Challenges and Opportunities for Modeling and Simulation

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obligatory Moore’s Law plot
nanoscale MOSFETs

ITRS 2022: $L_{\text{PHYS}} = 8 \text{ nm}$

- SiON $\sim 1.1 \text{ nm}$
- channel $\sim 40 \text{ nm}$
device simulation

- Monte Carlo simulation
  - with quantum corrections

- Drift-diffusion

molecular electronics

\[ \vec{J} = n q \mu_n \dot{E} + q D_n \nabla \dot{n} \]

\[ \mu = \frac{q \tau}{m^*} \]
generic model of a nanodevice

\[ \gamma = \frac{h}{\tau} \]

S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
(“Concepts of Quantum Transport” nanohub.org)
Landauer-Datta

\[ I_D = \frac{2q}{h} \int T(E) M(E) \left( f_1 - f_2 \right) dE \]

or

\[ I_D = \frac{2q}{h} \int \gamma (E) \pi \frac{D(E)}{2} \left( f_1 - f_2 \right) dE \]
S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
(“Concepts of Quantum Transport” nanohub.org)
limits of MOSFETs

from M. Luisier, ETH Zurich / Purdue
spintronics

Theory: Datta group Purdue

Electron Transport: NEGF Approach

Magnetization

Torque

Spin-NEGF

LLG Equation

Dynamics of Magnets

Top Electrode

CoFeB (3)

MgO (0.85)

CoFeB (3)

Ru (0.85)

CoFe (2.5)

Bottom Electrode

Experiment: Cornell

21st century electronics

molecular electronics

carbon nanotube electronics

flexible electronics

spin torque devices

nanowire bio-sensors

nanowire thermoelectrics

CoFe (2.5)
Ru (0.85)
CoFeB (3)
MgO (0.85)
CoFe (2.5)

Al Gate
HfO₂
10 nm SiO₂

p++ Si

nanonets

L₆

L₈

G

SD

SWNT

carbon nanotube

electronics

nanowire PV

molecular electronics

flexible electronics

nanowire thermoelectrics
MOSFETs and variability

Random Dopant Fluctuations

1997 MOSFET (Texas Instruments)

nanostructured solar cells (Alam group)

Phase segregation dominated by Spinodal decomposition

Holes

electron

anneal time
1) Transistors
   - quantum transport with dissipation
   - dealing with randomness and variability

2) Beyond transistors
   - from the atomistic/nano scales to the (often random) micro- and macro scales.

3) Other challenges
builders (experimentalists) vs. analysts

http://www.endex.com/gf/buildings/bbridge/bbgallery/

Eugene Fergason, in *Engineering and the Mind’s Eye*, 1994
why we simulate

Three reasons to simulate:

1) to **explore** uncharted territory

2) to **resolve** well-posed questions

3) to make good **design** choices

what we’re after

Two kinds of results:

1) answers, insight, understanding

2) numbers and software

(after Brian Hayes, on “inquisitive computing” in American Scientist, 2008)
role cyberinfrastructure

www.nanoHUB.org

signature service:
online simulation to connect simulation tool developers and users
cloud computing for science and engineering

Rappture +

Simulation Code

Simulation tool user

= Maxwell’s Daemon

Physical Machine

Virtual Machine

rendering farm

grid

Content Database

nanoHUB.org

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cyber-enabled research

Arvind Raman
ME, Purdue
Virtual Environment for Dynamic AFM

- Comprehensive suite of AFM simulation tools
- Includes realistic tip sample interaction models
- Sophisticated cantilever dynamics models
- Liquid/ambient/vacuum conditions
- Soft/hard organic/inorganics samples
- Used by individual researchers…
- and AFM industry (Agilent, Veeco, Asylum)

“I have been using VEDA now for almost a year and have found it to be extremely useful. … Finally, I have also been very happy with the ability to run these sometimes rather computationally expensive calculations remotely. I joked about it last year .. but since then I have actually run several calculations on my iPhone while traveling.”
Roger Proksch, CEO and co-founder, Asylum Research
another view

“The purpose of computing is insight - not numbers.”

-Richard W. Hamming
“Electronics from the Bottom Up”

“Research on molecular and nanoscale electronics is providing a new understanding of electronic conduction at the smallest scale. The objective of “Electronics from the Bottom-Up” is to convey these new insights, understanding, and conceptual approaches to students and working engineers worldwide.”

19,259 nanoHUB.org EBU students last year.

New partnership with World Scientific.
nanoHUB.org

>90,000 users/year
the biggest challenge in computational science

Where’s the Real Bottleneck in Scientific Computing?

Gregory V. Wilson

Scientists would do well to pick up some tools widely used in the software industry

American Scientist, pp.5,6, Jan/Feb 2006.

Software Carpentry:
Essential Software Skills for Research Scientists
https://www.nanohub.org/resources/1811
There are plenty of challenges, but many more opportunities!