

Frontiers of Characterization and Metrology for Nanoelectronics

Challenges and Opportunities for Modeling and Simulation

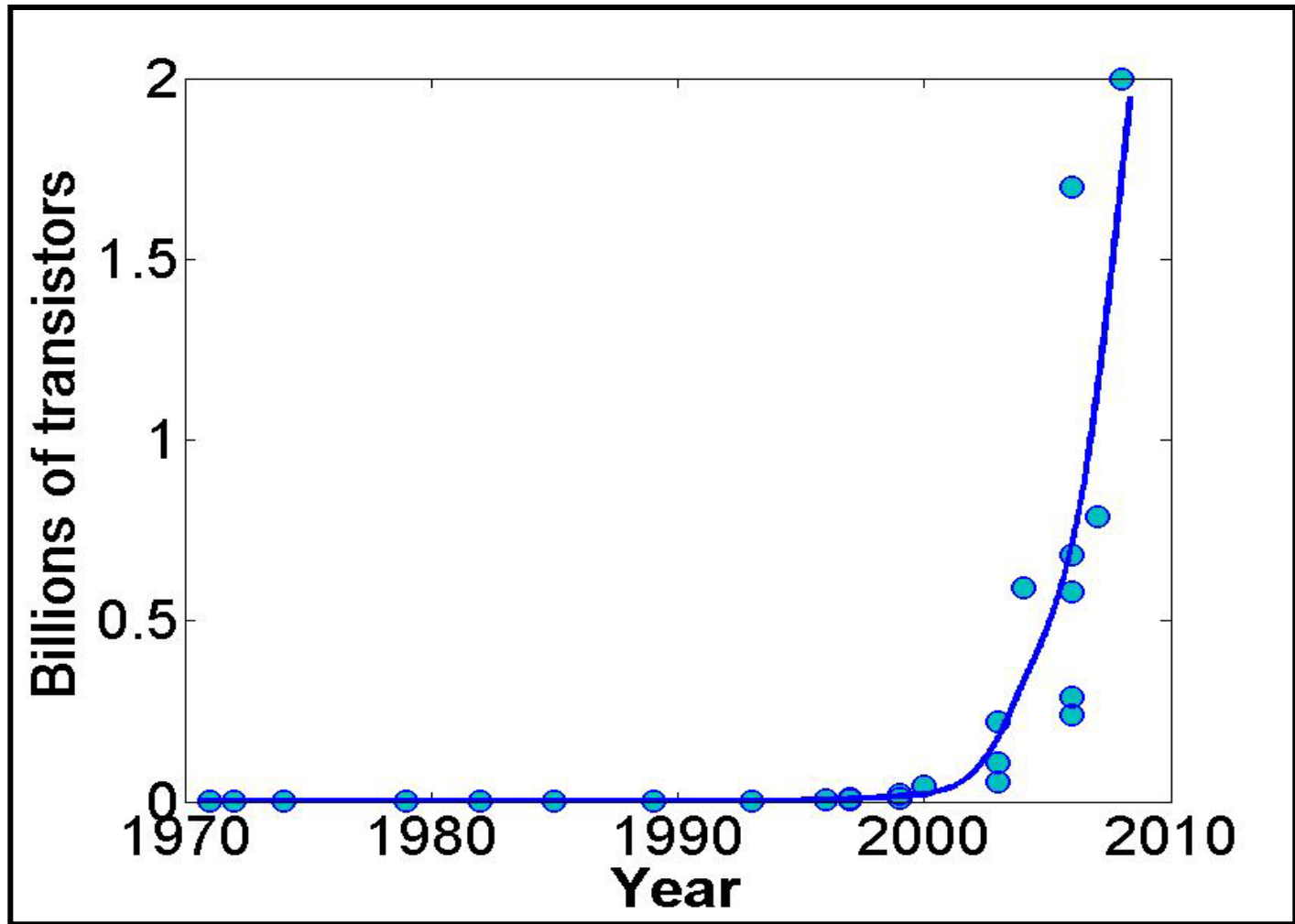
Mark Lundstrom

Network for Computational Nanotechnology

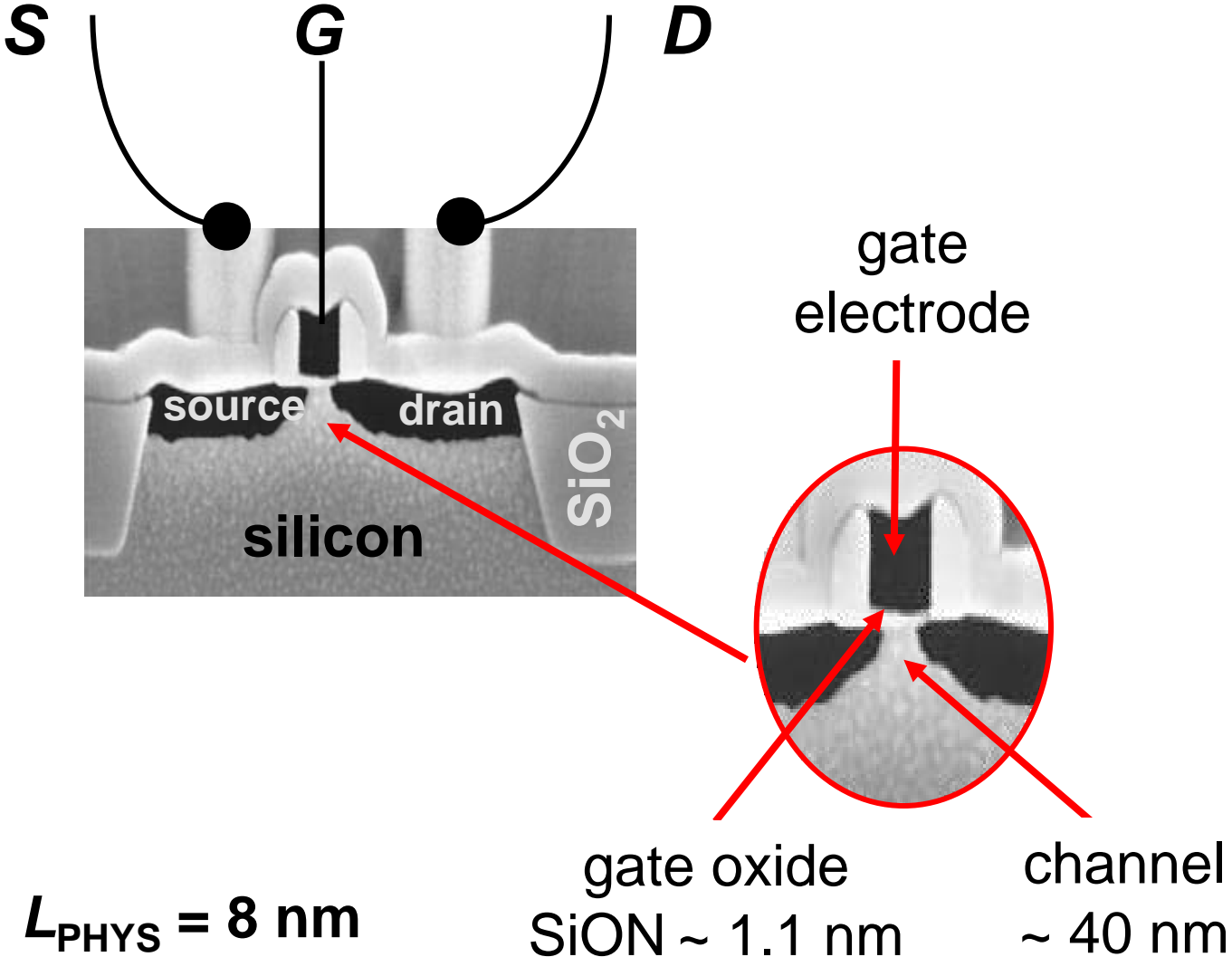
Purdue University

West Lafayette, Indiana USA

obligatory Moore's Law plot



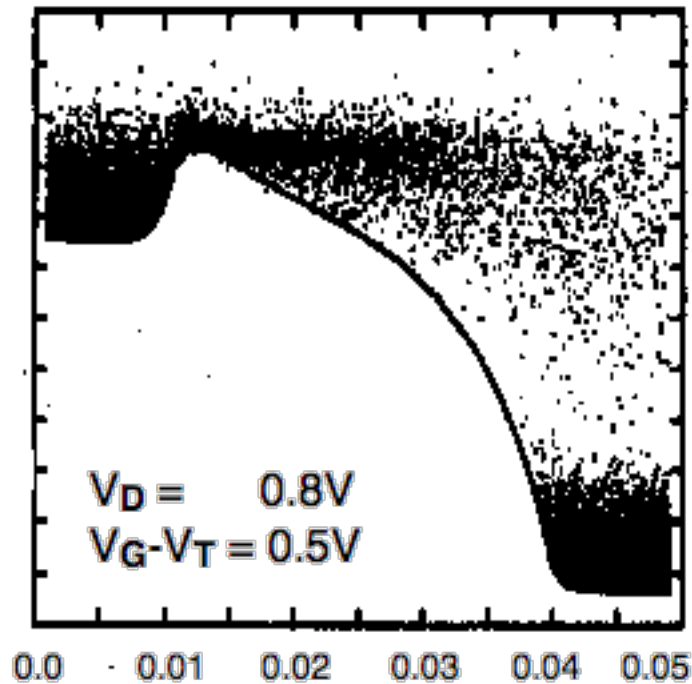
nanoscale MOSFETs



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

**gate oxide
SiON ~ 1.1 nm** **channel
~ 40 nm**

device simulation

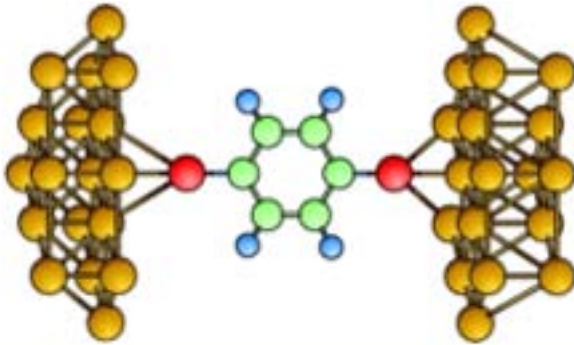


Position along Channel (μm)

Frank, Laux, and Fischetti, IEDM
Tech. Digest, p. 553, 1992.

- **Monte Carlo simulation**
-with quantum corrections
- **Drift-diffusion**

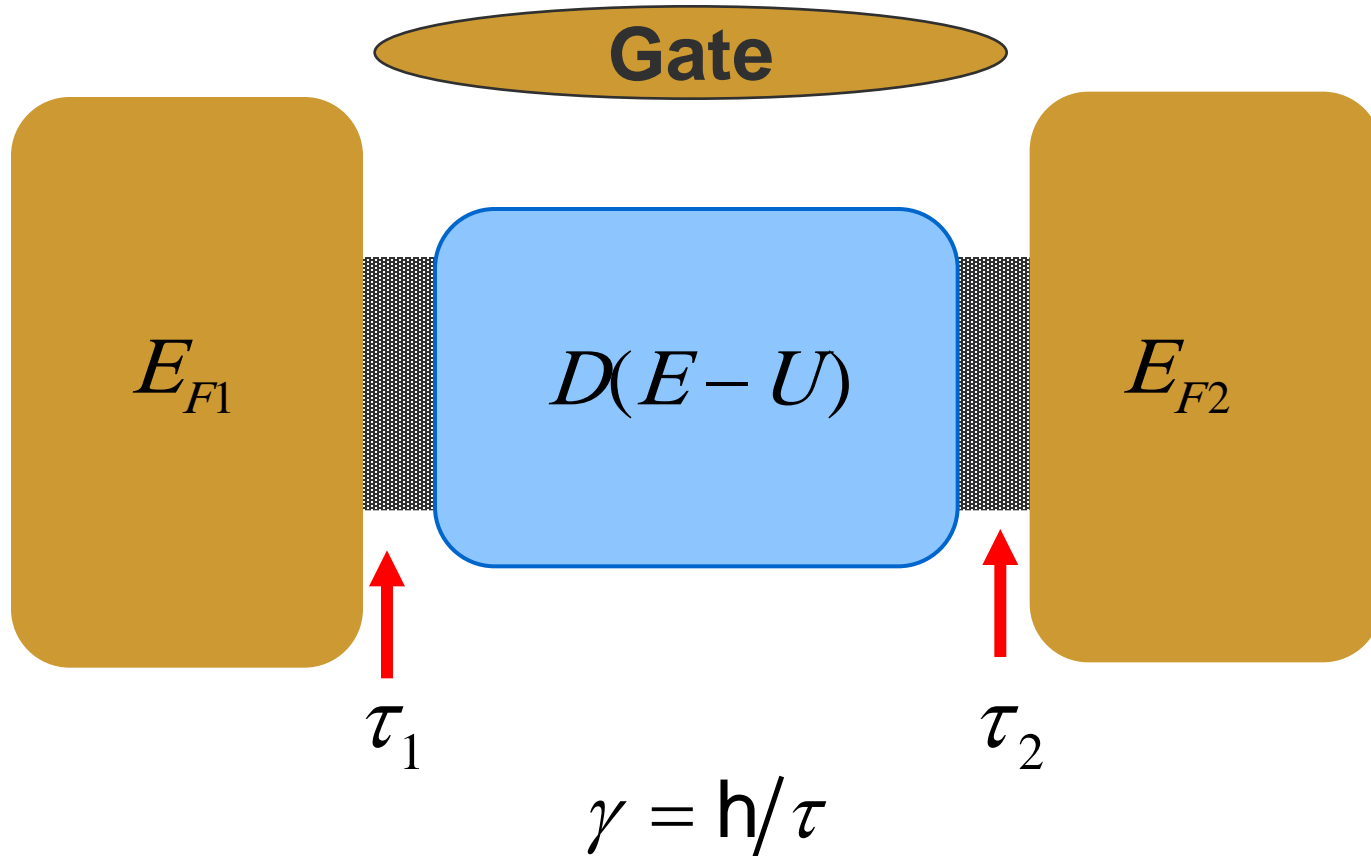
molecular electronics



$$\vec{J} = nq\mu_n \vec{E} + qD_n \nabla n ?$$

$$\mu = \frac{q\tau}{m^*} ?$$

generic model of a nanodevice



S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
("Concepts of Quantum Transport" nanohub.org)

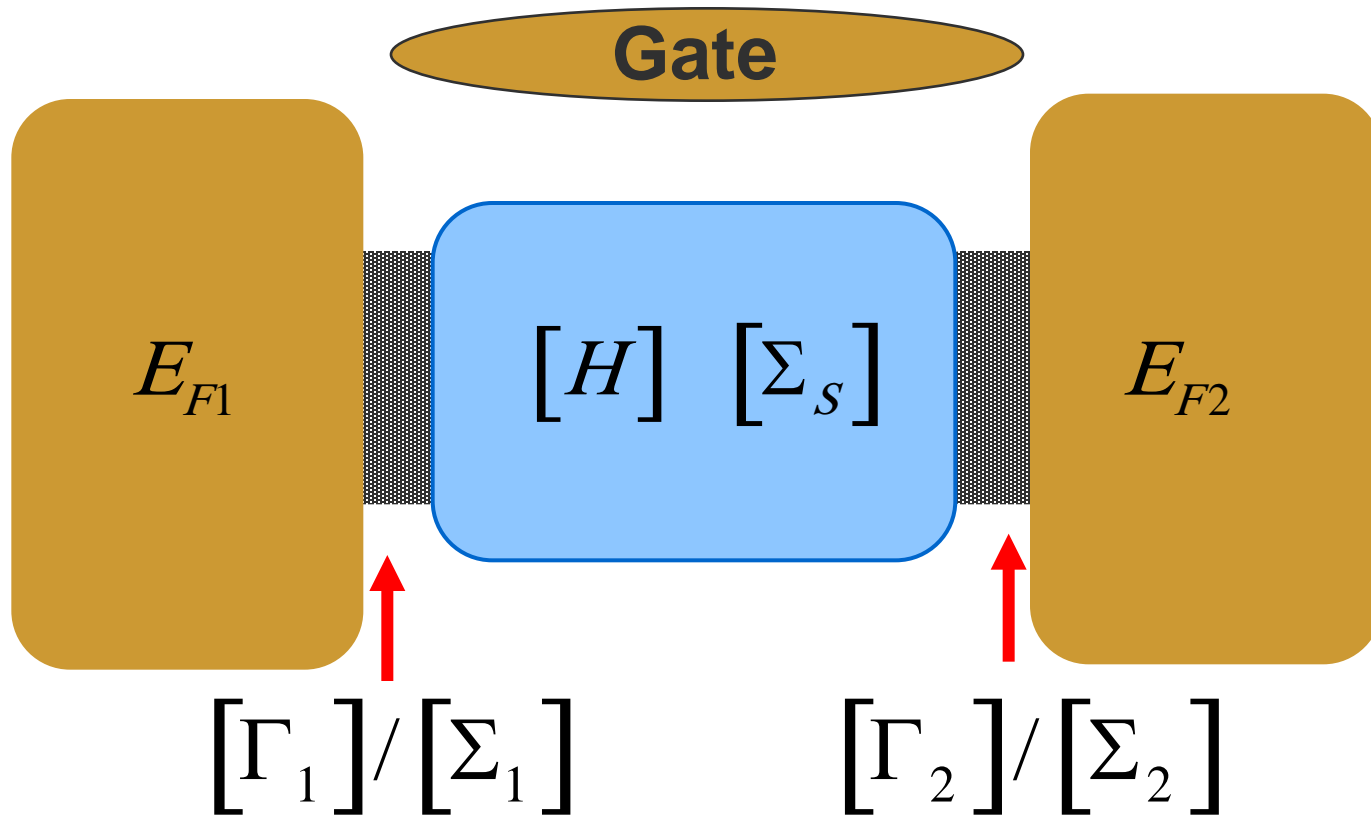
Landauer-Datta

$$I_D = \frac{2q}{h} \int T(E) M(E) (f_1 - f_2) dE$$

or

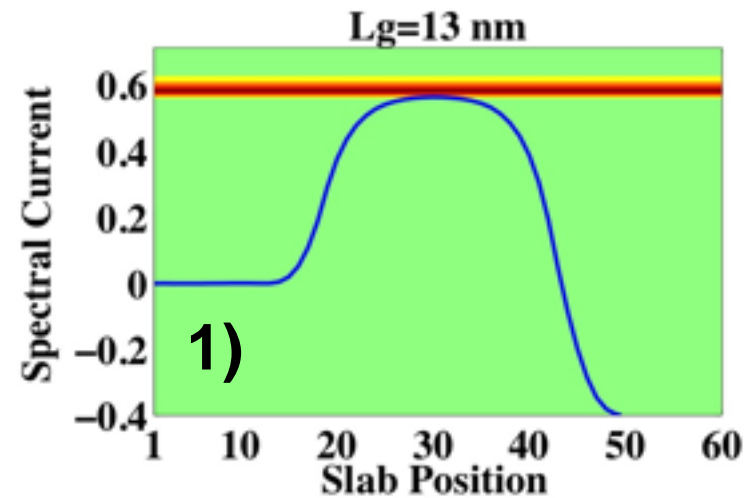
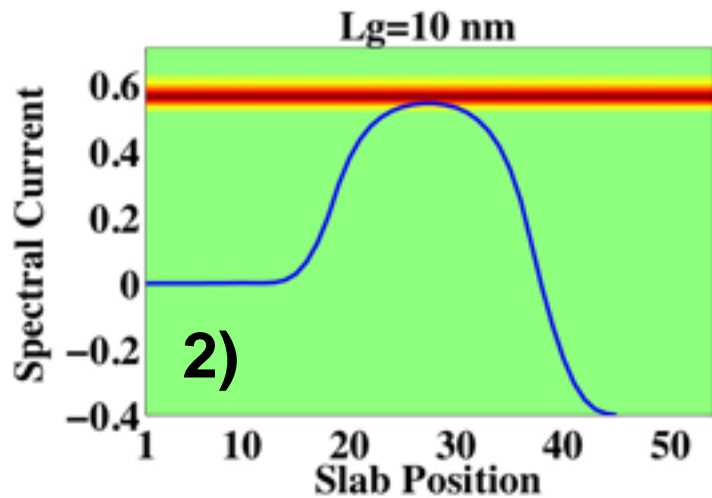
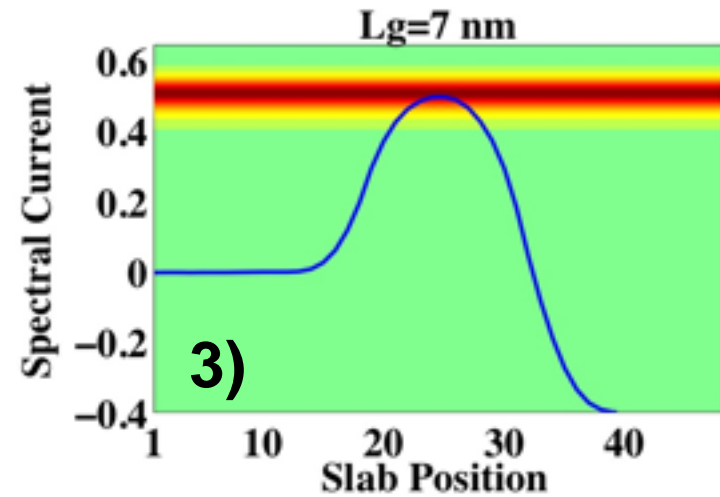
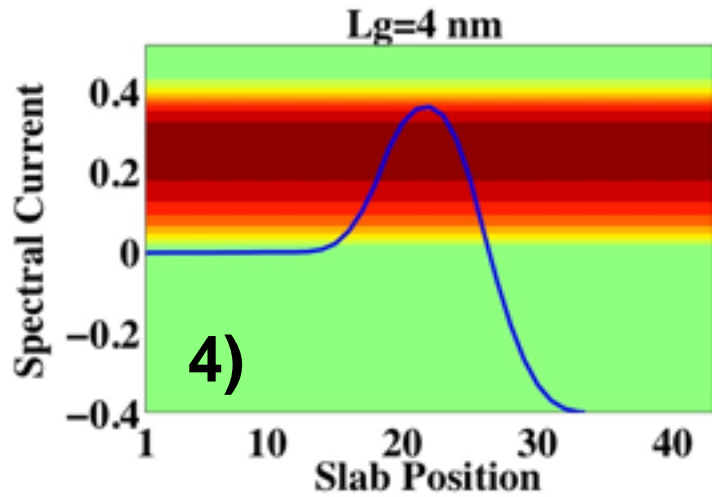
$$I_D = \frac{2q}{h} \int \gamma(E) \pi \frac{D(E)}{2} (f_1 - f_2) dE$$

generic model --> NEGF



S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
("Concepts of Quantum Transport" nanohub.org)

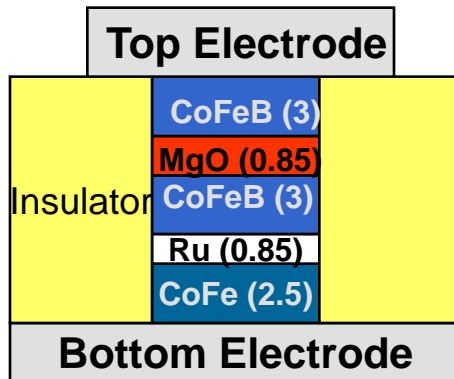
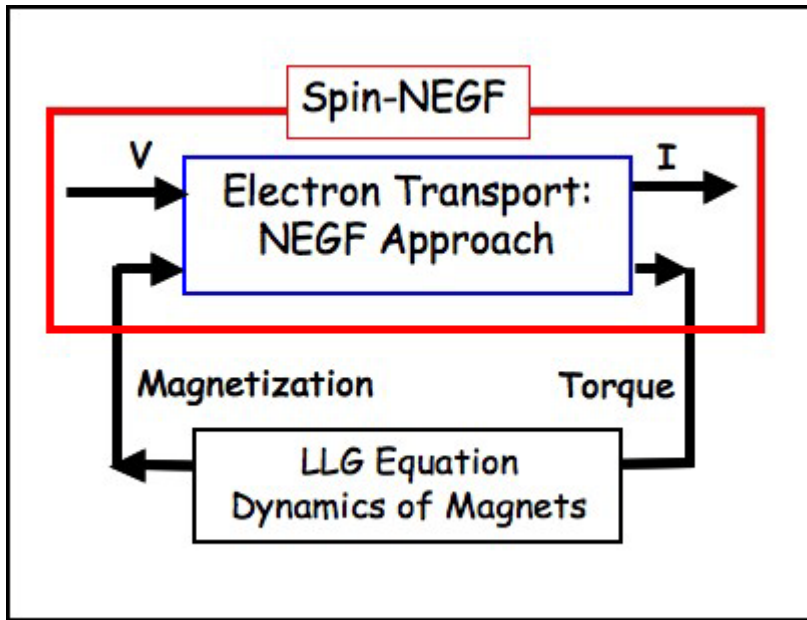
limits of MOSFETs



from M. Luisier, ETH Zurich / Purdue

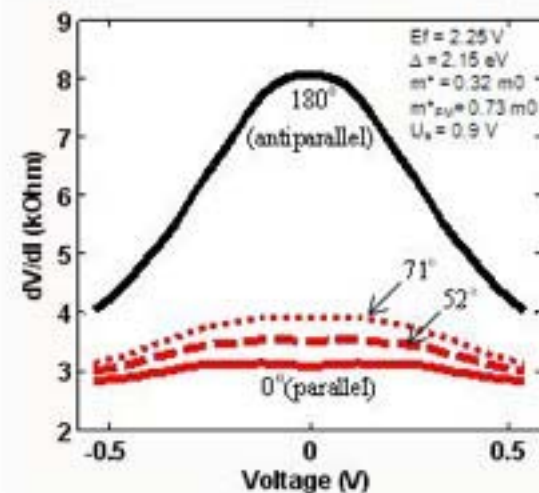
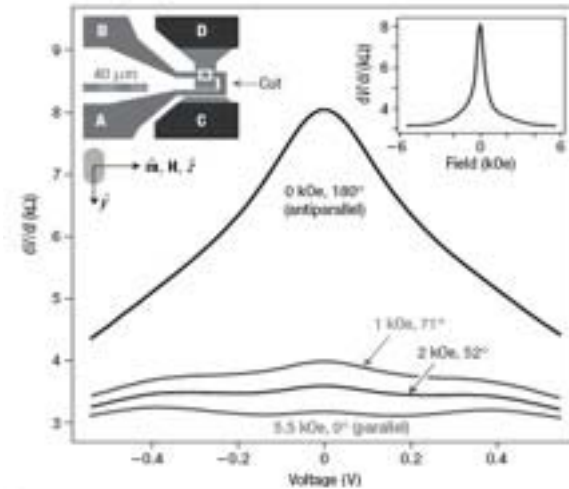
spintronics

Theory: Datta group Purdue



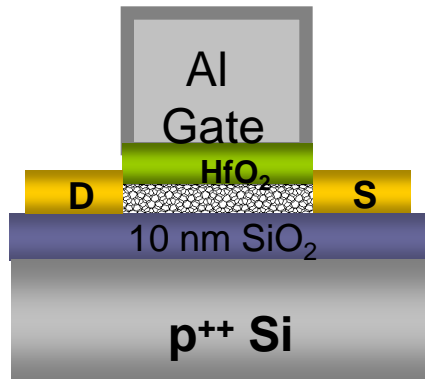
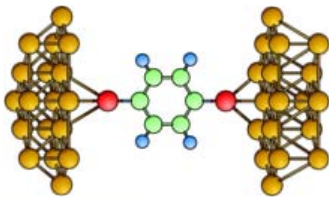
Experiment: Cornell

Sankey et al. *Nat. Phys.*, 4, 67 (2008)

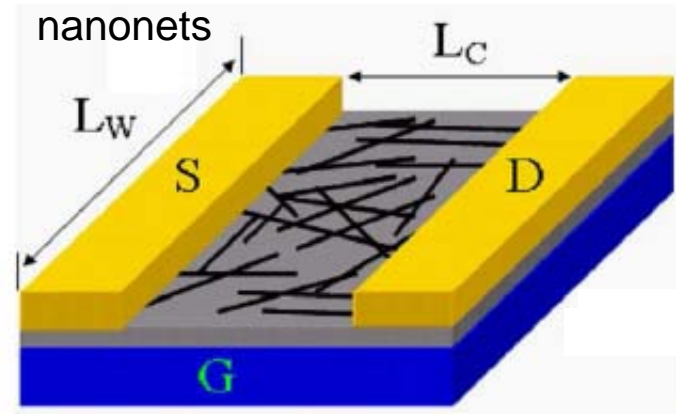


21st century electronics

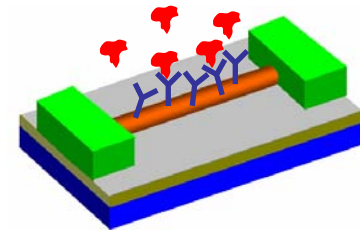
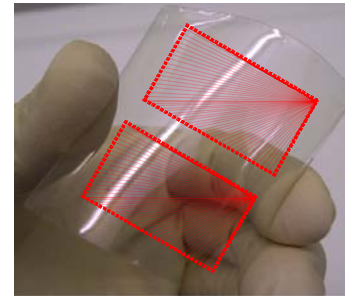
molecular electronics



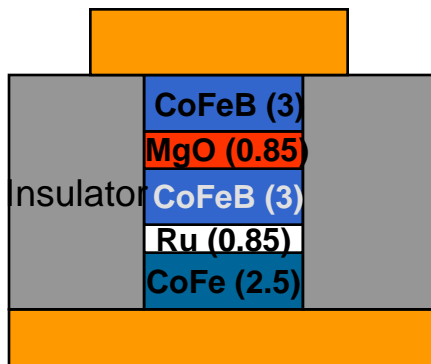
carbon nanotube electronics



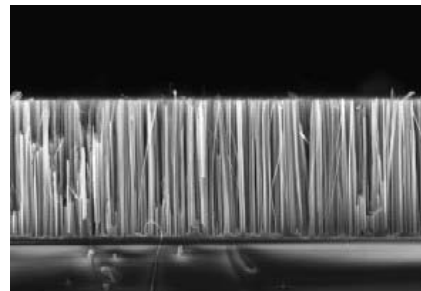
flexible electronics



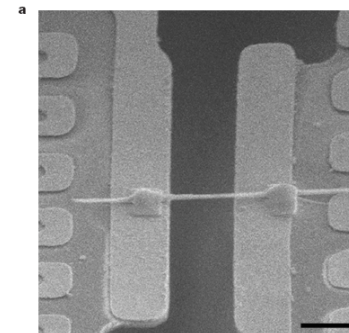
nanowire bio-sensors



spin torque devices



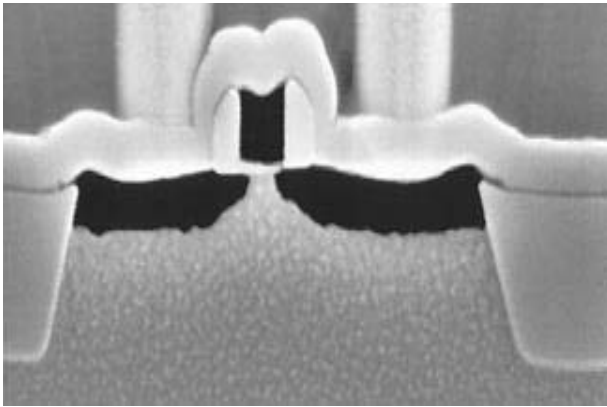
nanowire PV



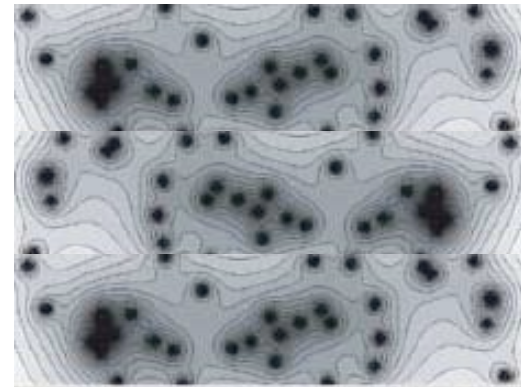
nanowire thermoelectrics

MOSFETs and variability

Random Dopant Fluctuations

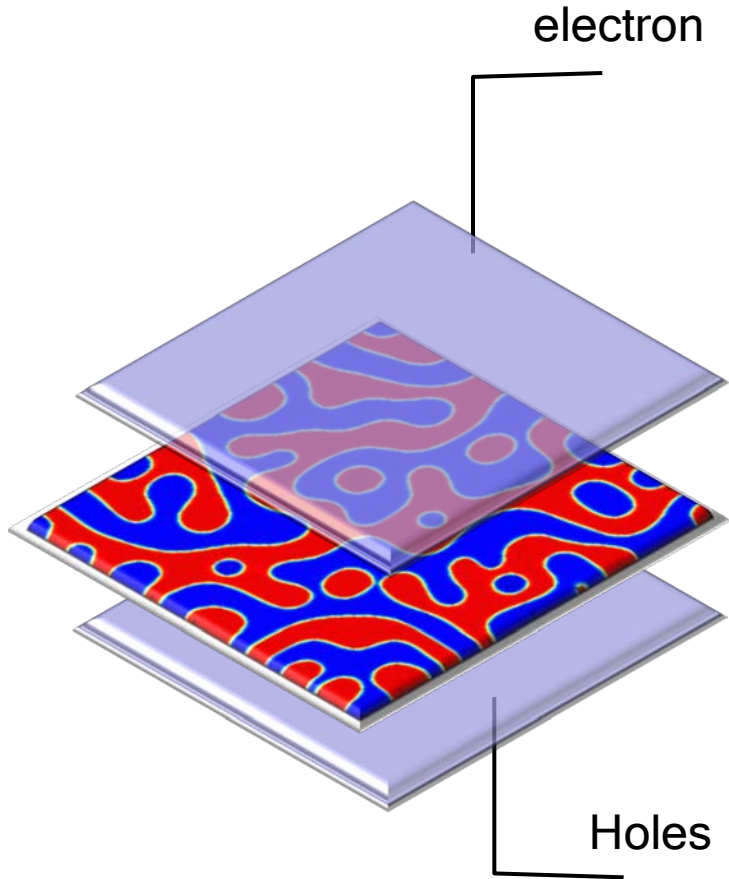


1997 MOSFET
(Texas Instruments)

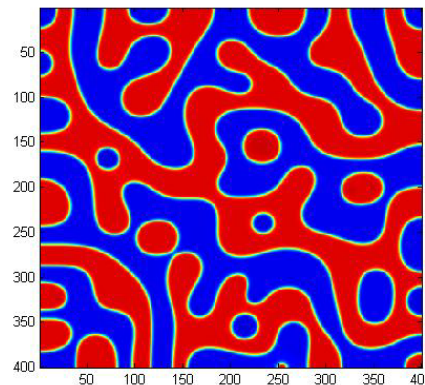
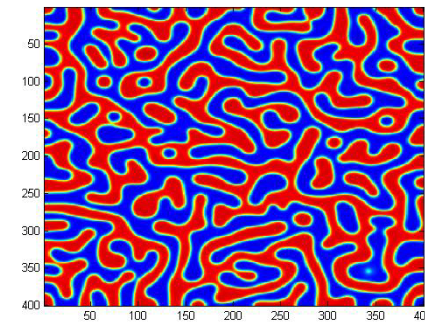
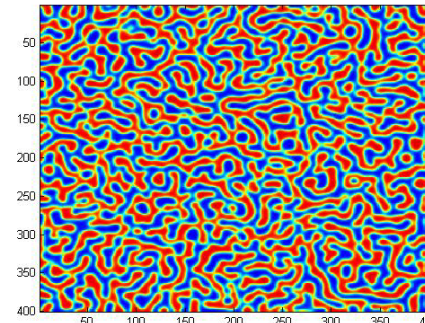


after Takahiro Shinada, et al.,
Nature, **437**,1128, 2005

nanostructured solar cells (Alam group)



Phase segregation dominated by Spinodal decomposition



anneal time

challenges

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 Ferguson, 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

-Leo Kadanov, *Computing in Science and Engineering*, 2004

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

The screenshot shows the nanoHUB.org website homepage. At the top, the logo reads "nanoHUB online simulation and more" with "by NCN member" next to it. A navigation bar includes links for Home, My nanoHUB, Resources, Contributors, Events, About, and Support. A search bar and a "Help" icon are also present. A status bar at the top right indicates "Logout (fundstro)", "141 guests, 25 members online - 4954022 hits last month", and "Whole".

The main content area features a large banner with the text "Over 60,000 annual users" and "Join the nanoHUB community". Below this, there are sections for "Take a tour", "A resource for nanoscience and technology", and "Learn more".

The page is organized into four main columns:

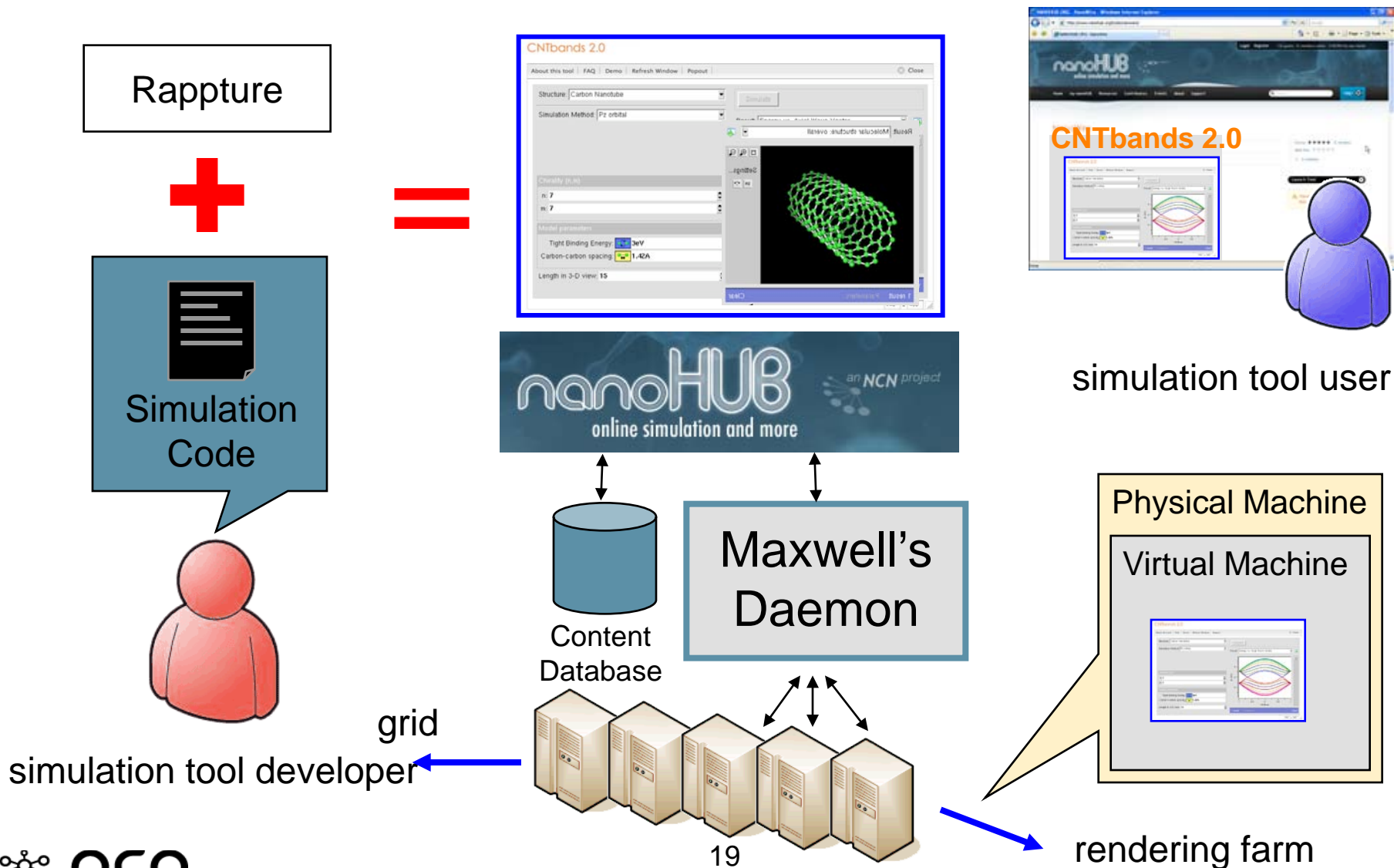
- Simulate:** Includes links for Nanoelectronics (Tools for nanoelectronics), NEMS/nanofluidics (Tools for NEMS and nanofluidics), and Nano-Bio Devices (Tools for nano-bio devices).
- Research:** Includes links for Seminars / Workshops (Cutting edge research), Collaborate (Work with your colleagues), Web Meetings (Right in your browser), and User Groups (Share with your colleagues).
- Teach & Learn:** Includes links for Tool Powered Curricula (Tools and Assignments for Classes), Nano 101 / Nano 501 (Introductory tutorials), Nanocurriculum (Curriculum on nanotechnology), and More Teaching Materials (Graduate, Undergrad).
- Contribute:** Includes links for Contribute Content (Upload your own materials), Give us Feedback (Success story? Suggestions?), Take a Poll (What would you like to be able to purchase with your points in the new nanoHUB store?), and Donations (Contribute your financial support).

At the bottom, there are sections for "Events", "Announcements", and "What's New on nanoHUB".

signature service:

online simulation to
connect simulation tool
developers and users

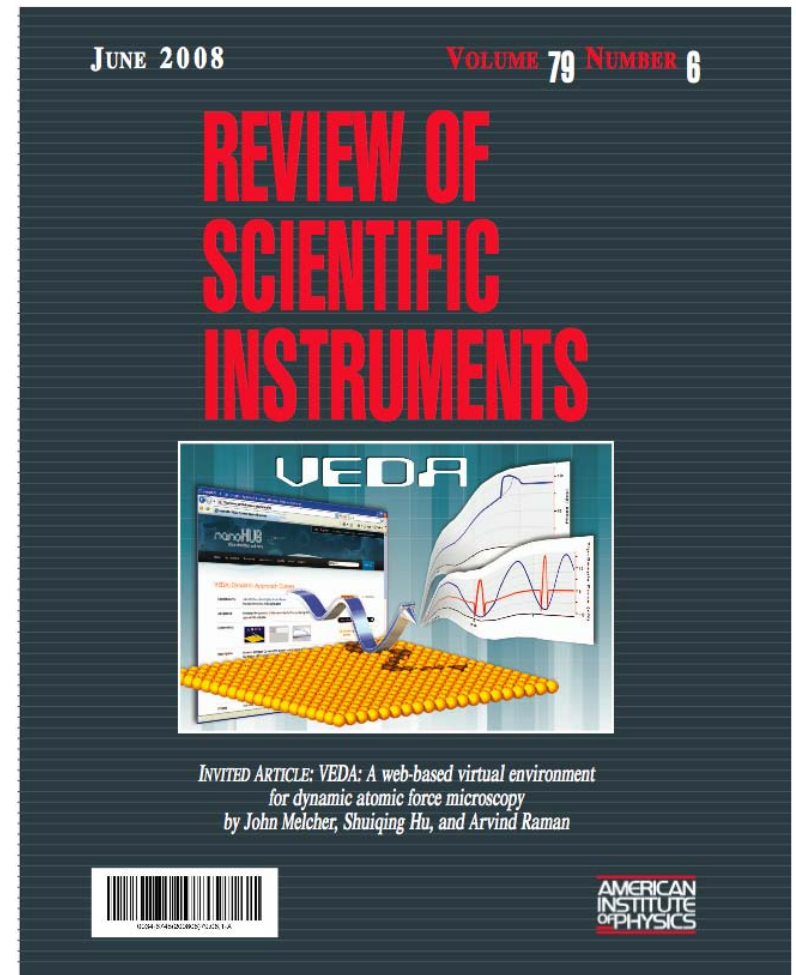
cloud computing for science and engineering



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”

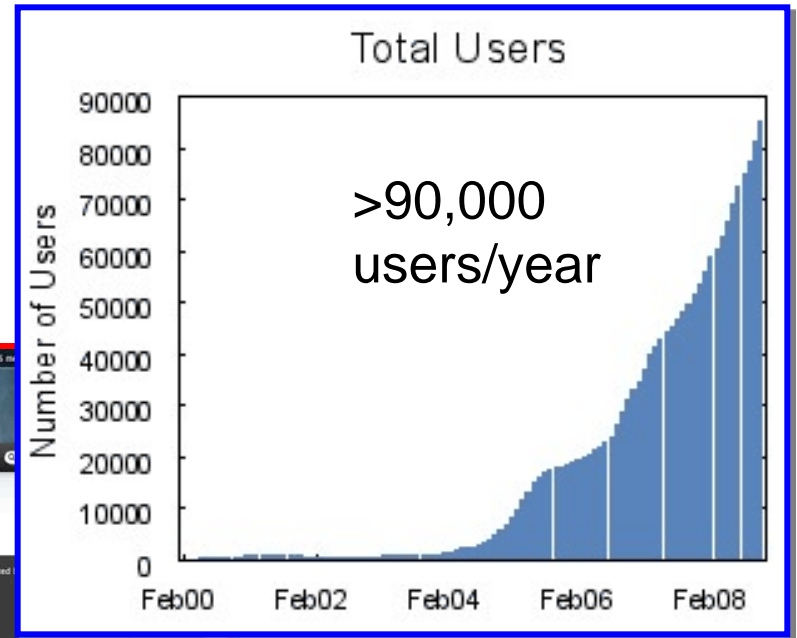
“Research on molecular and nanoscale electronics is providing a new understanding of electronic conduction at the smallest scale. The objective of “Electronics from the Bottom-Up” is to convey these new insights, understanding, and conceptual approaches to students and working engineers worldwide.”

19,259 nanoHUB.org EBU students last year.

New partnership with World Scientific.

nanoHUB.org

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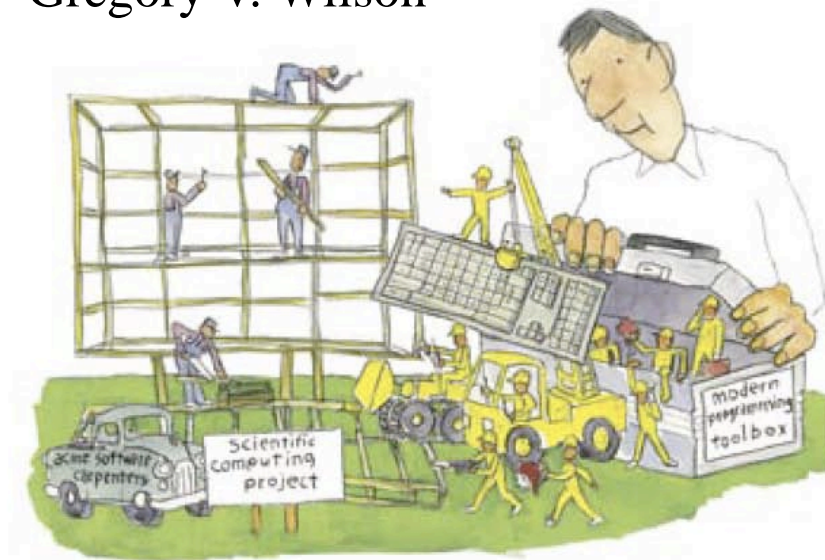


the biggest challenge in computational science

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>

conclusion

**There are plenty of challenges, but
many more opportunities!**