significant germanium enrichment occurs, allowing carrier confinement.

• These may be used as electrical devices such as SETs or Quantum Cellular Automata cells.
SiGe Quantum Fortresses

• Undirected nucleation also occurs, increasing the quantum dot density beyond the original pattern
Quantum Fortress Patterning

- Current experiments are attempting to grow capped, aligned samples which can be contacted using e-beam lithography and metal deposition
- Grid of Dots with fiducial marks created to facilitate electrical testing
Quantum Fortress QCA

FIB are used to deposit Pt contacts to ease the alignment requirements of the E-beam lithography.
Metal-dot QCA implementation

Metal tunnel junctions

Al/AlO$_2$ on SiO$_2$

electrometers

70 mK

“dot” = metal island
Metal-dot QCA cells and devices

- Demonstrated 4-dot cell

QCA Shift Register

$V_{IN}^+$
$V_{CLK1}$
$V_{CLK2}$
$V_{IN}^-$

$G_{top}$
$G_{bot}$
electrometers

$V^{+}$
$V^{-}$
$V_{CLK1}$
$V_{CLK2}$

Input
CLK$_1$
Latch$_1$
CLK$_2$
Latch$_2$

Time (msec)
Electron Switching in QCA

Metal Dots

Measure conductance

Molecular Dots

Measure capacitance

\[ G_{1-2}(\text{mS}) \]

Diagonal Voltage (mV)

(1,0)  (0,1)

Voltage
Double-dot click-clack

Hua & Fehlner

Notre Dame Center for Nano Science and Technology

Sandia National Laboratories
Magnetic QCA cell

- Dots are permalloy islands
- Limited to > ~20 nm sizes

CMOS analogue of QCA

- “Dots” are CMOS nodes
- Instead of charge quantization use transistor action
- Room temperature
- Slow performance
- Test-bed for architecture and power dissipation ideals
Silicon P-dot QCA cell

Demonstration of a silicon-based quantum cellular automata cell

Centre for Quantum Computer Technology, School of Electrical Engineering and School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia

C. Yang and D. N. Jamieson
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 metal-doped (n⁺) phosphorus-implanted nanoscale dots, separated from source and drain reservoirs by nominally undoped tunnel barriers. Metallic cell control gates, together with Al–AlOₓ single electron transistors for noninvasive cell-state readout, are located on the device surface and capacitively 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.
QCA chip isometric view

- Clock distribution plane
- QCA plane (molecules, Quantum fortresses...)
- Ground plane

\[ \phi_1, \phi_2, \phi_3, \phi_4 \]
Implementations

Four layers:
1. Upper insulating;
2. QCA
3. Lower insulating
4. Substrate

\[ C = \varepsilon_0 \varepsilon_r A / d \]

\[ R = \rho d / A \]

\[ C_{\text{tot}} = C_L + k C_m \]
Clock with RLC resonant circuit

- Parallel RLC circuit
- Ideally at resonating frequency no current is drained from the voltage supply
- The dissipation is related to the parasitic resistance in through the layers of the clocked circuit and the resistance of the clock wires
- To achieve a resonating frequency of 1 THz the LC product should be $\sim 10^{-24}$
- Consequently $L \sim \text{pH}$ and $C \sim \text{pF}$
System + Application Architectures

Grounded in device physics & simulation

Incorporate clock driven dataflow

Device architecture maps well to many system architectures…

Reconfigurable

<table>
<thead>
<tr>
<th>AND Plane</th>
<th>OR Plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>A A' B B' C C'</td>
<td>A B C + A B C + A B C</td>
</tr>
</tbody>
</table>

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...

Minterm-In

Literal-In

Select Bit (S)

= 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
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
Applications and $100M Supercomputers

**System Performance**

<table>
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<tr>
<th>Performance</th>
<th>Applications</th>
<th>Technology</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Zettaflops</td>
<td>Plasma Fusion Simulation [Jardin 03]</td>
<td>④ Quantum Computing Requires Rescaled Graph (see later slide)</td>
</tr>
<tr>
<td>100 Exaflops</td>
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<tr>
<td>100 Teraflops</td>
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**Applications**

- Full Global Climate [Malone 03]
- Compute as fast as the engineer can think [NASA 99]
- MEMS Optimize

**Technology**

- Nanotech + Reversible Logic µP (green) best-case logic (red) →
- Architecture: IBM Cyclops, FPGA, PIM →
- Red Storm/Cluster →

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