Overview of Simulation Strategies for Nanoelectronics

E. B. Rudnyi, CADFEM GmbH
J. G. Korvink, IMTEK, University of Freiburg
Outline

⇒ Introduction to Nanoelectronics

⇒ Nanoelectronics in ITRS

⇒ Molecular Simulation

⇒ Conclusion
Moore’s Law

 ⇒ Exponential growth.
 ⇒ Cost per function reduction:
     → 25-29% per year.
 ⇒ Market growth:
     → On average 17% per year.
 ⇒ The law holds for about 45 years.
 ⇒ ITRS
     → Industry want to keep with this law further.

Gordon E. Moore, 1965

Cramming more components onto integrated circuits
Papers on Nanoelectronics: Web of Science

⇒ 925 papers:
  → Refereed journals.
⇒ Search includes:
  → Title,
  → Keywords,
  → Abstract.
Papers on Nanoelectronics: IEEE

- 1681 papers.
- Only IEEE publications.
- IEEE conferences are included.
CRC On-Line Book Chapters

⇒ 163 Hits
What is Nanoelectronics?

⇒ Electronics on a nanometer scale (feature size less than 100 nm)

⇒ Si-based (CMOS) and beyond-CMOS

⇒ Is “electro” important?
  → Information processing
What technical capabilities need to be developed for the industry to stay on Moore’s Law and the other trends?
Contributors

2005 ITRS Members by Region

- USA (709) 55%
- Japan (223) 17%
- Korea (60) 5%
- Taiwan (172) 13%
- Europe (124) 10%

2005 ITRS Members by Affiliation

- Chip makers (677) 53%
- Equipment / Materials Suppliers (263) 20%
- Consortium / Research Institute / University (274) 21%
- Others (74) 6%

Figure 1 Composition of the ITRS Teams—1288 Global Participants
Structure

⇒ Executive Summary (89 pages)

⇒ 11 Focus International Technology Working Groups
   → ...
   → Emerging Research Devices / Emerging Research Materials
   → ...

⇒ 4 Crosscut International Technology Working Groups
   → ...
   → Modeling and Simulation
ITRS Product Technology Trend

Near-term
Years: 2005 to 2013

Long-term
Years: 2014 to 2020
# Scaling CMOS

## Table 76a  Lithography Technology Requirements—Near-term Years

<table>
<thead>
<tr>
<th>Year of Production</th>
<th>2005</th>
<th>2006</th>
<th>2007</th>
<th>2008</th>
<th>2009</th>
<th>2010</th>
<th>2011</th>
<th>2012</th>
<th>2013</th>
</tr>
</thead>
<tbody>
<tr>
<td>DRAM ½ pitch (nm) (contacted)</td>
<td>80</td>
<td>70</td>
<td>65</td>
<td>57</td>
<td>50</td>
<td>45</td>
<td>40</td>
<td>36</td>
<td>32</td>
</tr>
<tr>
<td>DRAM and Flash</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DRAM ½ pitch (nm)</td>
<td>80</td>
<td>70</td>
<td>65</td>
<td>57</td>
<td>50</td>
<td>45</td>
<td>40</td>
<td>35</td>
<td>32</td>
</tr>
<tr>
<td>Flash ½ pitch (nm) (un-contacted poly)</td>
<td>76</td>
<td>64</td>
<td>57</td>
<td>51</td>
<td>45</td>
<td>40</td>
<td>36</td>
<td>32</td>
<td>28</td>
</tr>
<tr>
<td>Contact in resist (nm)</td>
<td>94</td>
<td>79</td>
<td>70</td>
<td>63</td>
<td>56</td>
<td>50</td>
<td>44</td>
<td>39</td>
<td>35</td>
</tr>
<tr>
<td>Contact after etch (nm)</td>
<td>85</td>
<td>72</td>
<td>64</td>
<td>57</td>
<td>51</td>
<td>45</td>
<td>40</td>
<td>36</td>
<td>32</td>
</tr>
<tr>
<td>Overlay [A] (3 sigma) (nm)</td>
<td>15</td>
<td>13</td>
<td>11</td>
<td>10</td>
<td>9</td>
<td>8</td>
<td>7.1</td>
<td>6.4</td>
<td>5.7</td>
</tr>
<tr>
<td>CD control (3 sigma) (nm) [B]</td>
<td>8.8</td>
<td>7.4</td>
<td>6.6</td>
<td>5.9</td>
<td>5.3</td>
<td>4.7</td>
<td>4.2</td>
<td>3.7</td>
<td>3.3</td>
</tr>
</tbody>
</table>

Manufacturable solutions exist, and are being optimized
Manufacturable solutions are known
Interim solutions are known
Manufacturable solutions are NOT known
CMOS and beyond CMOS

⇒ CMOS is the workhorse of the industry.
⇒ Yet, scaling of CMOS has technological and physical limits.
⇒ The semiconductor industry’s future success continues to depend on new ideas.
⇒ Chapter on Emerging Research Devices including Emerging Research Materials.
Taxonomy for Nano Information Processing

- Digital
  - Boolean
  - Analog
  - Electric charge
    - Scaled CMOS
    - 1D FETs
    - RTDs
    - SETs

- Computational models
  - Bio inspired
  - Quantum

- Architectures
  - Reconfigurable
  - Bio inspired
  - Quantum

- State variables
  - Molecular state
  - Phase state
  - Spin orientation
  - Molecular
  - Ferromagnetic
  - Spintronic

- Devices
  - Bio inspired
  - Quantum
Devices and Architectures

⇒ Devices:
  → Carbon nanotube and nanowires,
  → Ferroelectric FET memory,
  → Molecular,
  → Nano floating gate memory,
  → Polymer memory,
  → Polymer transistor,
  → Resonant tunneling devices,
  → Spin transistor.

⇒ Architectures:
  → Quantum Cellular Automata,
  → Cellular Nonlinear Networks,
  → Reconfigurable Implementations,
  → Biologically Inspired Implementation.
Emerging Technologies and CMOS
Potential Solutions for Logic Devices (CNT and NW)

<table>
<thead>
<tr>
<th>Rank</th>
<th>Description</th>
</tr>
</thead>
</table>
| 3    | Substantially exceeds CMOS  
* or is compatible with CMOS architecture  
** or is monolithically integrable with CMOS wafer technology  
***or is compatible with CMOS operating temperature (i.e., Substantially Better than Silicon Logic) |
| 2    | Comparable to CMOS  
* or can be integrated with CMOS architecture with some difficulty  
** or is functionally integrable (easily) with CMOS wafer technology  
***or requires a modest cooling technology, T ≥ 77K (i.e., Comparable to Silicon Logic) |
| 1    | Substantially (2×) inferior to CMOS  
* or can not be integrated with CMOS architecture  
** or is not integrable with CMOS wafer technology  
***or requires very aggressive cooling technology, T < 77K (i.e., Substantially Worse that Silicon Logic) |
Modeling and Simulation: Technology CAD for CMOS

⇒ High-frequency device and circuit modeling

⇒ Front-end process modeling

⇒ Integrated modeling of equipment and materials

⇒ Lithography simulation

⇒ Thermo-mechanical-electrical modeling for interconnections and packages
Modeling and Simulation: Molecular Simulation

- Ultimate nanoscale CMOS simulation
- Nano-scale modeling of novel devices
- Modeling of new materials

- Nanoscale simulation capability including accurate atomistic and quantum effects

- **Algorithms:**
  - Efficient atomistic/quantum models; ab-initio or molecular dynamics based topography simulations;
  - Multi-scale simulation (atomistic-continuum); fast coupling of equipment-topography-electrical-reliability models; hierarchical full-chip simulation.
Model Order Reduction for EDA

⇒ Current EU projects:
  → COMSON (COupled Multiscale Simulation and Optimization in Nanoelectronics)
    http://www.comson.org/
  → CHAMELEON RF, (Comprehensive High-Accuracy Modelling of Electromagnetic Effects in Complete Nanoscale RF blocks)
    http://www.chameleon-rf.org/
  → O-MOORE-NICE, (Operational MOdel Order REduction for Nanoscale IC Electronics)
Course: Molecular Simulation for MST

⇒ J. G. Korvink, E. B. Rudnyi
  → http://evgenii.rudnyi.ru/teaching.html#md
⇒ Introductory course for MST engir
⇒ 12 lectures, 3 computational labs
From the First Principles

⇒ Ab initio (from the beginning)
⇒ Input: A few fundamental constants
  → electron mass, proton mass, Plank constant, speed of light, ...
⇒ Output: Everything

⇒ Computationally expensive

⇒ Blue Gene: IBM Petaflop computer
  → Protein folding
Hierachy

⇒ Potential Energy Surface (0 K)
  → Electronic Schrödinger Equation
  → Semiempirical methods
  → Molecular Mechanics

⇒ Adding Entropy and Temperature
  → Molecular Dynamics
  → Monte Carlo

⇒ QSAR (empirical correlations)
Schrödinger Equation

\[ H = T_{\text{nucl}} + T_{\text{elec}} + U_{\text{nucl-nuc}} + U_{\text{elec-elec}} + U_{\text{elec-nuc}} \]

Nuclei \((R)\) and electrons \((r)\):

\[ \Psi(R, r) \quad H\psi = E\psi \]
Potential Energy Surface

⇒ Born-Oppenheimer Approximation
⇒ Proton is 1836 times heavier than electron.

→ Factorize for nuclei part

\[ \Psi(R, r) = \Psi(R) \psi(r; R) \]

→ Schrödinger equation for electrons

\[ H_{el} \psi(r; R) = E_{el}(R) \psi(r; R) \]
PES Example
Quantum Chemistry Methods

Molecular orbitals

\[ \Psi(1,2,\ldots,N) \approx \psi(1)\psi(2)\ldots\psi(N) \]

Atomic orbitals

\[ \psi = \sum_i c_i \varphi_i \]
What kind of software is needed?

As the main challenge in nanoscale technology derive from quantum phenomena across nanoscale junctions, interfaces and surfaces, it is critical to be able to accurately model such phenomena from quantum theory.
Semiempirical Methods

⇒ Consider valence electrons only

⇒ Neglect some integrals

⇒ Parameterize the others

⇒ Accuracy depends on the parameterization
Molecular Mechanics

⇒ Empirical force field
  → Bonding: stretching, bending, torsion, cross-terms;
  → Not-bonding: van der Waals, electrostatic, hydrogen, etc...

⇒ Accuracy depends on the force field employed
Molecular Dynamics and Monte Carlo

⇒ **Input:**
  → Potential energy surface

⇒ **Output:**
  → Heat conductivity, viscosity, …

⇒ **Time average**
  → Integrating in time

⇒ **Ensemble average**
  → Sampling according to Boltzmann distribution
Multiscale Simulation

Silicon Gear Teeth


Sub-micron Microresonator

Two Million Particle Device

Dynamic Region

Gear Shaft

FE

CGMD

Handshake

MD

FE/CG MD

Force of Gravity (N) in Angstroms

Time (10^8 seconds)
Conclusion

⇒ Beyond CMOS: New ideas for nanoelectronics

⇒ Molecular simulation is a natural way to check new ideas

⇒ Tight collaboration between industry and academia
EUNANAIA.

ENIAC is the European Technology Platform for Nanoelectronics

The principal mission of ENIAC is to:

- Provide a strategic research agenda for the nanoelectronics sector, with respect to R&D;
- Set out strategies and roadmaps to achieve this vision through the Strategic Research Agenda and other associated documents;
- Stimulate increased and more effective and coherent public and private investment in R&D in the nanoelectronics sector;
- Contribute to improving convergence between EC, national, regional and private R&D actions on nanoelectronics within the European Research Area Framework;
- Enhance networking and clustering of the R&D capacity in Europe;
- Promote European commitment to R&D thus ensuring Europe as an attractive location for researchers;
- Interact with other policies and actors at all levels that influence the competitiveness of the sector such as education and training, competition, IPR, finance and investment, etc.

How to express your interest

You are invited to submit an Expression of Interest that should include a short overview of the organisation's activities in the nanoelectronics sector as well as the motivation for participating in ENIAC. A short CV of the person from the organisation that would be the contact point (including a web link) should also be included.
NanoFab - neue Wege in der Nanoelektronik