NCN: Global Initiative About "Electronics from the Bottom-up" Mythbusting Scientific Knowledge Transfer

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NCN vision 2002

accelerate the transformation of nanoscience to nanotechnology through simulation

NCN vision 2002

enable new modes of discovery, innovation, learning, and engagement that accelerate the transformation of nanoscience to nanotechnology through simulation tightly linked to experimental research and education

1965 Gordon Moore

http://www.intel.com/technology/moorelaw
Intel in 2009

Device Size: 
Tens of nanometers

Device Integration: 
>2 Billion

Stanford SUPREM

Berkeley

Simulation Program with Integrated Circuit Emphasis

from: Larry Nagel, BCTM ’96
• Started as a class project
• Developed as a teaching tool
• Quality control: pass Pederson
• Dissemination:
  ▶ Public domain code
  ▶ Pederson carried tapes along
  ▶ Students took it along to industry and academia
• Released 1972

Stanford

Stanford University Process Modeling

• Stanford wanted to mimic Berkeley success
• Combine various existing models
• Dissemination:
  ▶ Public domain code
  ▶ Community workshops
  ▶ Students took it along to industry and academia

Birth of an Industry

Intel Capitalization: $85B
Total Industry: $280B

Process Simulation

Device Size

Years
**Goals - Impact Metrics**

- **Services:**
  - Modeling and Simulation Software
  - Seminars, tutorials, classes

- **Goals:**
  - Knowledge transfer
    - Use in class rooms
  - Knowledge generation
    - Use in research
    - Use by experimentalists
  - Economic impact
    - Use in industry
  - Professional Development / Community building

**Mythbusting Scientific Knowledge Transfer**

User Perceptions / Beliefs:
- Cannot use research software for education
  - It would take a long time
- You cannot use someone else’s code to conduct research
  - Experimentalists will not use computational research codes
- Codes are too hard to install
- Codes get out of date
- You cannot provide enough compute cycles
Mythbusting
Scientific Knowledge Transfer

Developer Perceptions / Beliefs:
• No incentive to share working code
• Scientists must rewrite their codes for web deployment
• Graphical user interfaces cannot be built by scientists/engineers
  ⇒ Scientists must hand-over their code to someone else
  ⇒ Scientists disowned
  ⇒ Scientists will never use their own code on the web platform

CI Operation Perceptions / Beliefs:
• Need one designated computer scientist per application to port to web and to support
  ⇒ $200k per application/year
• A University cannot create and serve a National Resource
• There is no infrastructure that is
  – Secure
  – Serves users and developers
  – Affordable
  – Scalable

Demonstration / Capability / Impact:
• 52 million atom electronic structure (101nm)^3.
• Quantum dots, nanowires, quantum computing...

Self-Assembly Process ⇒ InAs deposition on GaAs substrate

InAs (0.60583 nm)

GaAs (0.56532 nm)

InAs deposition on GaAs substrate

First Layer (wetting layer) ~ 1ML

InAs

GaAs

GaAs
Capping with Intermediate Alloy

InAs GaAs

Objective:
• Optical emission at 1.5μm without GaN
• Understand experimental data on QD spectra in selective overgrowth

Approach:
• Model large structure
  • 60nm x 60nm x 60nm
  • 9 million atoms
  • No changes to the previously published TB & VFF parameters

Result:
• Theory (red line) matches a sequence of 17 experiments (black dots/lines)
  • Bi-modal In-As,Ga-As bond dist.
  • change in quantum dot aspect ratio
  • Quantitative model of complex system

Over 220 tools online!

Introduction to semiconductor device education with ABACUS

Over 2,700 Resources!

Advancing Quantum Mechanics for Engineers with AQME

What is an artificial atom

What is resonant tunneling

What is the relation between confinement potential and the state spectrum

What are MOSFET subbands

What is the silicon crystal structure

What are highly doped PIN-junctions

Where is voltage drop in a MOSFET

220 tools

55 courses

2,000 seminars and teaching materials
Sociology
How do Users Behave?

- **Questions:**
  - How many students in the class?
  - Which tools?
  - Intensity of use
  - Sustained use
  - Percentage of service: Education vs. Research use

- **Some Statistics**
  - 8,600 users ran 345,000 simulations Academic Year 2009/2010
  - 116 classes / 97 institutions in Academic Year 2009/2010
    - Info Obtained from self-registration, manual follow-up
    - 575 citations in the literature
    - Info obtained from Google Scholar and manual analysis
Formal Education vs. Research

AY 09/10:
116 Courses,
97 institutions,
~2,100 students
95% outside NCN

Myth Busted!
Proof of use in EDUCATION!
Knowledge Transfer out of Research
Voluntary / Viral Use

Transition to the Classroom
Takes a Long Time

Mythbusting Scientific Knowledge Transfer

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Virtual Org.
Proof of Use in Experimental Work!
Not Just Computational Theory!

User Myth: No Good Research!

575 nanoHUB citations
469 in nano research
142 30% expt. data
55 12% experimentalists

Academy of Engineering Member
Faculty member 3 years after PhD

Mythbusting Scientific Knowledge Transfer

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Virtual Org.

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Virtual Org.
Web-enabling Tools

- Vendor
- Scientist
- Web Developer

2 years -> 1 week
100 : 1 ratio

Developer Activities

- Versions
- Tools
- Developers

Next Generation Publications
Research Incentives

Tool Usage ➔ reading papers

Dragica Vasileska

Computational Electronics
Semiclassical and Quantum Device Modeling and Simulation

17 tools
11,570 users
123 citations

Next Generation Faculty:

Shaikh Ahmed

- Infused nanoHUB into existing classes
- Built a new nanoelectronics curriculum
- Used nanoHUB for research

6,183 users
8 tools

Recently Dr. Ahmed was promoted to tenured Associate Professor. I would like to emphasize that Dr. Ahmed's use of nanoHUB in education and research, which earned him national and international visibility, did play a significant positive role in his early promotion case.

Glafkos Galanos
Chair, Dept. of Electr. and Comp. Eng, SIUC
Mythbusting
Scientific Knowledge Transfer

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Typical Dissemination Paths

Problems:

- REALLY LONG stove pipe
- Web content: afterthought
  - usually stale
- Data shared by email
- Tools spread by hiring

nanoHUB Technical Solution

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nanoHUB.org
The World’s Largest Nano User Facility

188,000 lecture users
830 lecturers
8,100 simulation users
300 sim developers

Impact:
• Research: 719 citations in the literature
• Education: 134 courses, 97 institutions (2010)
• Collaboration: 300 simulation tool developers

Users in 2010
172 countries

How do we get Growth?
NEW CONTENT

Annualized
New Resources
nanoHUB Users

Introduction of seminars and classes

nanoHUB.org
Fully Operational Cloud for End Users

Systemic Use in Research:
• Citation map shows
  Social network of researchers
• Enable other researchers to utilize
  recent PhD thesis nano-modeling software
• Can measure tool impact

Systemic Use in Education:
• Cohorts of students behave similarly
• Can measure classroom sizes
• Can measure tool impact
• Time from research to classroom use
  as small as 2 years!

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The World’s Largest Nano User Facility
Fully Operational Cloud for End Users

NSF Impact through an UNUSUAL Investment:
• Operational, reusable cyberinfrastructure
  • NOT research into cyberinfrastructure, results are NOT papers
• Harvesting of existing research capabilities
  • Conversion into useful tools ➔ Software-as-a-service-Cloud
  • Enable new fundamental research and education as a service
• Commit to serious assessment
  ➔ Focus on users, developers, and operation
• NOT a promise of future delivery, delivery TODAY

12/6/11