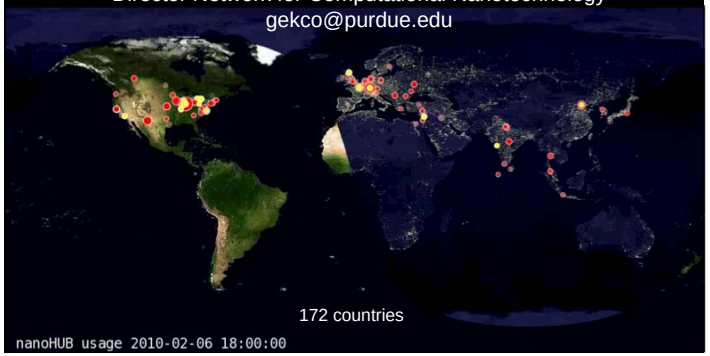
NCN: Global Initiative About "Electronics from the Bottom-up"

Mythbusting Scientific Knowledge Transfer

Gerhard Klimeck
Director Network for Computational Nanotechnology
gekco@purdue.edu



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

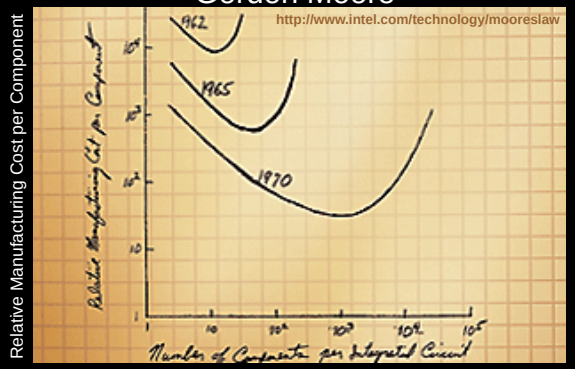
transformation of nanoscience to nanotechnology

through simulation

tightly linked to experimental research and education

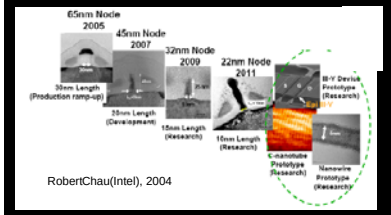
1965

Gordon Moore



4

Intel in 2009



RobertChau(Intel), 2004

Device Size:
Tens of nanometers

Stanford SUPREM

Device Integration:
>2 Billion

Berkeley SPICE

5

Berkeley

Simulation Program with Integrated Circuit Emphasis.

from: Larry Nagel, BCTM '96

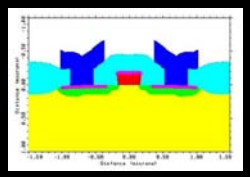
- Started as a class project
- Developed as a teaching tool
- Quality control: pass Pederson
- Dissemination:
  - Public domain code
  - Pederson carried tapes along
  - Students took it along to industry and academia

- Released 1972

6

Stanford

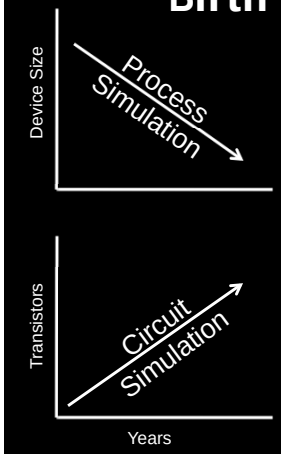
Stanford University PRocEss Modeling



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

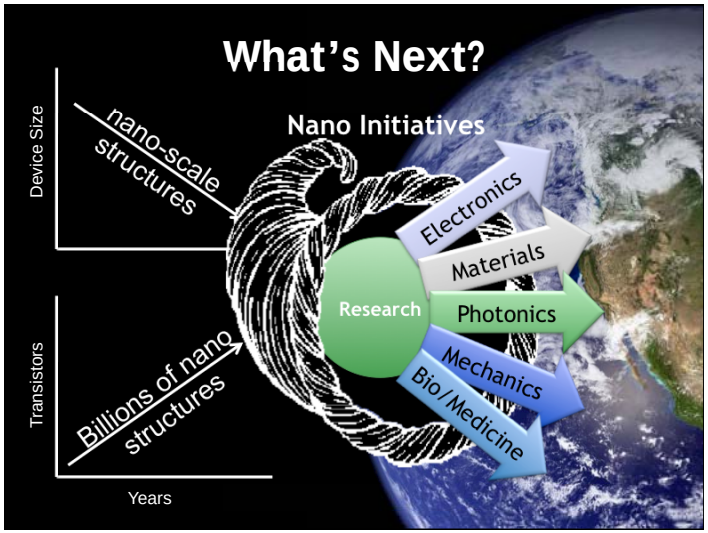
7

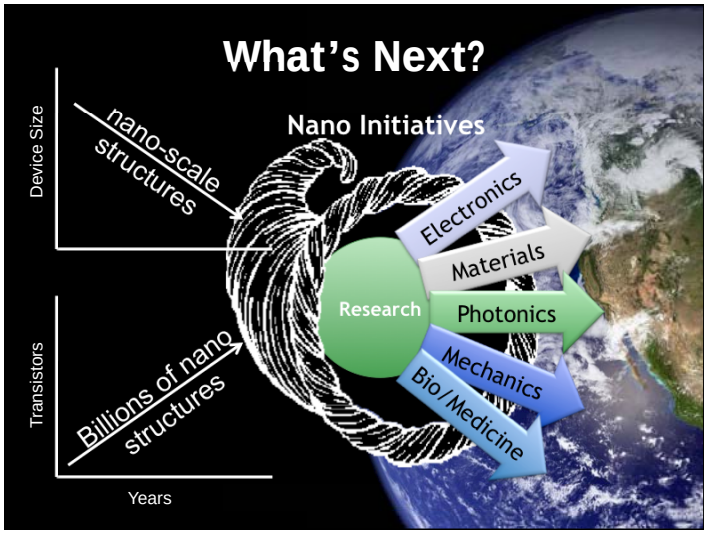
Birth of an Industy



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

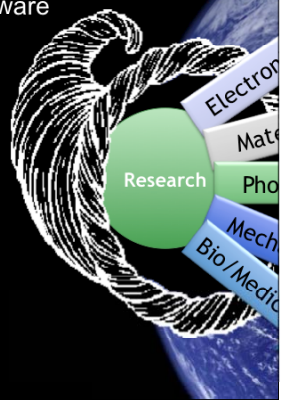
8





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

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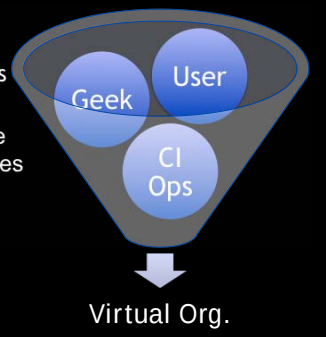

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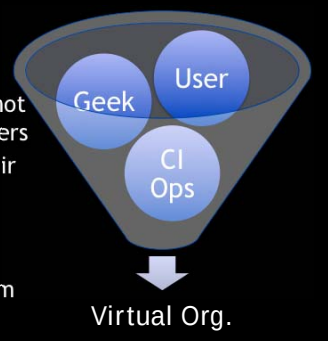

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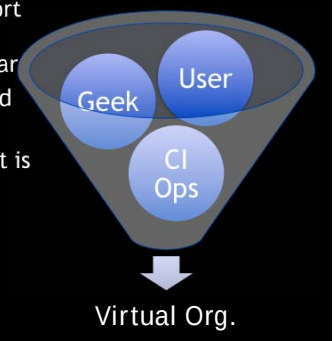
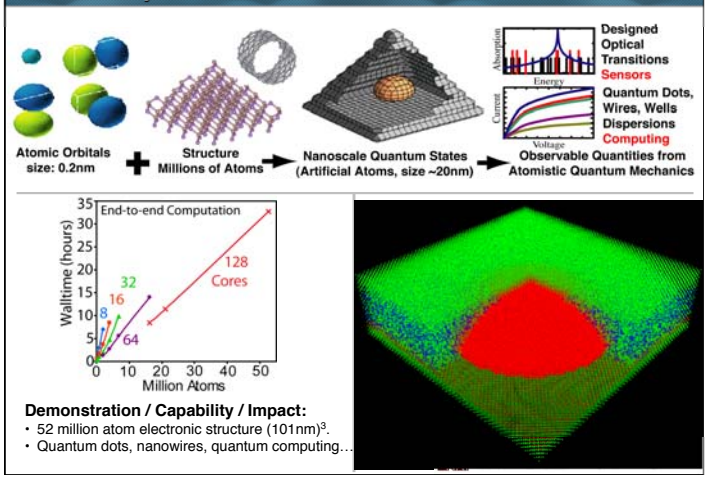
  - Serves users and developers
  - Affordable
  - Scalable



Bottom-Up Electronic Device Simulations

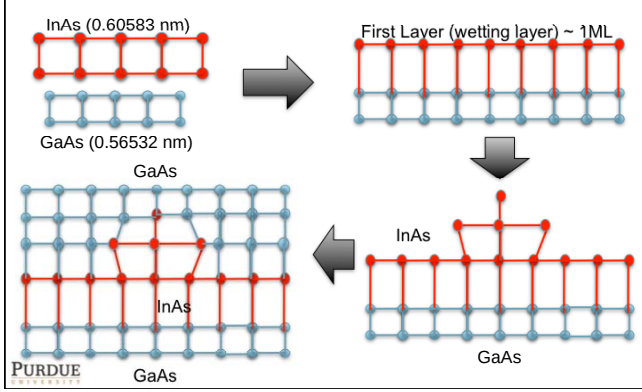


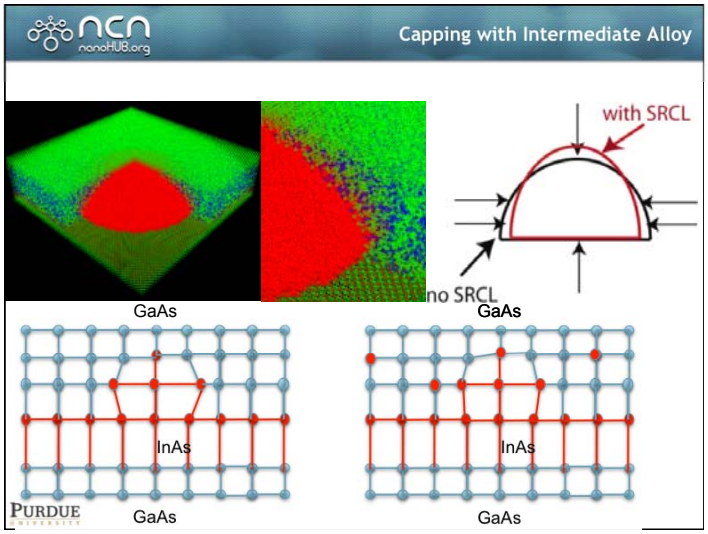
Demonstration / Capability / Impact:

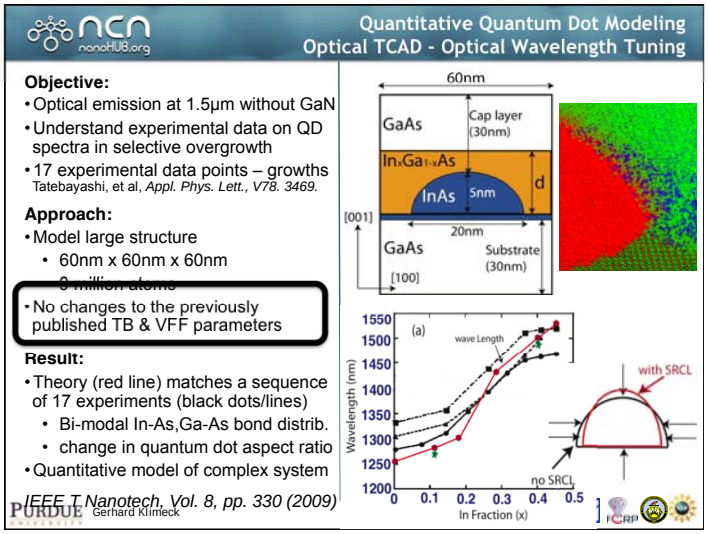
- 52 million atom electronic structure (101nm)^3.
- Quantum dots, nanowires, quantum computing…

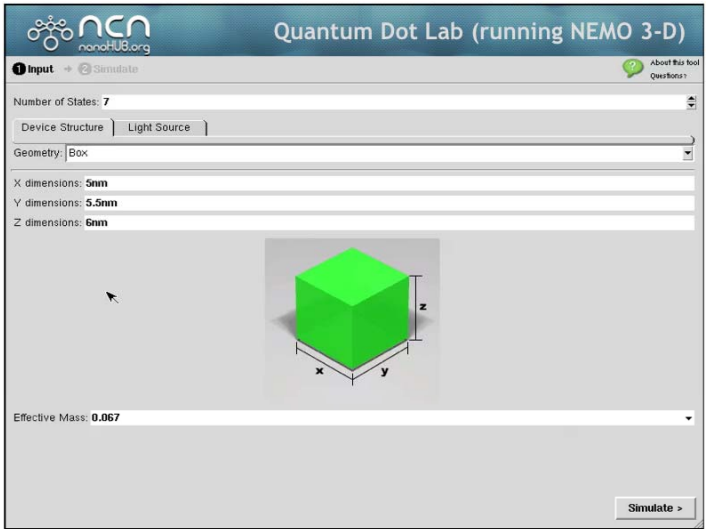
How do we get QDs? ➔ Stranski-Krastanow Growth

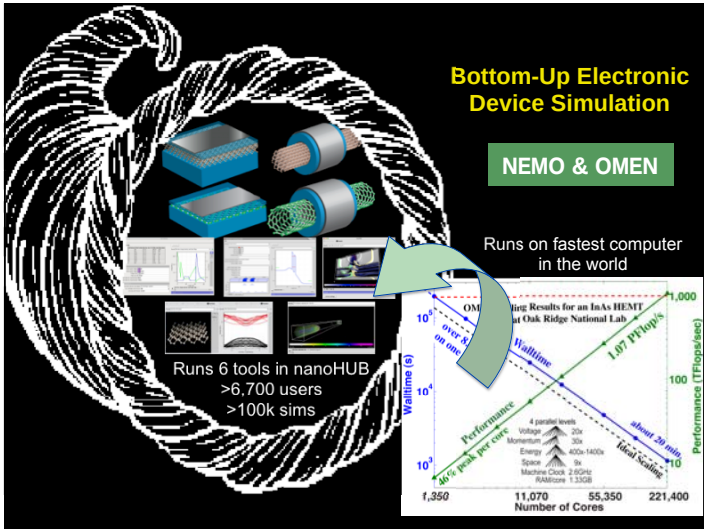
Self-Assembly Process ➔ InAs deposition on GaAs substrate



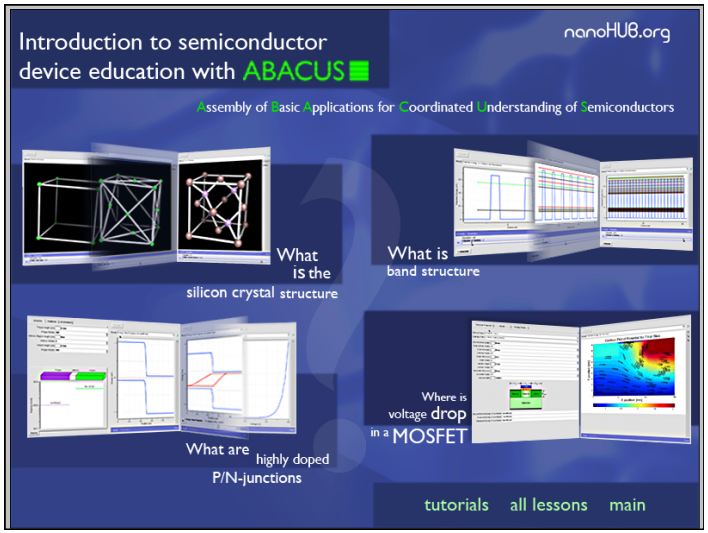

Capping with Intermediate Alloy
with SRCL
no SRCL
GaAs
GaAs
InAs
InAs
GaAs
GaAs
PURDUE

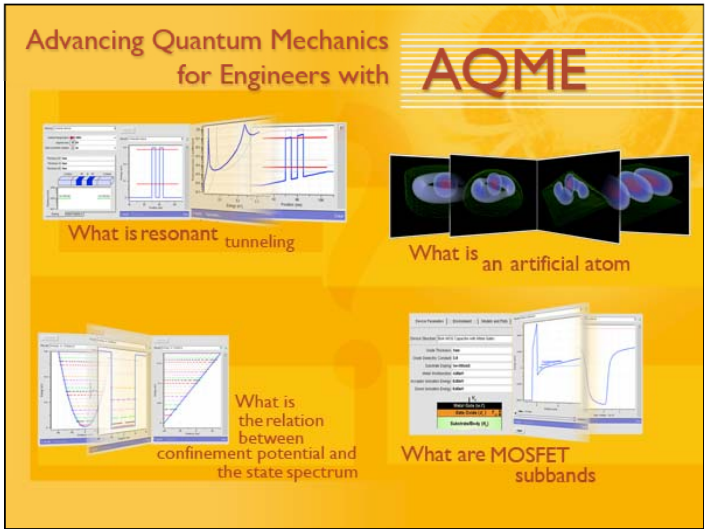

Quantitative Quantum Dot Modeling
Optical TCAD - Optical Wavelength Tuning
Objective:
• Optical emission at 1.5μm without GaN
• Understand experimental data on QD spectra in selective overgrowth
• 17 experimental data points – growths
Tatebayashi, et al, Appl. Phys. Lett., V78. 3469.
Approach:
• Model large structure
• 60nm x 60nm x 60nm
• 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 distrib.
• change in quantum dot aspect ratio
• Quantitative model of complex system
IEEE T Nanotech, Vol. 8, pp. 330 (2009)
60nm
GaAs
Cap layer (30nm)
InAs
5nm
d
20nm
GaAs
Substrate (30nm)
[001]
[100]
Wavelength (nm)
In Fraction (x)
with SRCL
no SRCL
PURDUE
Gerhard Klimeck


Quantum Dot Lab (running NEMO 3-D)
Input
Simulate
Number of States: 7
Device Structure
Light Source
Geometry: Box
X dimensions: 5nm
Y dimensions: 5.5nm
Z dimensions: 6nm
Effective Mass: 0.067
Simulate >

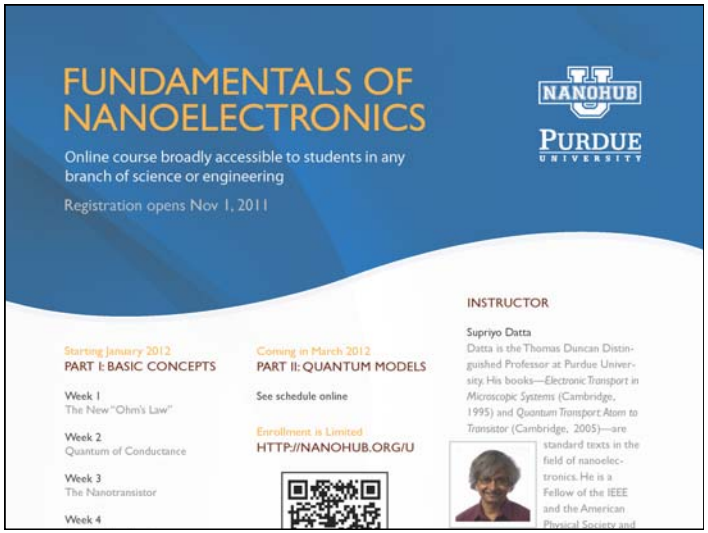

Bottom-Up Electronic Device Simulation
NEMO & OMEN
Runs on fastest computer in the world
Runs 6 tools in nanoHUB
>6,700 users
>100k sims
Walltime (s)
Performance (TFlops/sec)
Number of Cores
1,350
11,070
55,350
221,400
1,07 PFlop/s
Ideal Scaling


Over 220 tools online!


Introduction to semiconductor device education with ABACUS
nanoHUB.org
Assembly of Basic Applications for Coordinated Understanding of Semiconductors
What is the silicon crystal structure
What is band structure
What are highly doped P/N-junctions
Where is voltage drop in a MOSFET
tutorials
all lessons
main


Advancing Quantum Mechanics for Engineers with AQME
What is resonant tunneling
What is an artificial atom
What is the relation between confinement potential and the state spectrum
What are MOSFET subbands

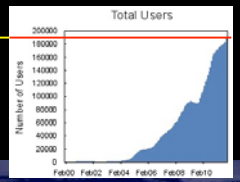

Over 2,700 Resources!
220 tools
55 courses
2,000 seminars and teaching materials

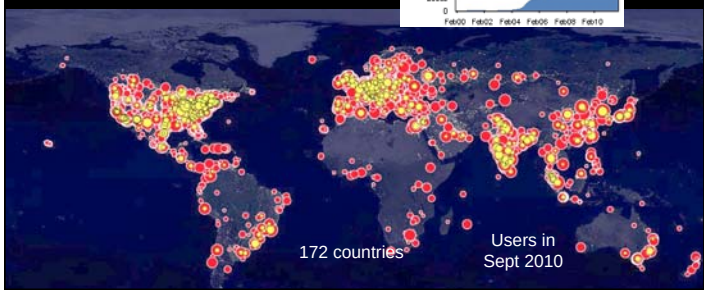


Nano App Store

188,000 users worldwide

As much traffic as www.purdue.edu
Users at all Top 50 US Engr Schools
19% of all .edu domains

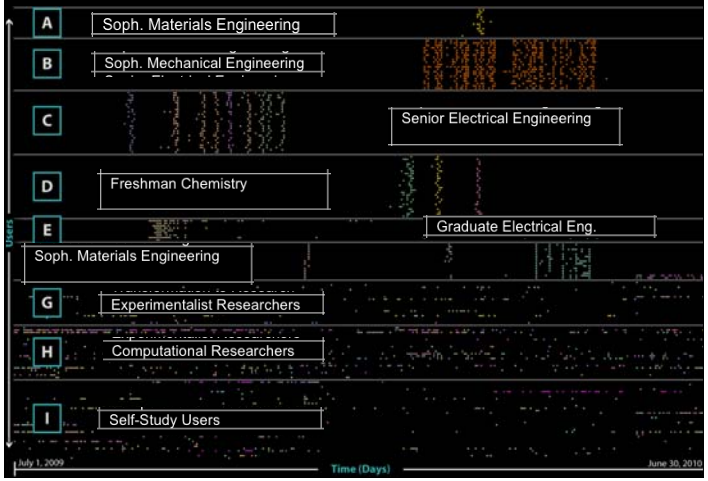


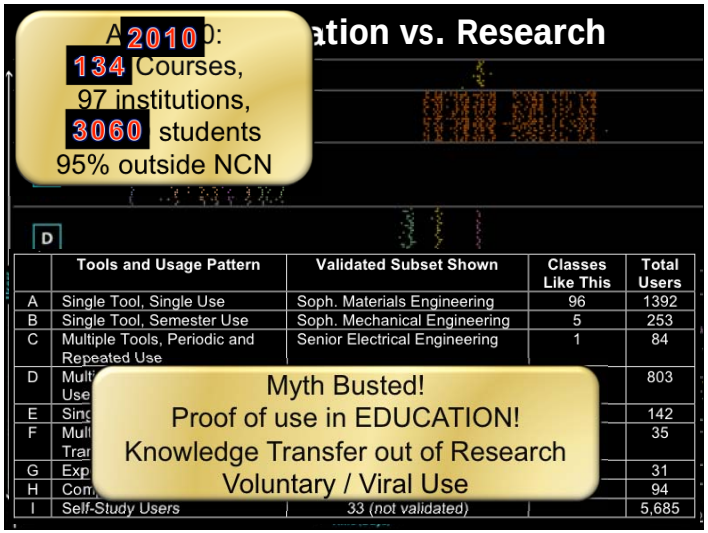


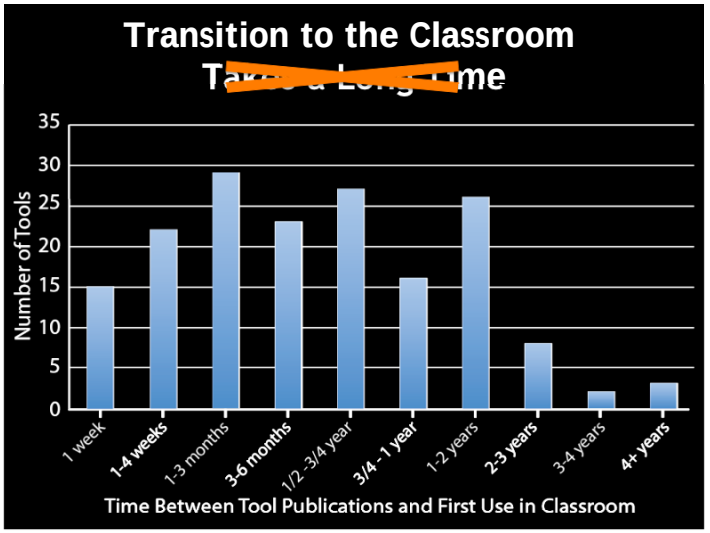
Sociology
How do Users Behave?

- 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







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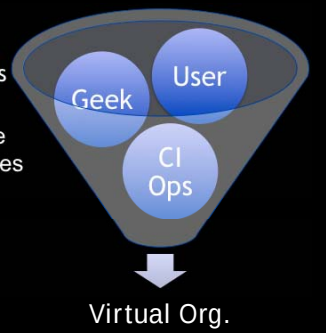

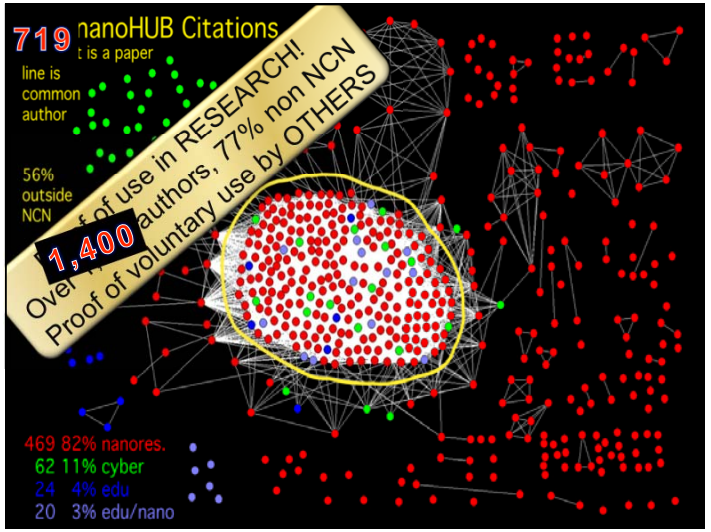

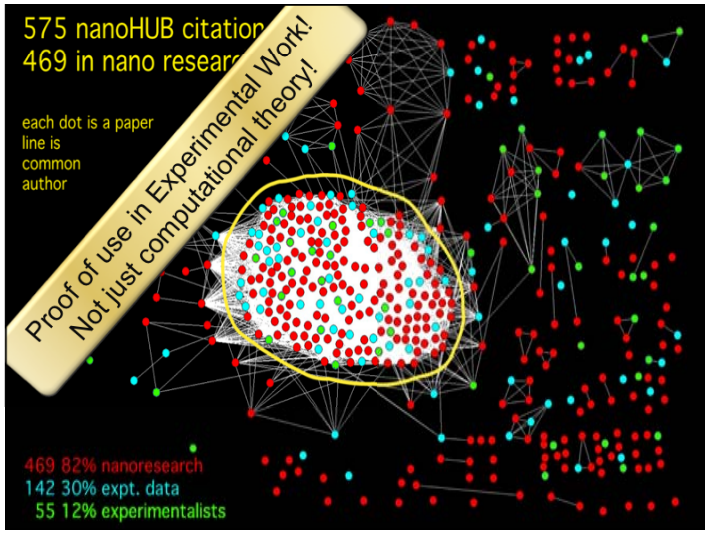

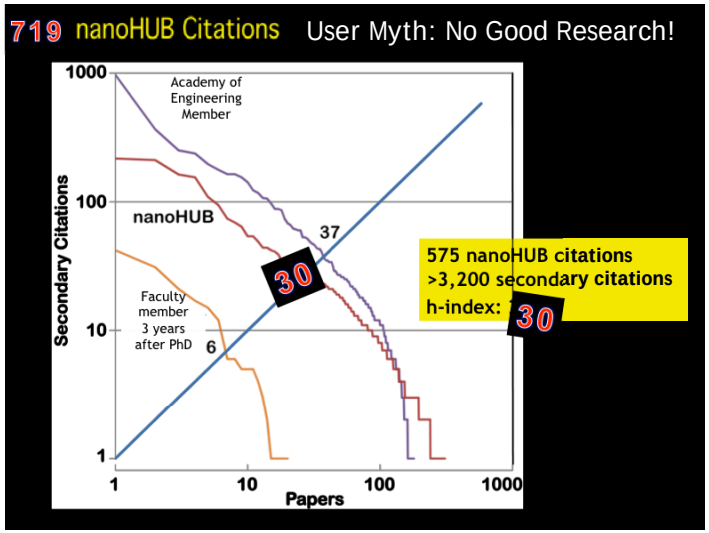

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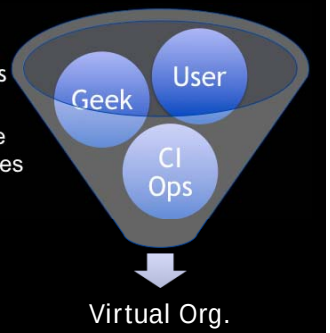

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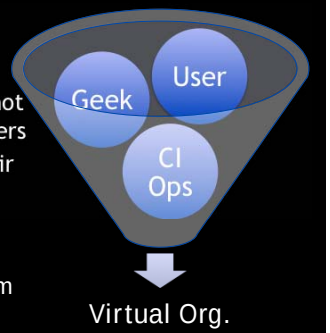
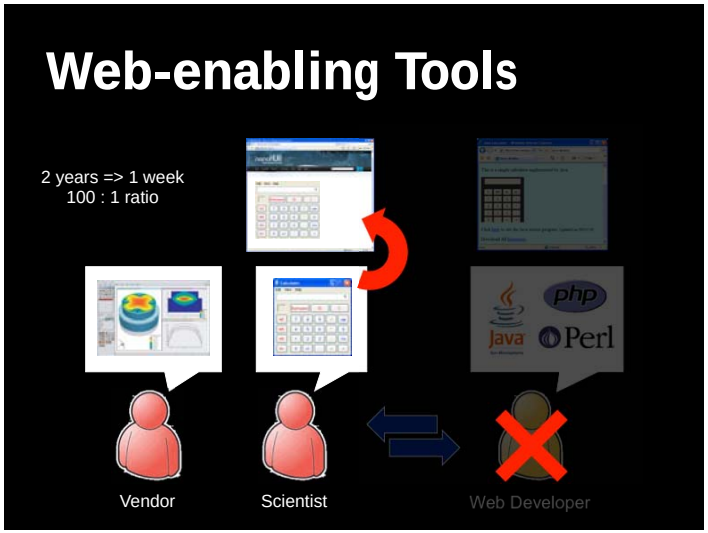
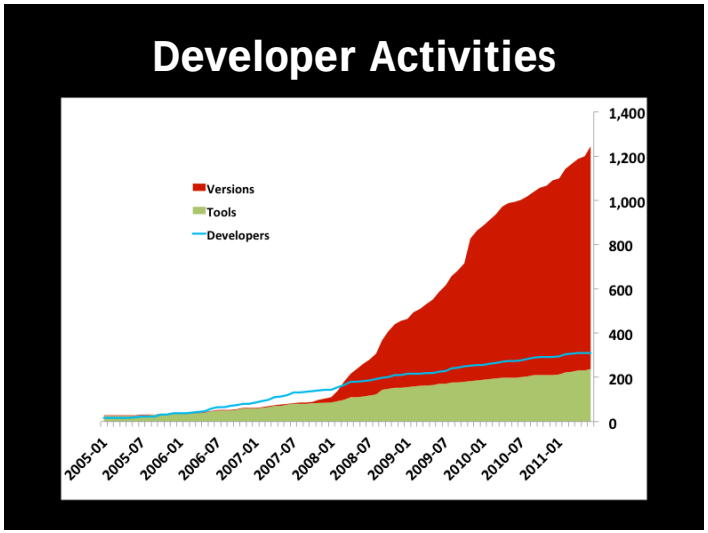
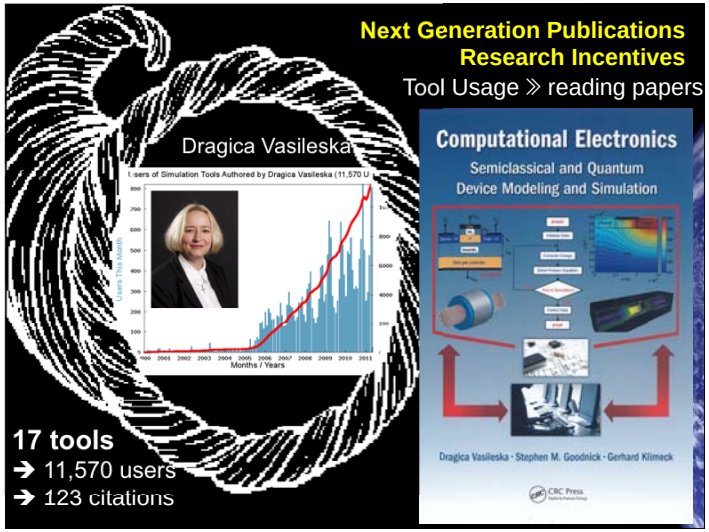
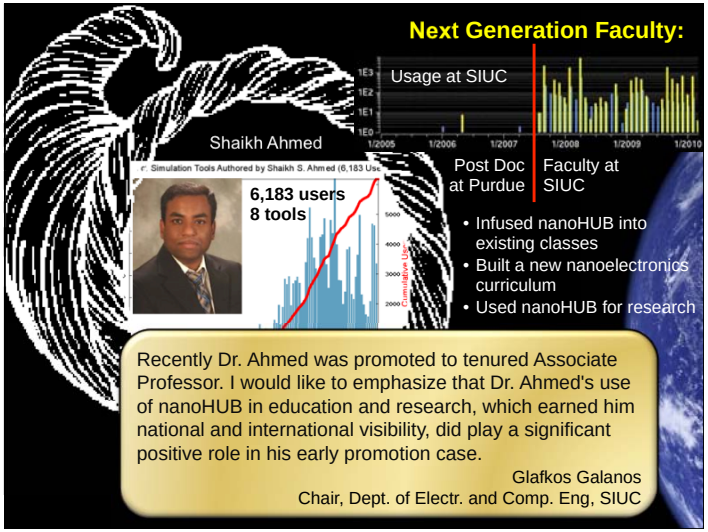



Web-enabling Tools
2 years => 1 week
100 : 1 ratio
Vendor
Scientist
Web Developer


Developer Activities
Versions
Tools
Developers
1,400
1,200
1,000
800
600
400
200
0
2005-01
2005-07
2006-01
2006-07
2007-01
2007-07
2008-01
2008-07
2009-01
2009-07
2010-01
2010-07
2011-01


Next Generation Publications
Research Incentives
Tool Usage ≫ reading papers
Dragica Vasileska
Computational Electronics
Semiclassical and Quantum
Device Modeling and Simulation
Dragica Vasileska · Stephen M. Goodnick · Gerhard Klimeck
17 tools
➔ 11,570 users
➔ 123 citations


Next Generation Faculty:
Usage at SIUC
Shaikh Ahmed
6,183 users
8 tools
Post Doc
at Purdue
Faculty at
SIUC
• Infused nanoHUB into existing classes
• Built a new nanoelectronics curriculum
• Used nanoHUB for research
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

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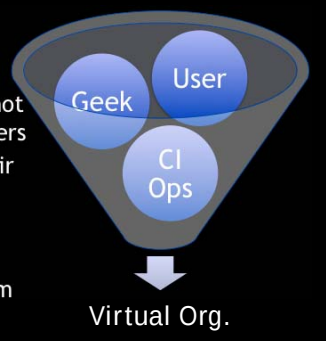

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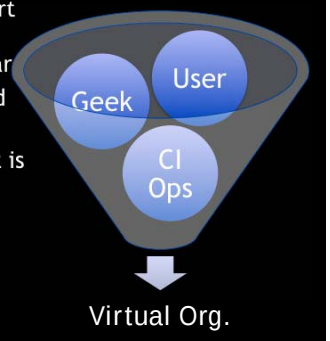
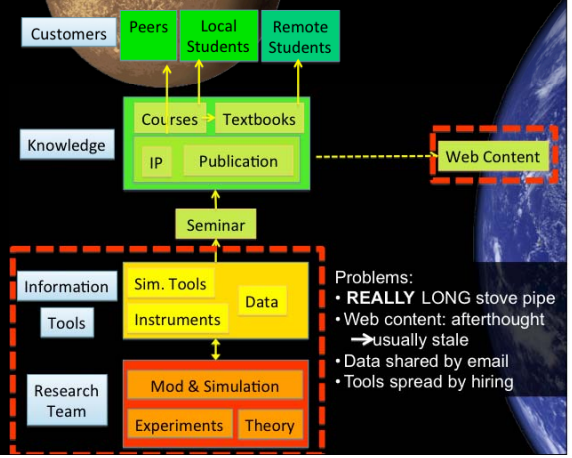
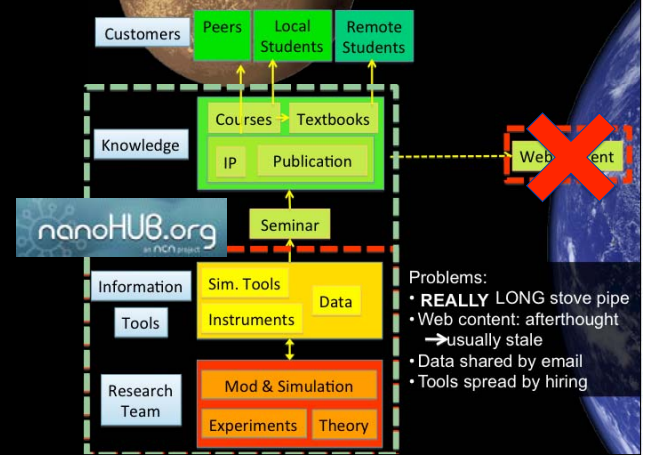


Typical Dissemination Paths



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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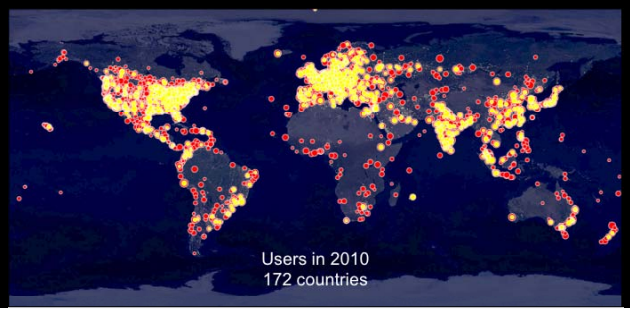
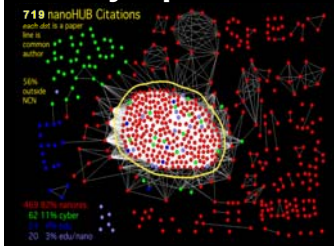
nanoHUB.org
The World's Largest Nano User Facility

188,000 lecture users
830 lecturers
11,000 simulation users
300 sim developers

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

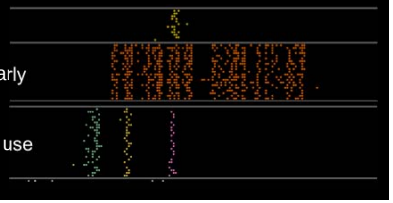


nanoHUB.org
Fully Operational Cloud for End Users

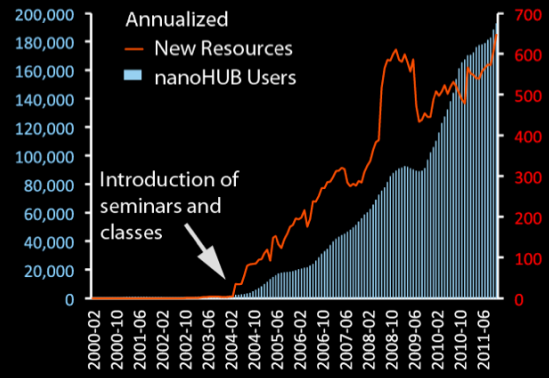


Systemic Use in Research:
- Citation map shows
  Social network of researchers
- Enable other researchers to utilize recent PhD thesis nano-modeling software
- Can measure tool impact

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



How do we get Growth?
NEW CONTENT



nanoHUB.org
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*
  - NO new fundamental research funded in NCN/nanoHUB
- Commitment to serious assessment
  => Focus on users, developers, and operation
  - NOT a promise of future delivery, delivery TODAY