Frontiers of Characterization and Metrology for Nanoelectroincs

Challenges and Opportunities for Modeling and Simulation

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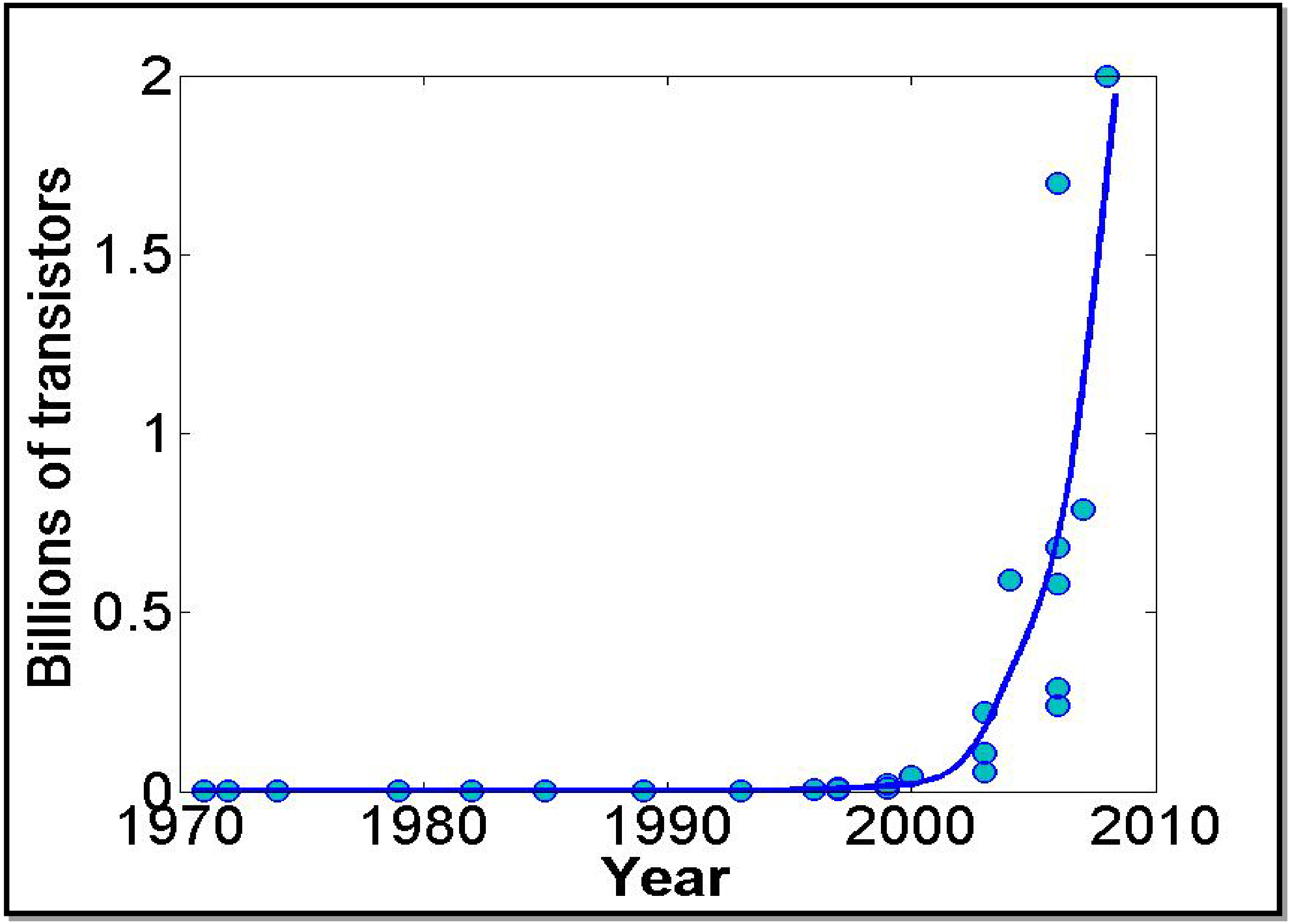
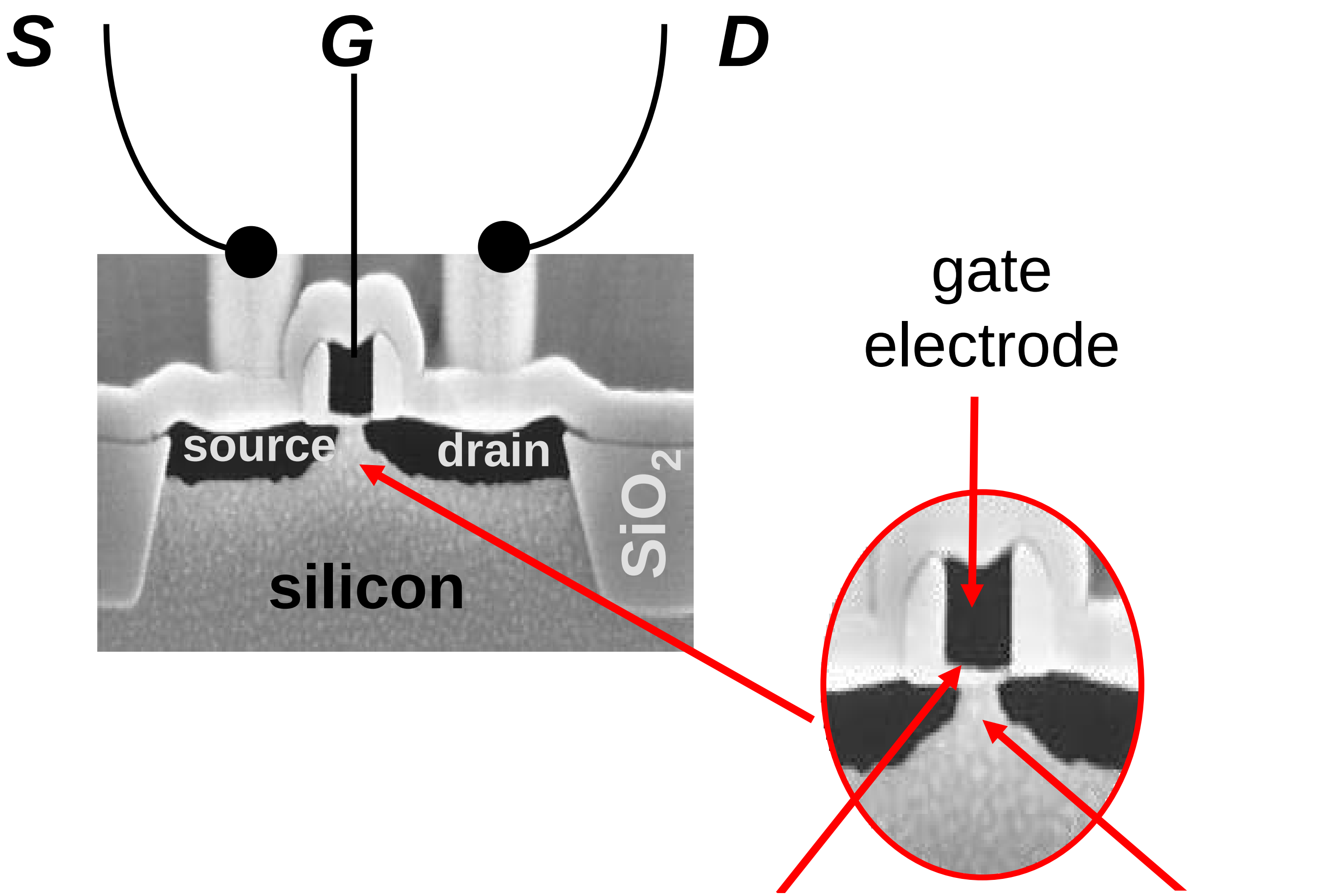
ncn nanoHUB.org

PURDUE UNIVERSITY

obligatory Moore's Law plot

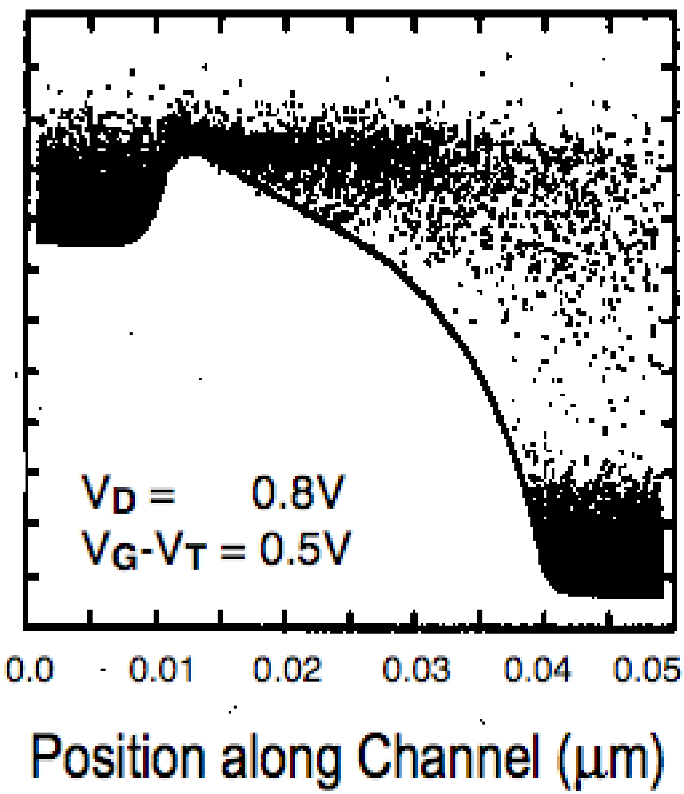


nanoscale MOSFETs



ITRS 2022: L_{PHYS} = 8 nm

device simulation

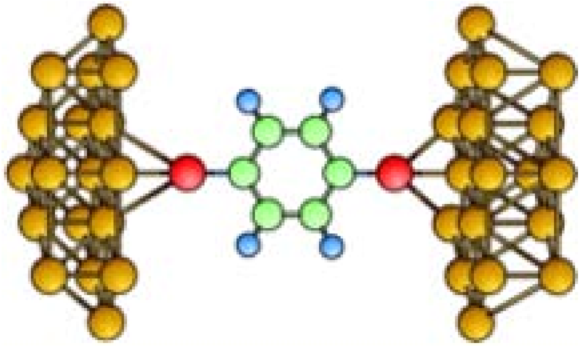


Frank, Laux, and Fischetti, IEDM Tech. Digest, p. 553, 1992.

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

- **Drift-diffusion**

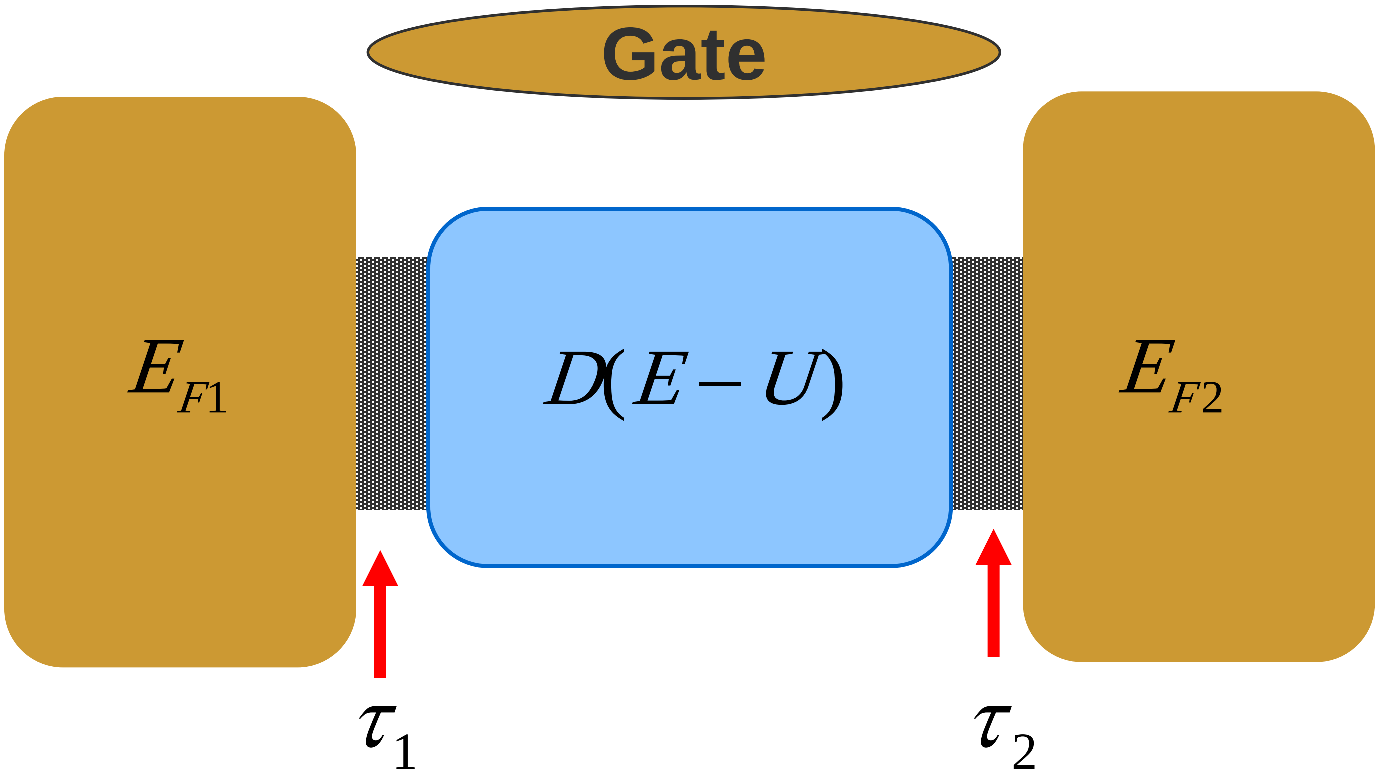
molecular electronics



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

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

generic model of a nanodevice



$$\gamma = \hbar/\tau$$

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

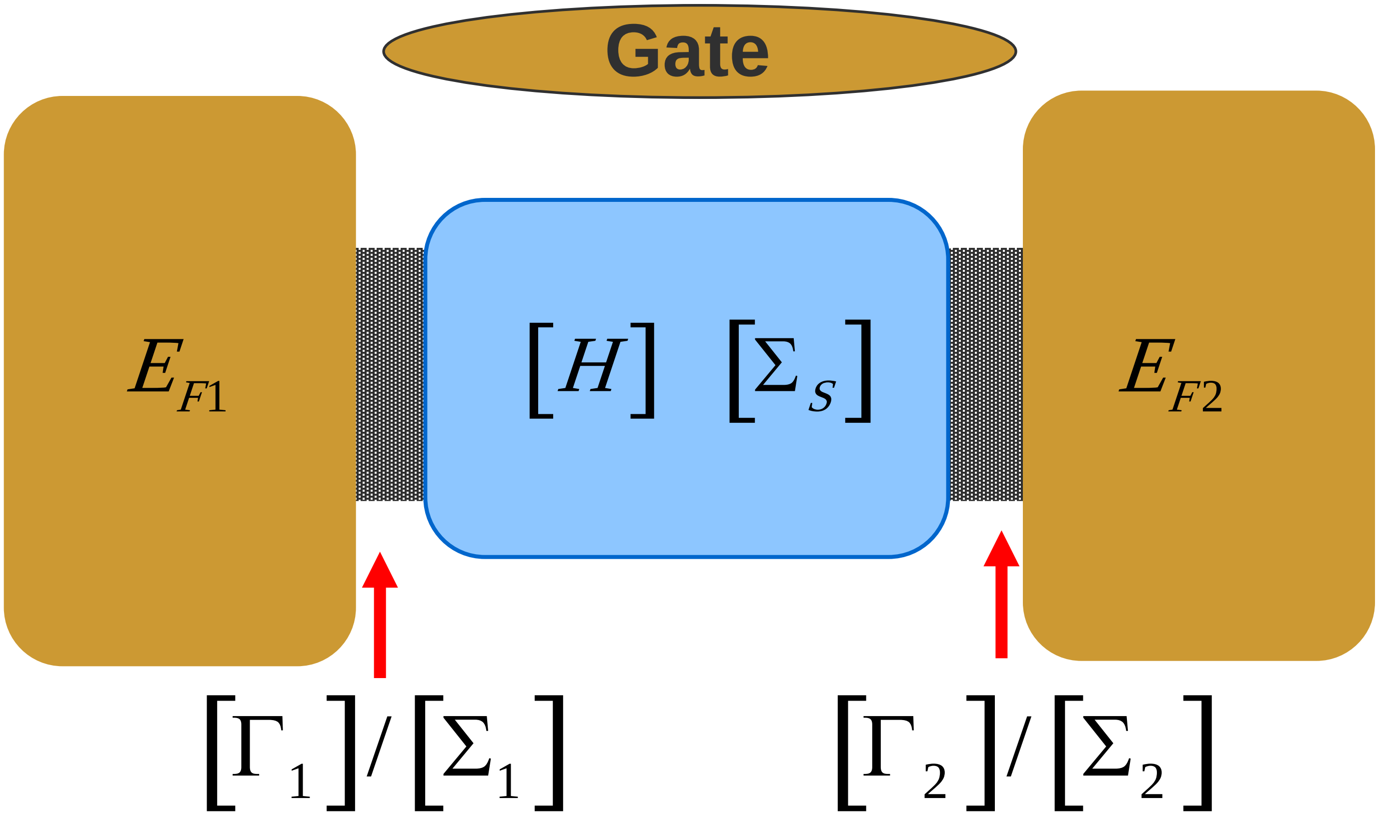
Landauer-Datta

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

or

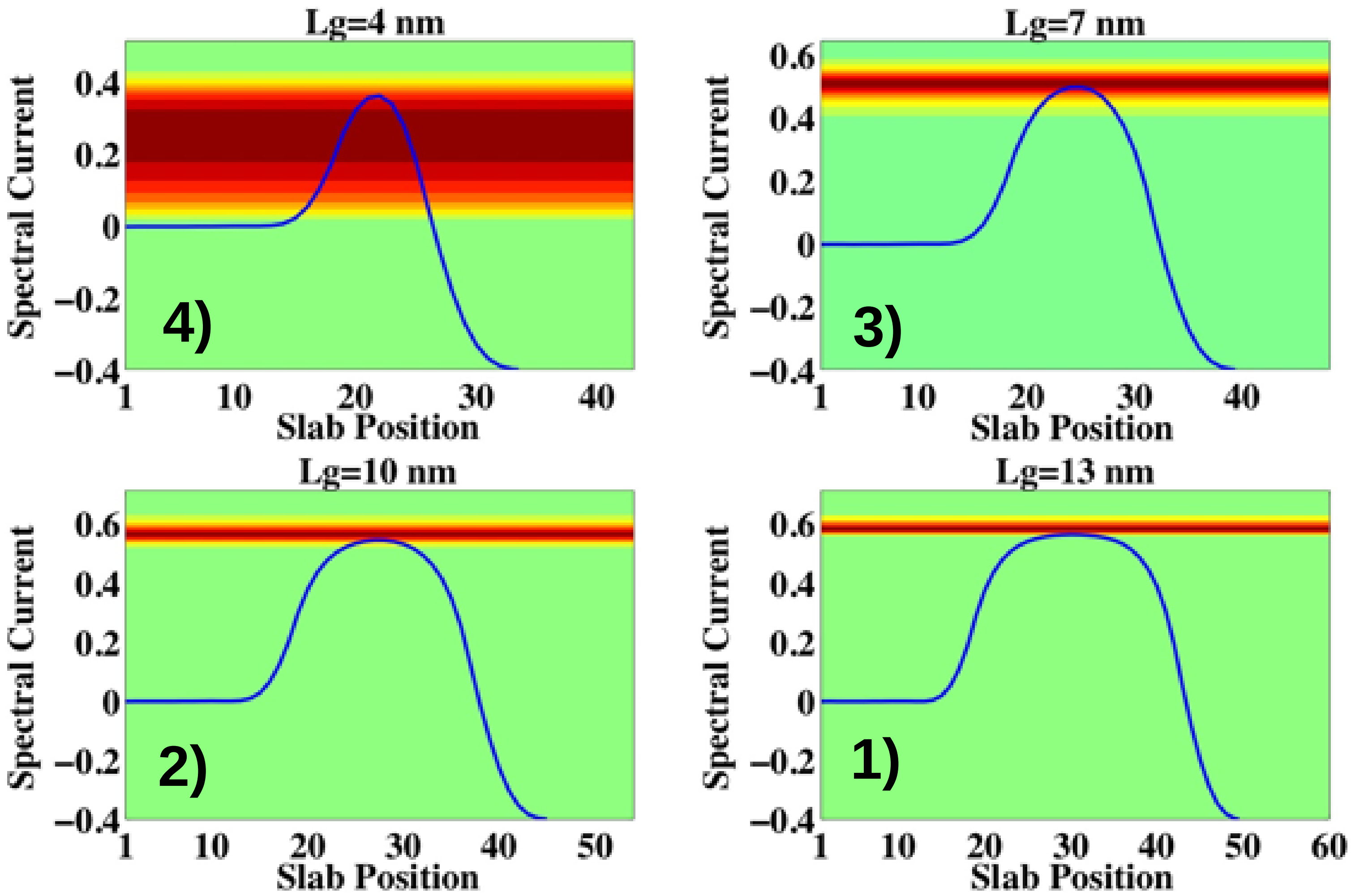
$$I_D = \frac{2q}{h}\int \gamma\left(E\right)\pi\frac{D\left(E\right)}{2}\left(f_1 - f_2\right)dE$$

generic model --> NEGF



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

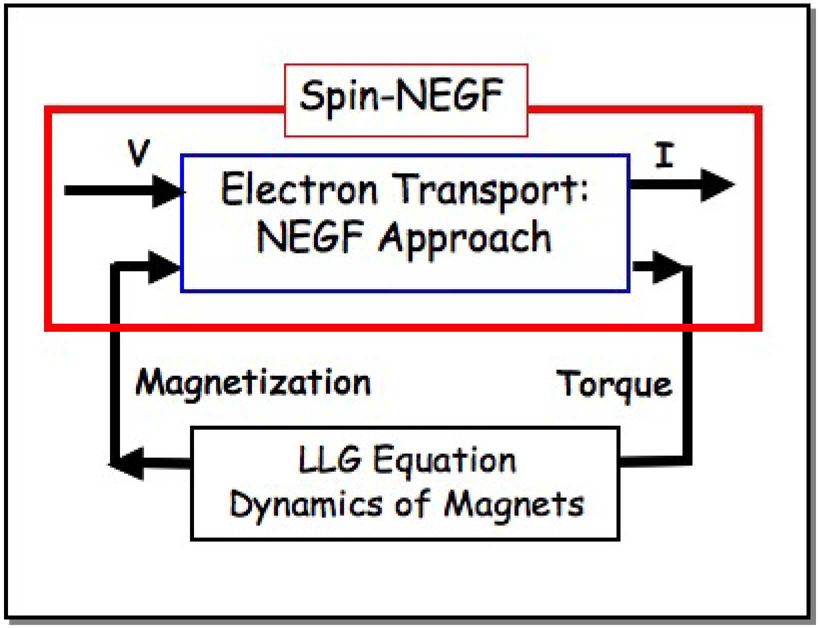
limits of MOSFETs

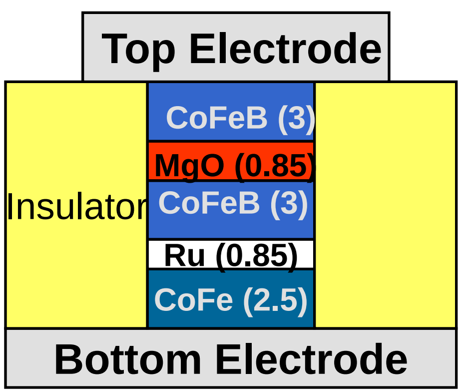


from M. Luisier, ETH Zurich / Purdue

spintronics

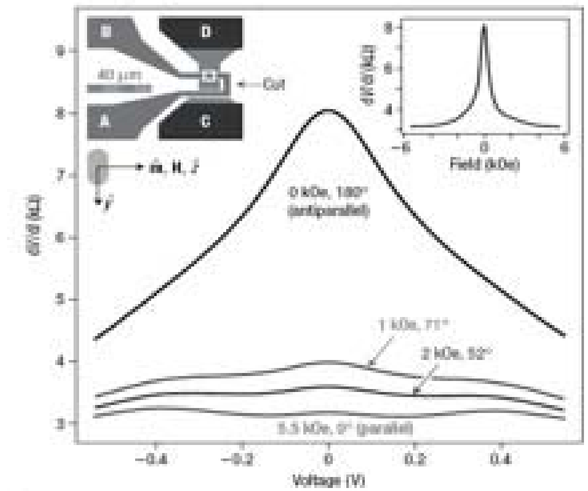
Theory: Datta group Purdue

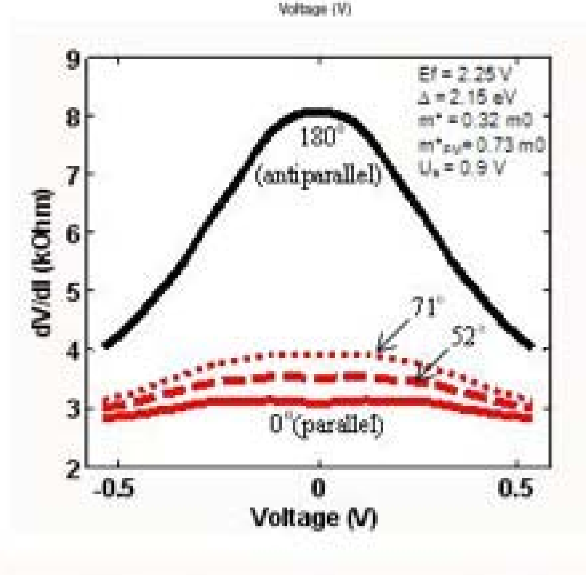




Experiment: Cornell

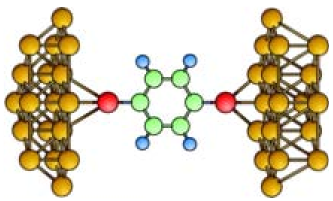
Sankey et al. *Nat. Phys.*, **4**, 67 (2008)

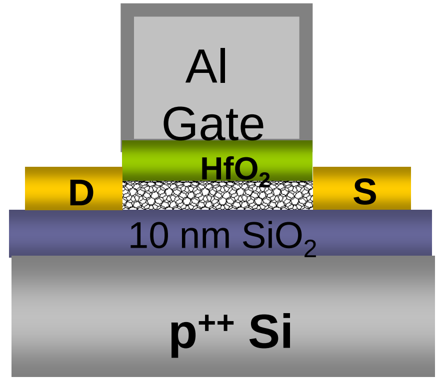




21st century electronics

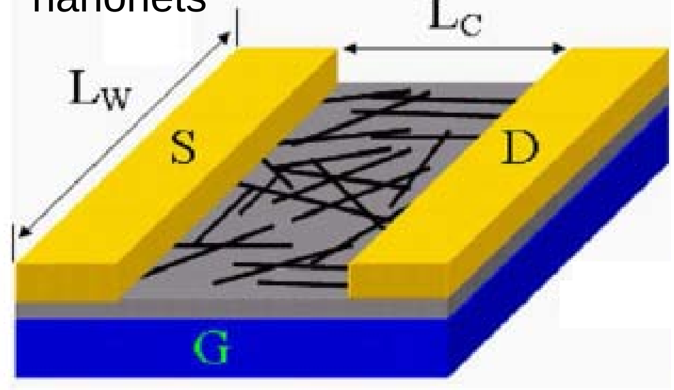
molecular electronics



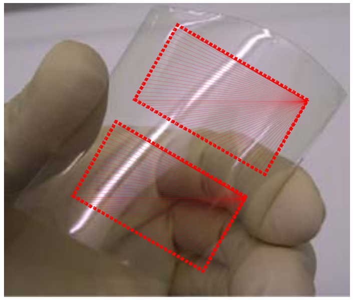


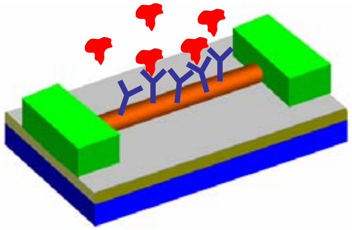
carbon nanotube electronics

nanonets

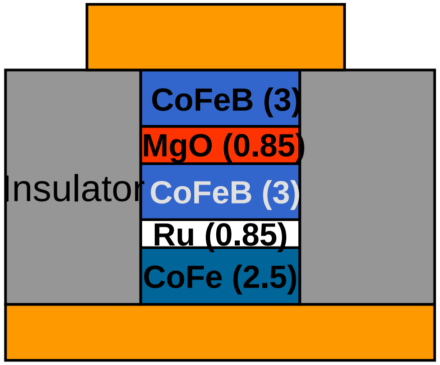


flexible electronics



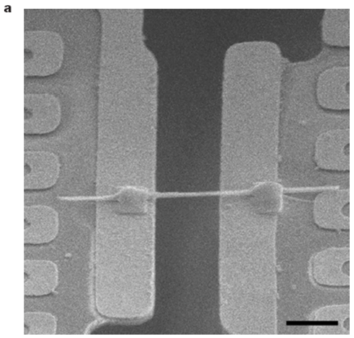


nanowire bio-sensors



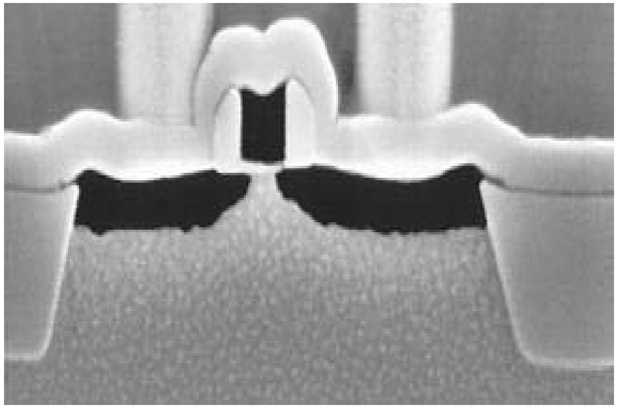
spin torque devices

nanowire PV



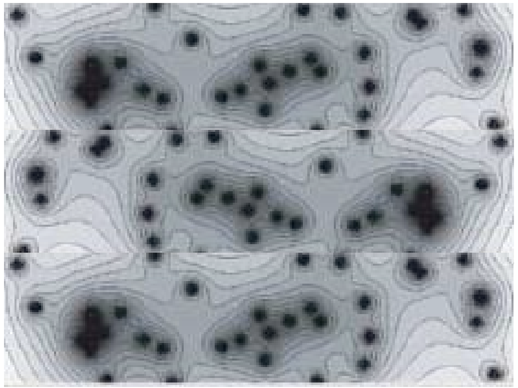
nanowire thermoelectrics

MOSFETs and variability



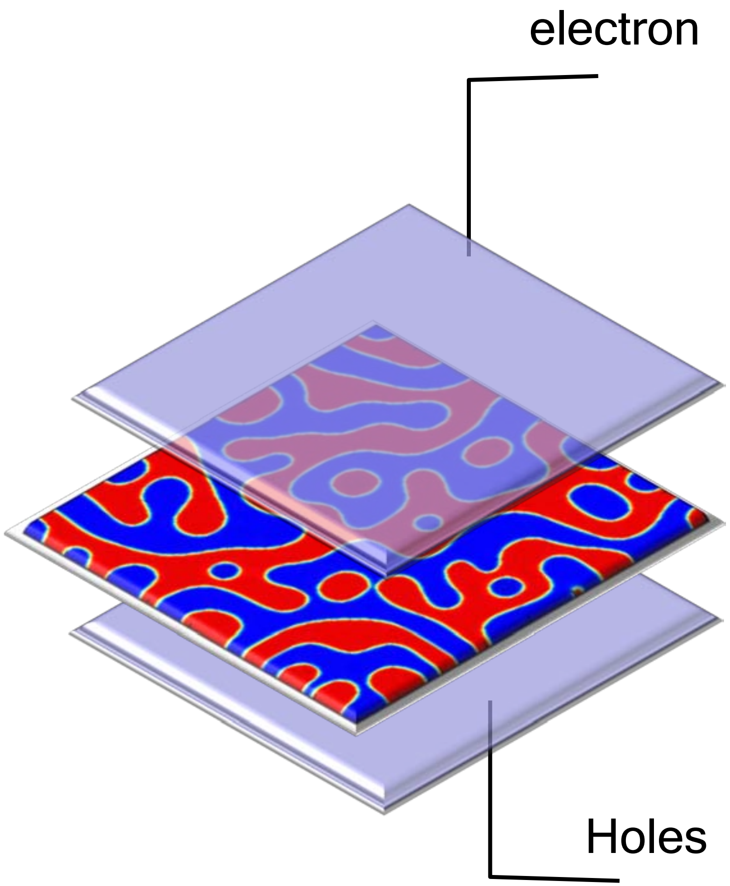
1997 MOSFET
(Texas Instruments)

Random **D**opant
Fluctuations

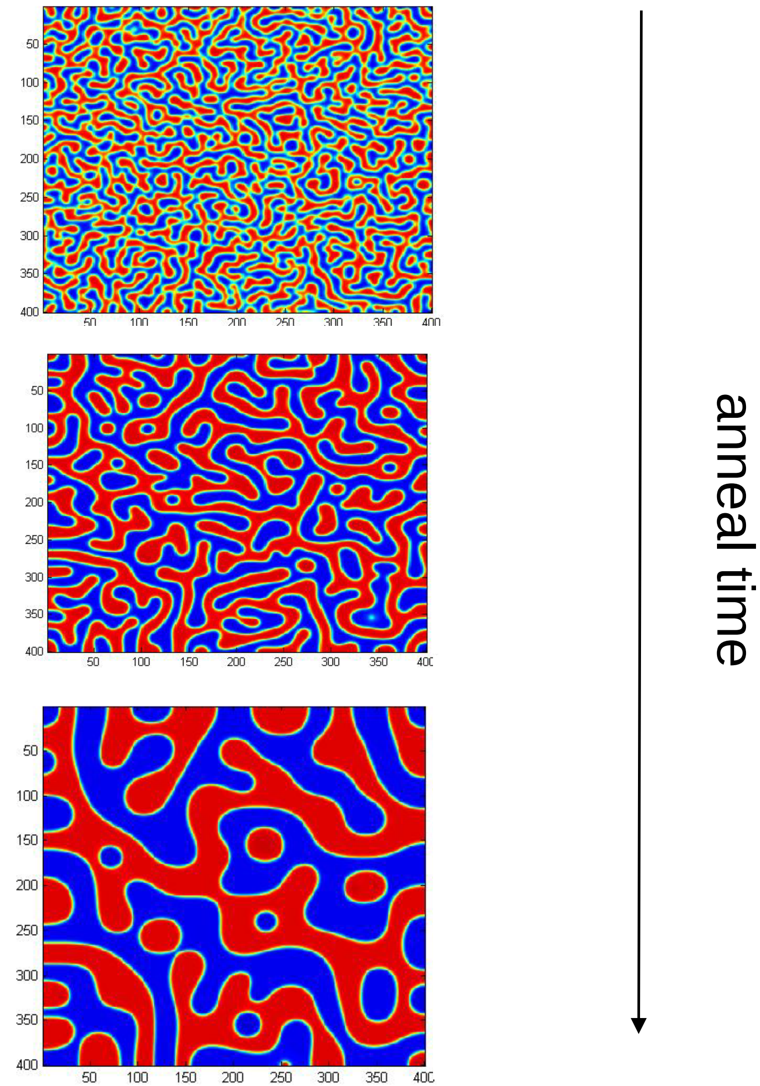


after Takahiro Shinada, et al.,
Nature, **437**,1128, 2005

nanostructured solar cells (Alam group)



Phase segregation dominated by
Spinodal decomposition



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 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

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

what we're after

Two kinds of results:

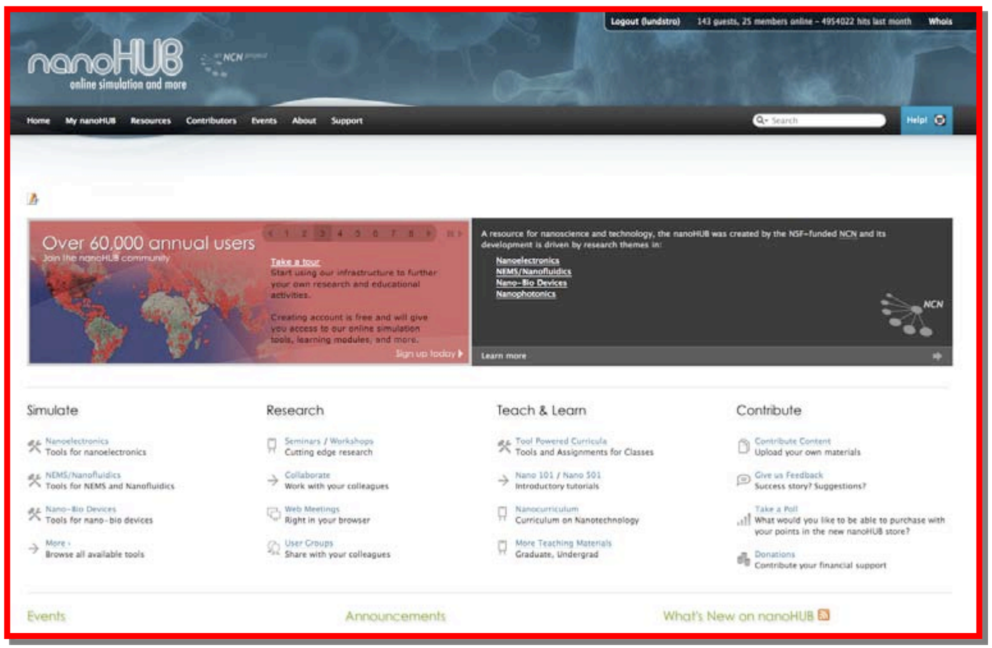
1) **answers, insight, understanding**

2) **numbers and software**

(after Brian Hayes, on "inquisitive computing" in *American Scientist*, 2008)

role cyberinfrastructure

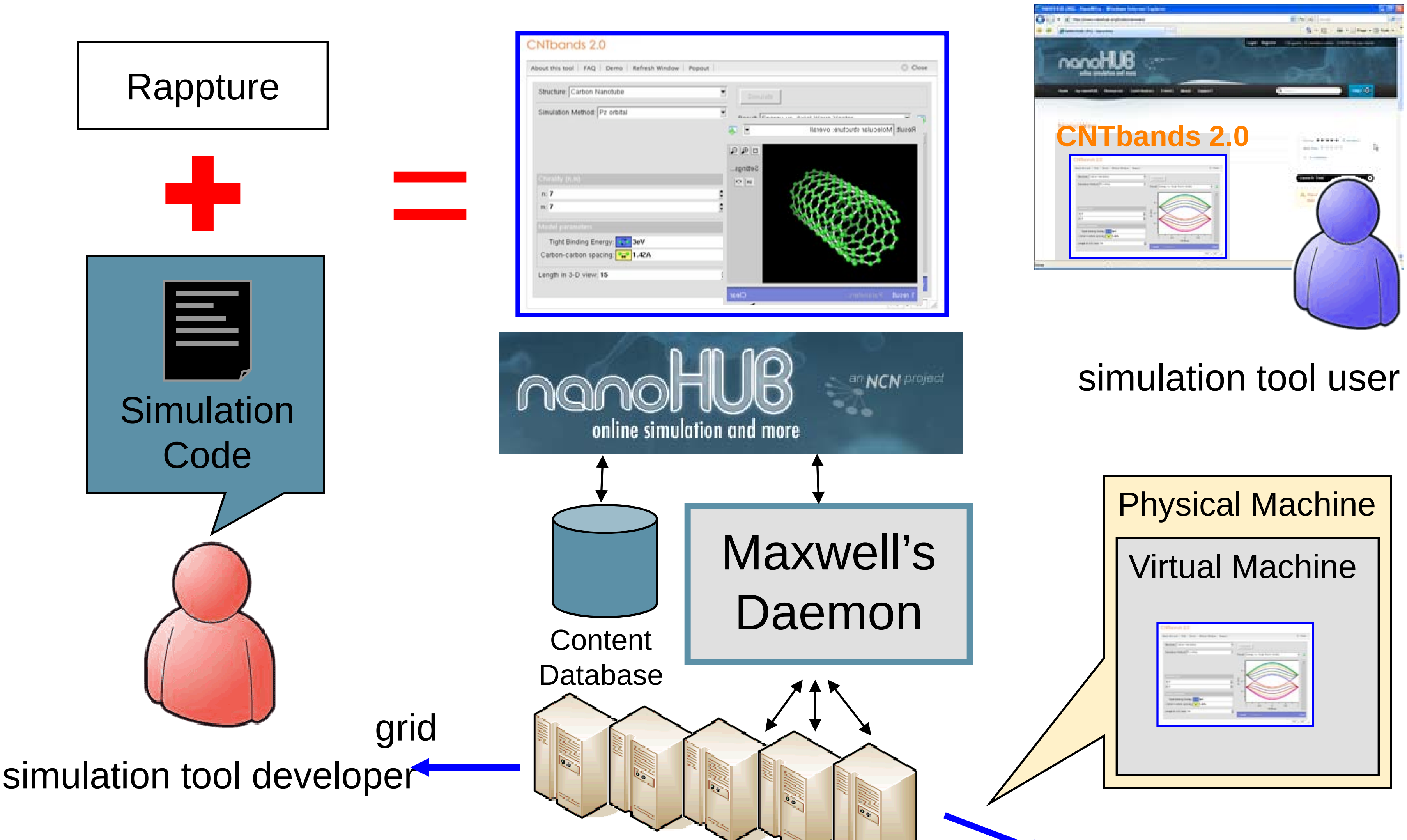
www.nanoHUB.org



***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 **E**nvironment for **D**ynamic **A**FM

- 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

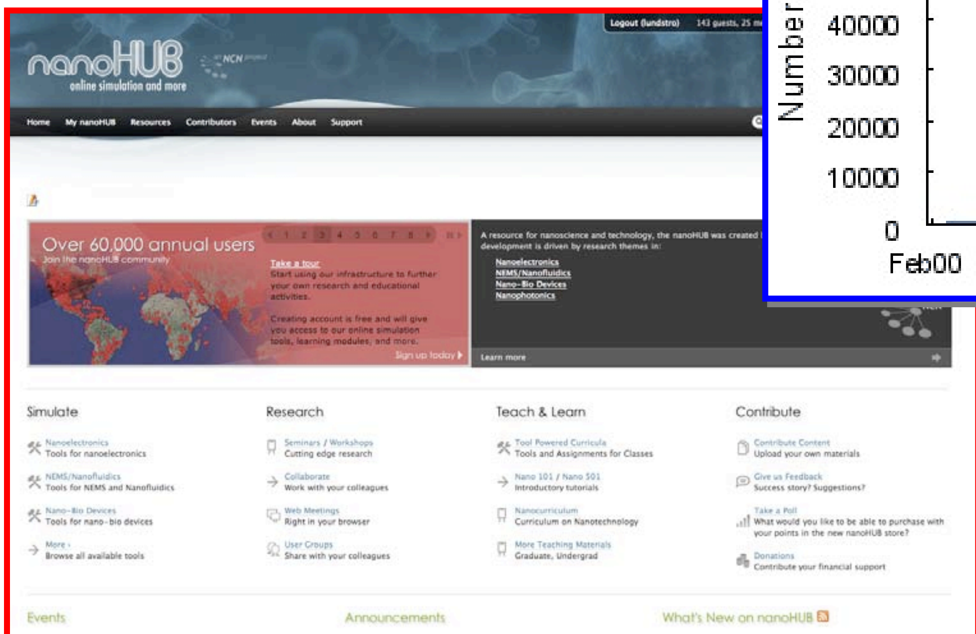
“Electronics from the Bottom Up”

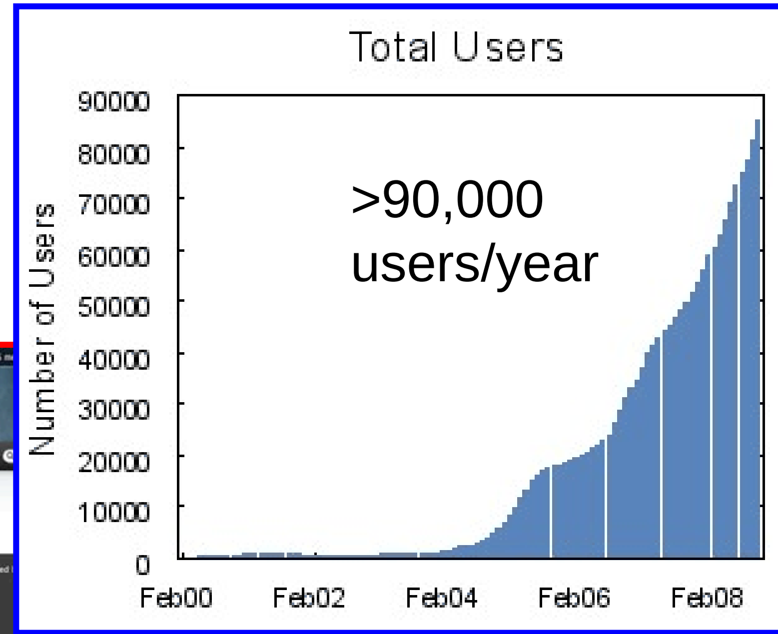
“Research on molecular and nanoscale electronics is providing a new understanding of electronic conduction at the smallest scale. The objective of “Electronics from the Bottom-Up” is to convey these new insights, understanding, and conceptual approaches to students and working engineers worldwide.”

19,259 nanoHUB.org EBU students last year.

New partnership with World Scientific.

nanoHUB.org





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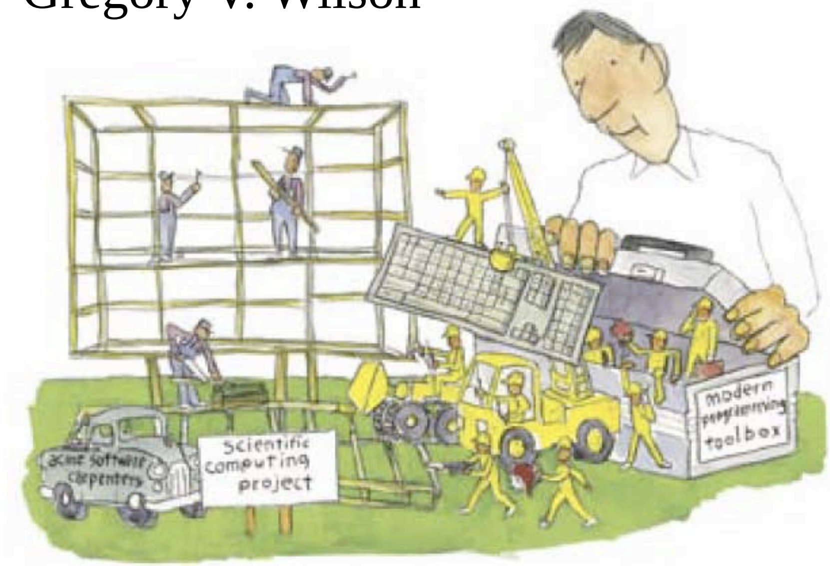
the biggest challenge in computational science

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!