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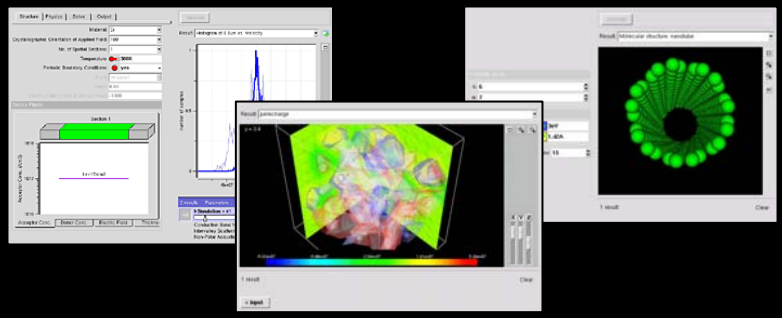
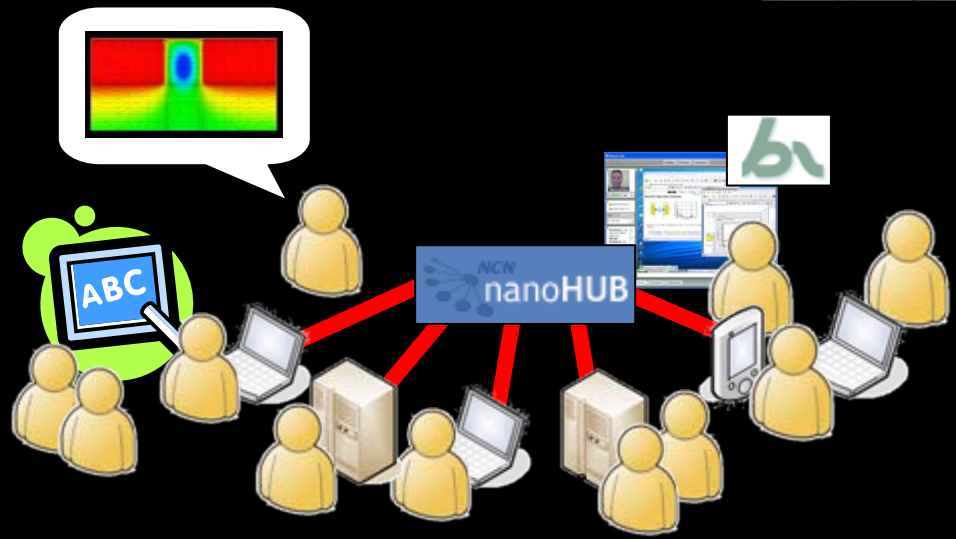
George Adams
Mark Lundstrom, Gerhard Klimeck, Michael McLennan
Network for Computational Nanotechnology
Purdue University

CNI Spring Task Force Meeting
April 8, 2008

What is nanoHUB?

Online simulation… *…and more!*





[Live Demo>>]

[PPT Demo>>]

NANOHUB.ORG - BioMOCA - Microsoft Internet Explorer provided by Insight Broadband

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Address http://www.nanohub.org/simulation_tools/biomoca_tool_information

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BioMOCA

Date posted	09 Jun, 2006
Contributor(s)	Reza Toghraee, Umberto Ravaioli
Type	Simulator
Tags (?)	nano/bio applications, nanomedicine
At a glance	Transport Monte Carlo simulation of conduction in biological Ionic Channels.

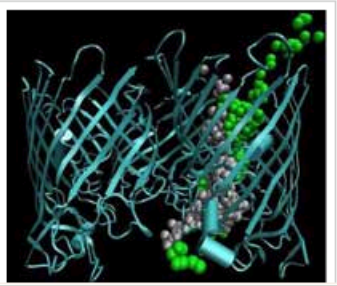
Rating: ★★★★★ (1 review)
Rate this: ☆☆☆☆☆

Launch Tool

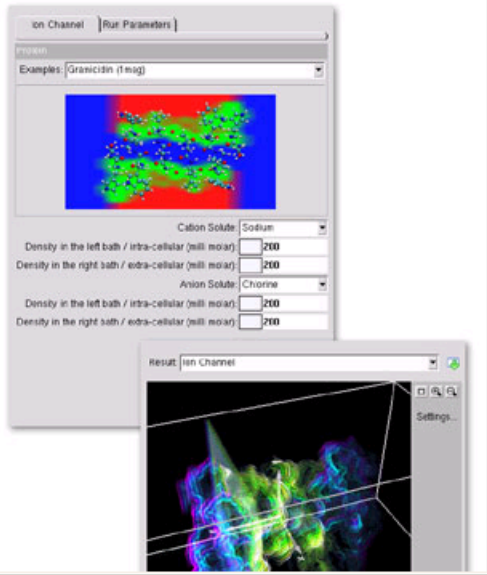
⚠ You must log in before you can run this tool.

Description

With the recent availability of high-resolution structure information for several key ion channel proteins and large-scale computational resources, Molecular Dynamics has become an increasingly popular tool for ion channel simulation. However, the CPU requirements for simulating ion transport on time scales relevant to conduction still exceed the resources presently available. To address the problem, we have developed Biology Monte Carlo (BioMOCA), a three-dimensional coarse-grained particle ion channel simulator based on the Boltzmann Transport Monte Carlo (BTMC) methodology.



The BioMOCA code has progressed steadily to become a flexible tool for investigation of ionic transport that can be used as a complement of more expensive Molecular Dynamics simulations. The picture shown



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BioMOCA

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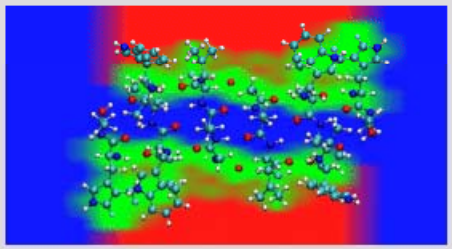
Ion Channel | Run Parameters

Protein

Examples: Gramicidin (1mag)



Cation Solute: Sodium

Density in the left bath / intra-cellular (milli molar): 200

Density in the right bath / extra-cellular (milli molar): 200

Anion Solute: Chlorine

Density in the left bath / intra-cellular (milli molar): 200

Density in the right bath / extra-cellular (milli molar): 200

Simulate >

Refresh Screen

Applet VncViewer started

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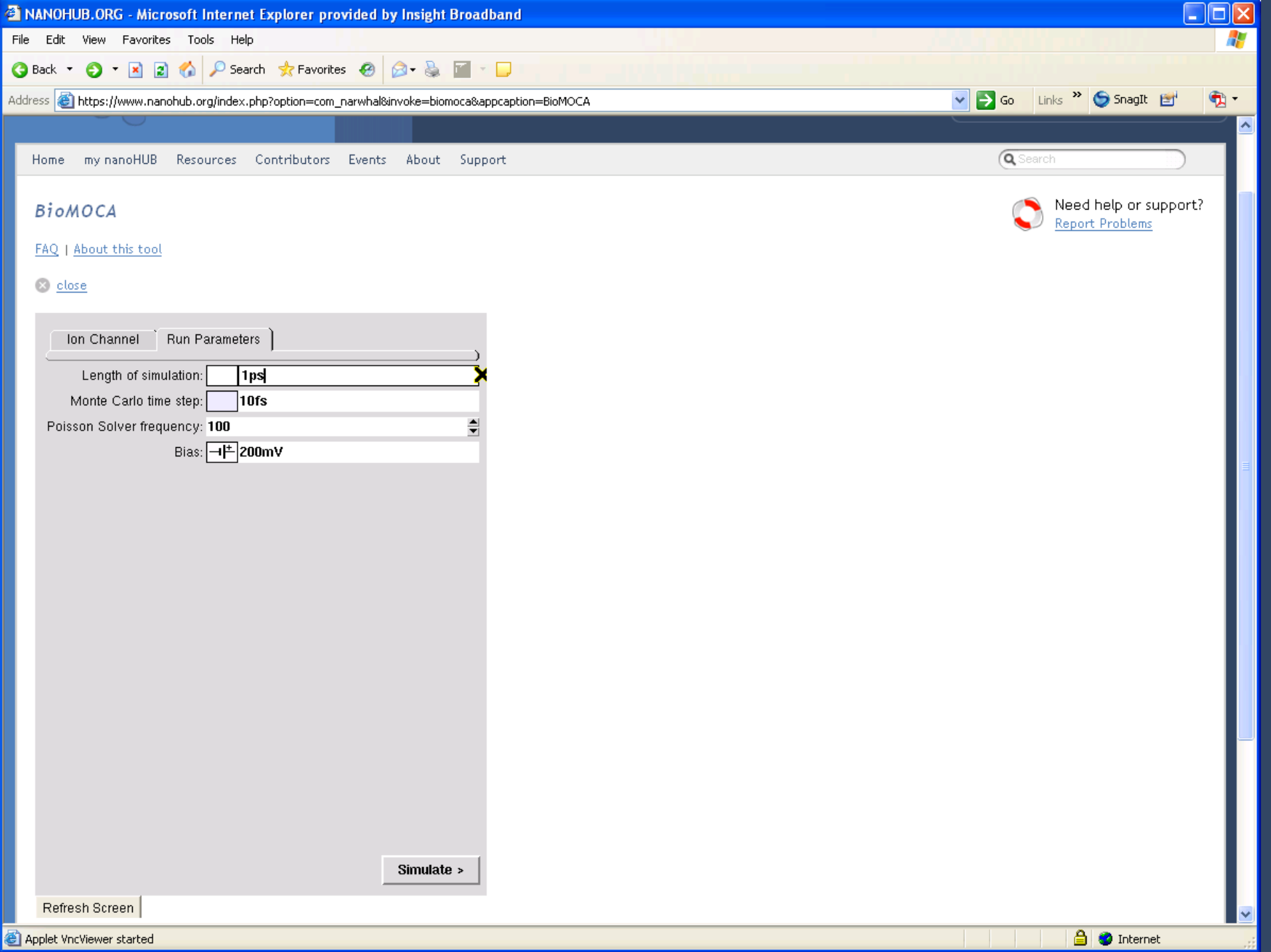
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Ion Channel
Run Parameters
Length of simulation: 1ps
Monte Carlo time step: 10fs
Poisson Solver frequency: 100
Bias: 200mV
Simulate >
Refresh Screen
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```
ATOM 529 CE2 TRP 15 0.250000 7.522000 -15.086000 -0.04
ATOM 530 CE3 TRP 15 0.341000 6.311000 -12.968000 -0.03
ATOM 531 CZ2 TRP 15 -0.638000 8.457000 -14.568000 0.00
ATOM 532 CZ3 TRP 15 -0.561000 7.248000 -12.446000 0.00
ATOM 533 CH2 TRP 15 -1.048000 8.304000 -13.233000 0.00
ATOM 534 H TRP 15 0.219000 3.319000 -13.292000 0.25000
ATOM 535 HA TRP 15 1.253000 3.094000 -16.039000 0.0000
ATOM 536 1HB TRP 15 2.467000 4.433000 -13.597000 0.000
ATOM 537 2HB TRP 15 3.253000 4.335000 -15.209000 0.000
ATOM 538 HD1 TRP 15 2.155000 5.943000 -17.222000 0.000
ATOM 539 HE1 TRP 15 0.785000 8.045000 -17.070000 0.300
ATOM 540 HE3 TRP 15 0.701000 5.499000 -12.354000 0.000
ATOM 541 HZ2 TRP 15 -1.036000 9.239000 -15.191000 0.00
ATOM 542 HZ3 TRP 15 -0.936000 7.144000 -11.437000 0.00
ATOM 543 HH2 TRP 15 -1.750000 8.986000 -12.773000 0.00
ATOM 544 C1 ETA 15 5.148000 0.421000 -15.604000 0.1500
ATOM 545 C2 ETA 15 3.657000 0.080000 -15.674000 0.2500
ATOM 546 N ETA 15 2.813000 1.244000 -15.775000 -0.4000
ATOM 547 O ETA 15 5.921000 -0.752000 -15.827000 -0.650
ATOM 548 1HN ETA 15 2.507000 1.491000 -16.687000 0.250
ATOM 549 HO ETA 15 5.736000 -1.339000 -15.086000 0.400
ATOM 550 1H1 ETA 15 5.410000 1.174000 -16.373000 0.000
ATOM 551 2H1 ETA 15 5.374000 0.849000 -14.601000 0.000
ATOM 552 1H2 ETA 15 3.383000 -0.525000 -14.780000 0.00
ATOM 553 2H2 ETA 15 3.492000 -0.565000 -16.560000 0.00
counter1 552
Poisson parameters:  nitscg = 140 epscg = 1e-06 dkrfac
PLANAR ELECTRODES setting V = 0.2 at z=zmin/zmaz
initialize geometry arrays.
```

Abort

< Input

Refresh Screen

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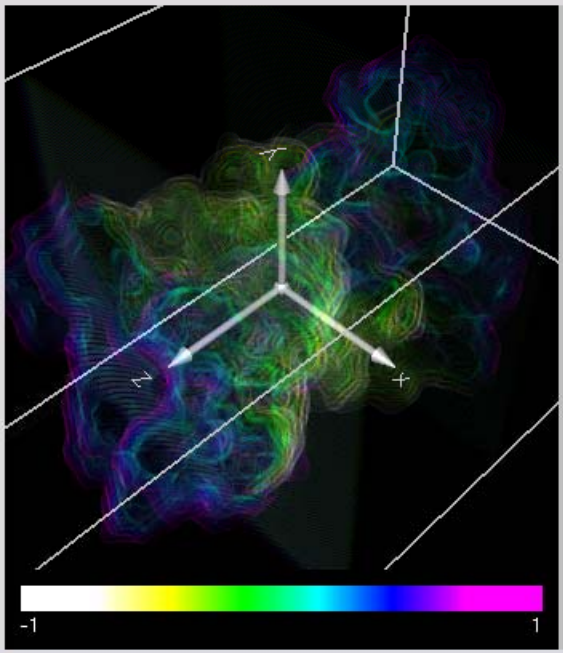
Result: Ion Channel



Settings...

Volume

X Y Z

1 result Parameters... Clear

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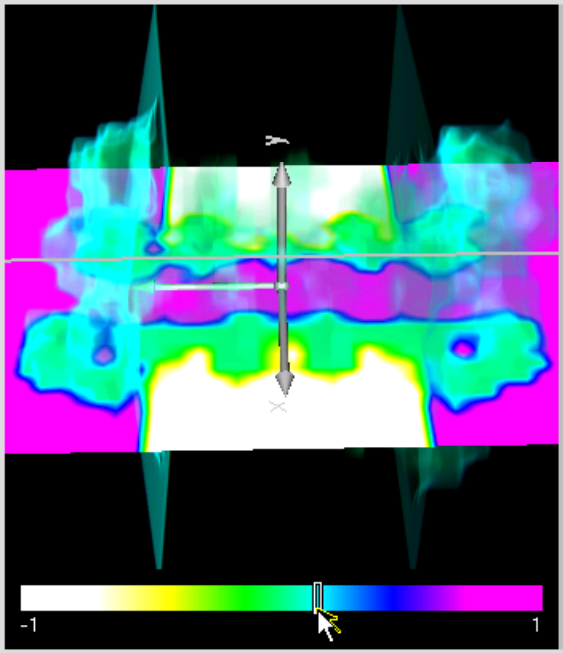
Result: Ion Channel



Settings...

Volume

X Y Z

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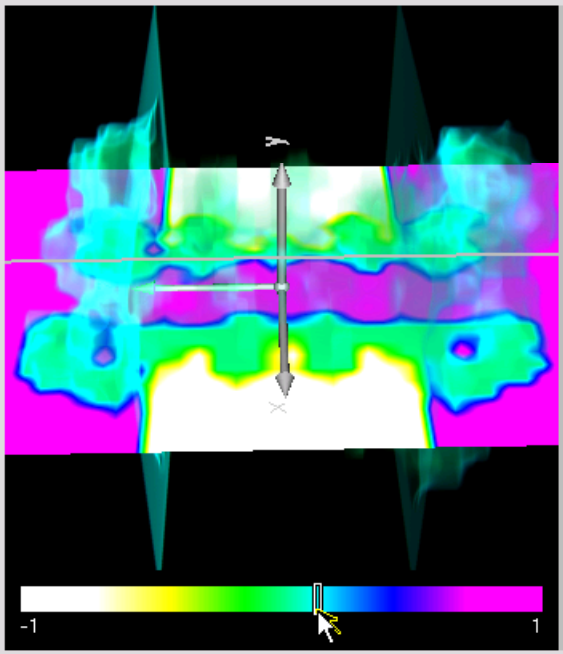
Result: Ion Channel



Volume
X Y Z

1 result Parameters... Clear

< Input

Refresh Screen

cancer

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- Receptor-Targeted Therapies for **Cancer** and Inflammatory Diseases
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  ... Receptor-Targeted Therapies for **Cancer** and Inflammatory Diseases ...
- 2005 Oncological Sciences Center Symposium
  22 Nov, 2005
  ... Progress and Problems in **Cancer** Treatment and Prevention ...
- Testicular **Cancer**
  20 Dec, 2005 | Contributor(s): Stephen D. Williams
- Ovarian **Cancer**: Progress and Challenge
  20 Dec, 2005 | Contributor(s): Daniela Matei
- Multianalyte Approaches to **Cancer** Diagnosis
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  01 Sep, 2005 | Contributor(s): Sigfrid Yngvesson
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- Sensitivity Amplification in Biosensors using Nanoparticles and Enzymatic Macromolecules
  01 Sep, 2005 | Contributor(s): Cagri Savran
  ... er from relatively low sensitivity. We present detection of **cancer** markers using the Quartz Crystal Microbalance and demonstrate that 2 order-

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Nanotechnology 501 Lecture Series

Nanosystems Biology

Date posted	09 Sep, 2004
Contributor(s)	James R. Heath
Time	2004-09-10 9:30 AM
Location	RAWLS, Room 1086, Purdue University, West Lafayette, IN
Type	Online Presentation
Tags (?)	nano/bio applications, nanofluidics, nanomedicine, nanowires, research seminar

Rating: ★★★★½ (2 reviews)

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Abstract

As we enter the 21st century, we stand at a major inflection point for biology and medicine-the way we view and practice these disciplines is changing profoundly. These changes are being driven by systems biology, a new approach to biology, and which will increasingly transform medicine from disease-driven and reactive to health-driven and predictive and preventative. Systems biology and predictive and preventative medicine are both are data driven and, accordingly, both require new tools for making large numbers of measurements. Microfluidics, nanotechnologies and molecular imaging will revolutionize our ability to generate comprehensive data sets that span from individual cells to patients. In this talk I will describe a systems biology approach toward disease, using cancer as the model. I will then describe our progress toward developing 'informative' diagnostic tools based upon the multiparameter analysis of blood cells and serum, with the goals of achieving early stage detection of various cancers.

Biography

James R. Heath is the Elizabeth W. Gilloon Professor and Professor of Chemistry at Caltech, and Professor of Molecular & Medical Pharmacology at UCLA. Heath received a B.Sc. degree in 1984 (Baylor) and his Ph.D. in Chemistry (Rice) in 1988 where he was the principal student involved in the Nobel Prize-winning discovery of C60 and the fullerenes. Heath was a Miller Fellow at UC Berkeley from 1988-91, and on the Technical Staff at IBM Watson Labs from 1991-94. In 1994 he joined the faculty at UCLA. He founded the California NanoSystems Institute in 2000 and served as its Director until moving to Caltech. Heath has

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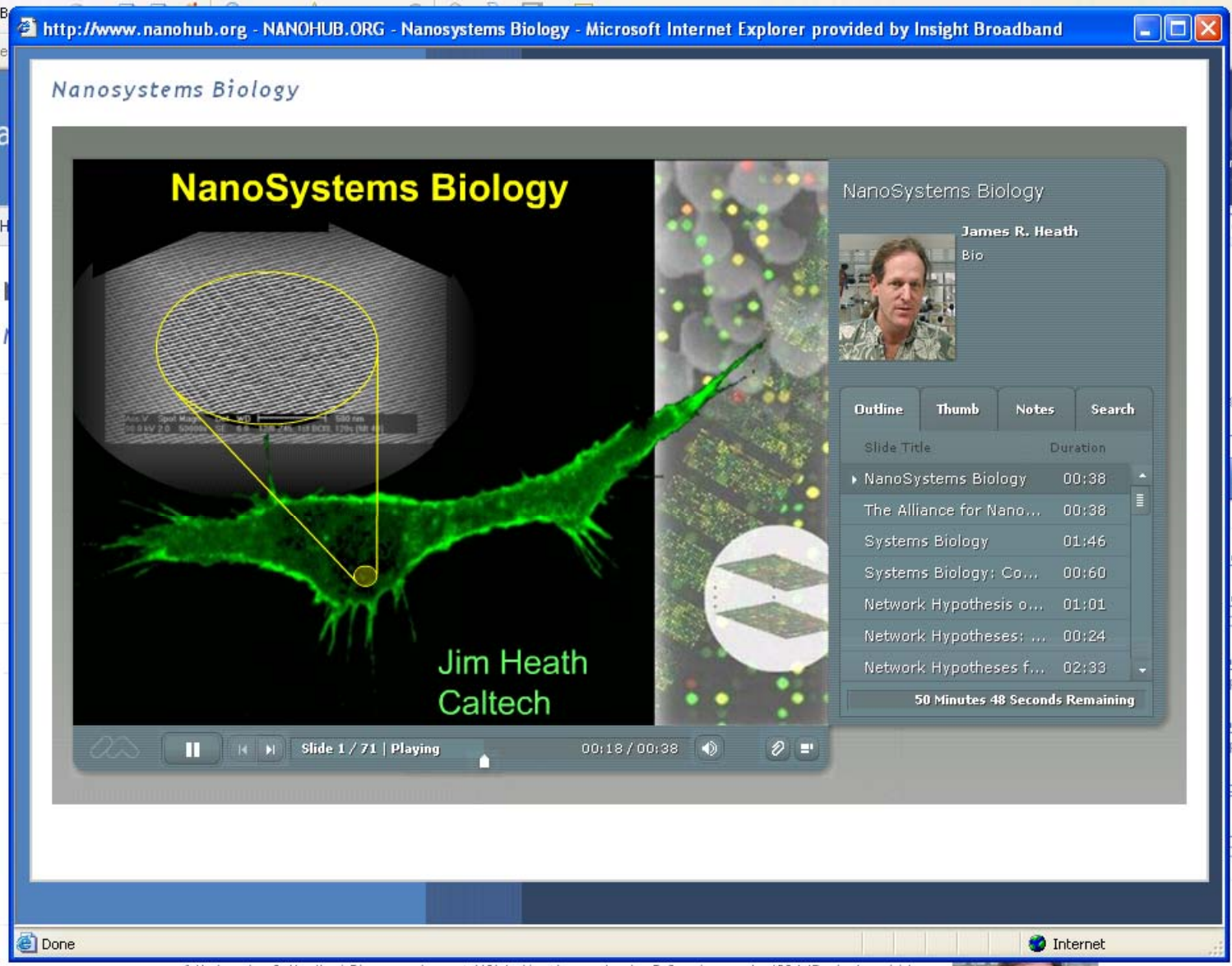
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Caltech
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James R. Heath
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Thumb
Notes
Search
Slide Title
Duration
NanoSystems Biology 00:38
The Alliance for Nano... 00:38
Systems Biology 01:46
Systems Biology: Co... 00:60
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Network Hypotheses f... 02:33
50 Minutes 48 Seconds Remaining
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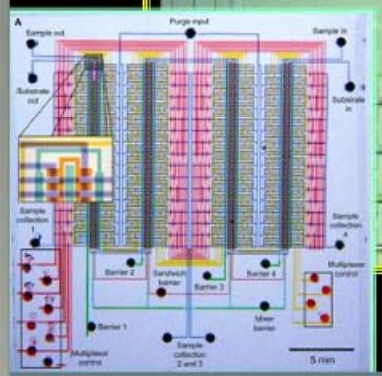
Nanosystems Biology

Integrated Channels, Valves & Pumps for Multiparameter Diagnostics & molecular imaging probe synthesis



Steve Quake group

NanoSystems Biology

James R. Heath

Bio

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probe

Slide Title	Duration
Integrated Channels, ...	01:19
Probe molecules	00:40
Moving beyond single...	01:28
Probe	00:19

25 Minutes 43 Seconds Remaining

Slide 23 / 71 | Playing 00:04 / 01:19

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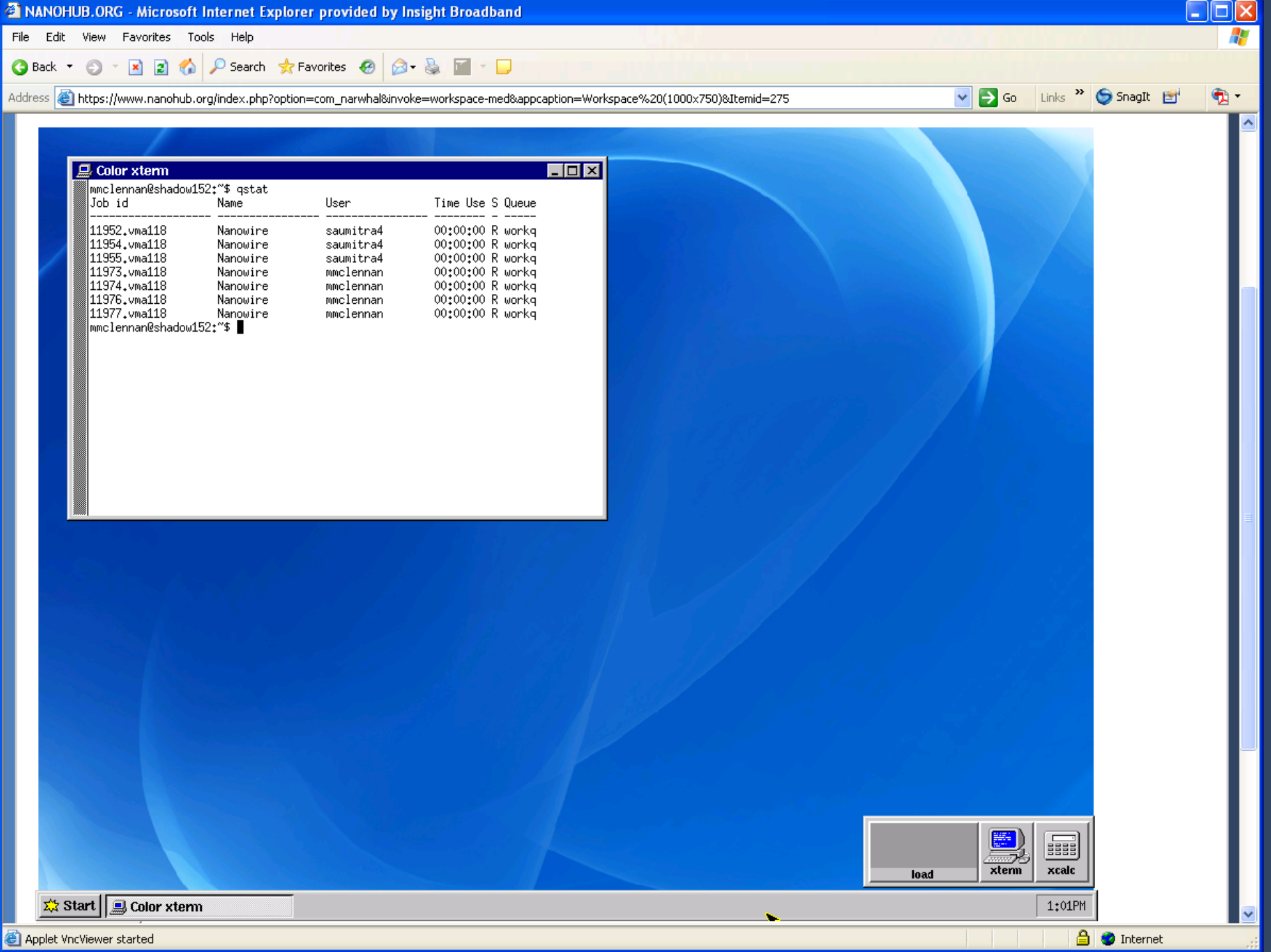
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Color xterm
mmclennan@shadow152:~$ qstat
Job id Name User Time Use S Queue
11952.vma118 Nanowire saumitra4 00:00:00 R workq
11954.vma118 Nanowire saumitra4 00:00:00 R workq
11955.vma118 Nanowire saumitra4 00:00:00 R workq
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11976.vma118 Nanowire mmclennan 00:00:00 R workq
11977.vma118 Nanowire mmclennan 00:00:00 R workq
mmclennan@shadow152:~$
load
xterm
xcalc
Start
Color xterm
1:01PM
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Color xterm

```
mmclennan@shadow152:~$ qstat
Job id              Name             User             Time Use S Queue
------------------- ---------------- ---------------- -------- - -----
11952.vma118        Nanowire         saumitra4        00:00:00 R workq
11954.vma118
11955.vma118
11973.vma118
11974.vma118
11976.vma118
11977.vma118
mmclennan@shado
Using /apps/nan
```

Silicon nanowire simulator

File

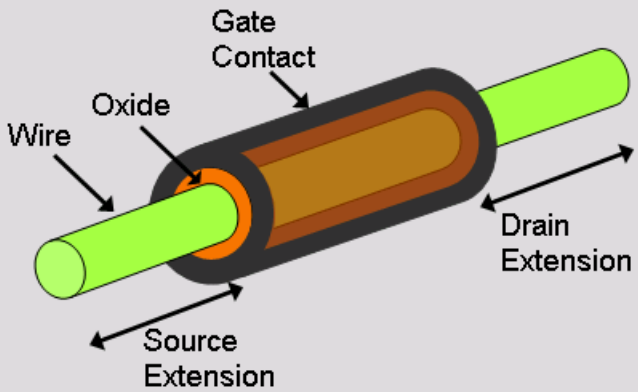
Geometry & doping | Gate | Drain | Simulation parameters

Simulate | new input parameter

Diameter of the silicon-nanowire:	5nm
Oxide thickness:	1nm
Gate length:	10nm
Source & drain extension length:	8nm
Source & drain doping (n):	2.0e26/m3
Channel doping (p):	0.0/m3

Silicon nanowire simulator

Press "Simulate" to view results.



load xterm xcalc

Start | Color xterm | Silicon nanowire simula... | 1:02PM

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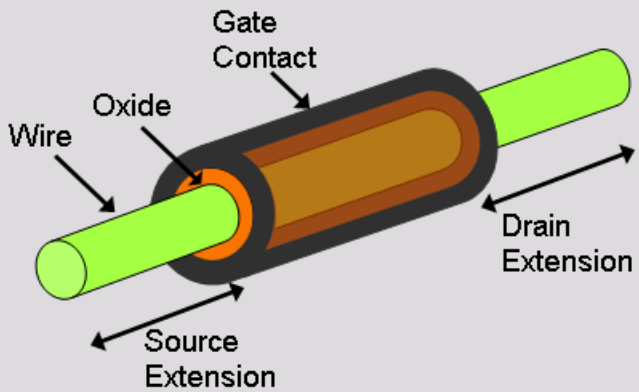
Gate length: 10nm

Source & drain extension length: 8nm

Source & drain doping (n): 2.0e26/m3

Channel doping (p): 0.0/m3

Press "Simulate" to view results.



Start

Refresh S

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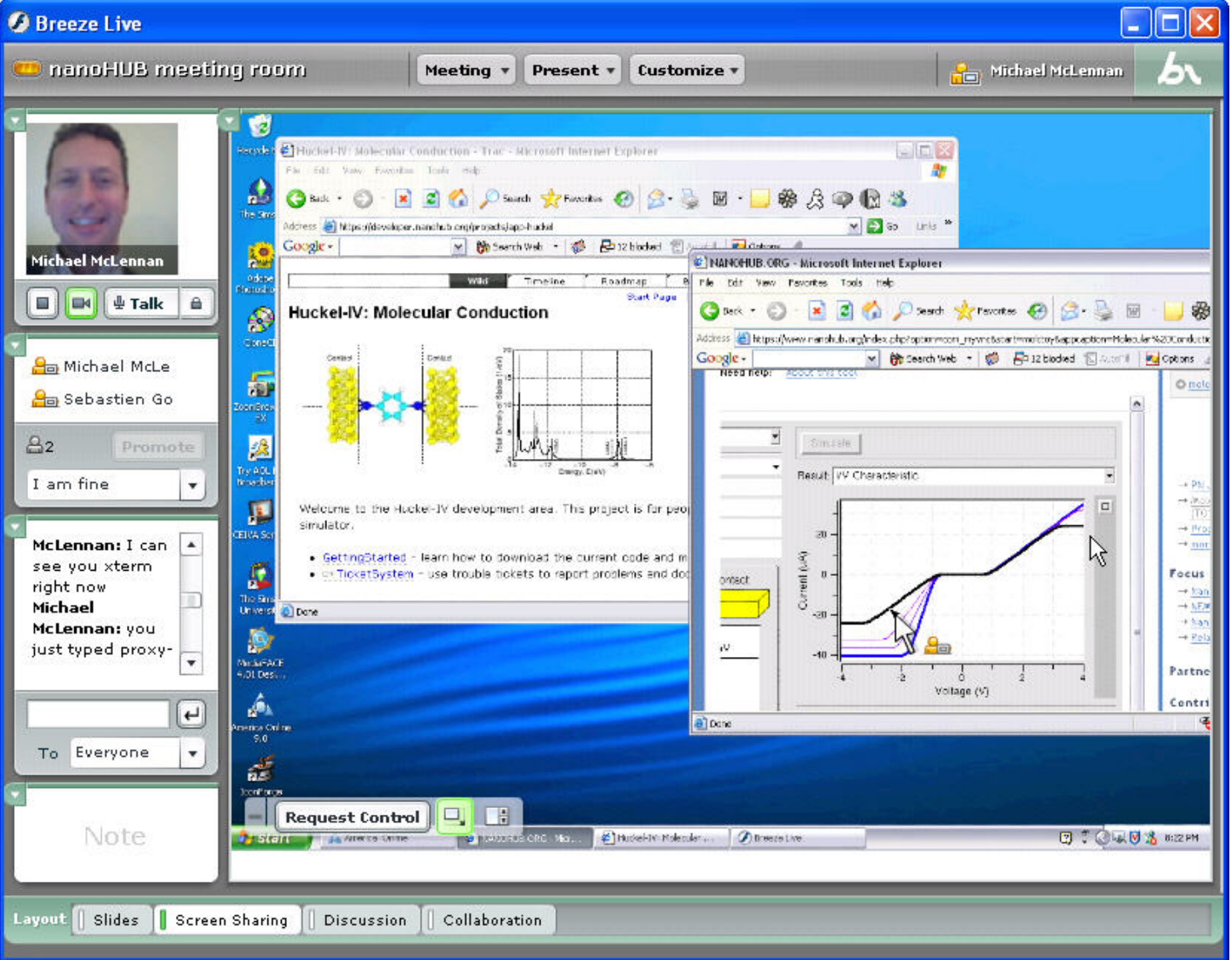
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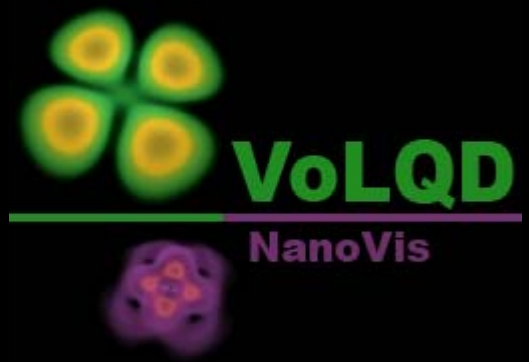
nanoHUB meeting room
Meeting
Present
Customize
Michael McLennan
Michael McLennan
Talk
Michael McLe
Sebastien Go
2
Promote
I am fine
McLennan: I can see you xterm right now
Michael McLennan: you just typed proxy-
To
Everyone
Note
Huckel-IV: Molecular Conduction - Trac - Microsoft Internet Explorer
Huckel-IV: Molecular Conduction
Welcome to the Huckel-IV development area. This project is for peo
simulator.
GettingStarted - learn how to download the current code and m
TicketSystem - use trouble tickets to report problems and doc
NANOHUB.ORG - Microsoft Internet Explorer
Result: IV Characteristic
Current (uA)
Voltage (V)
Request Control
Layout
Slides
Screen Sharing
Discussion
Collaboration

Free Account

(just confirm your email address)

Interactive Visualization

integrated seamlessly

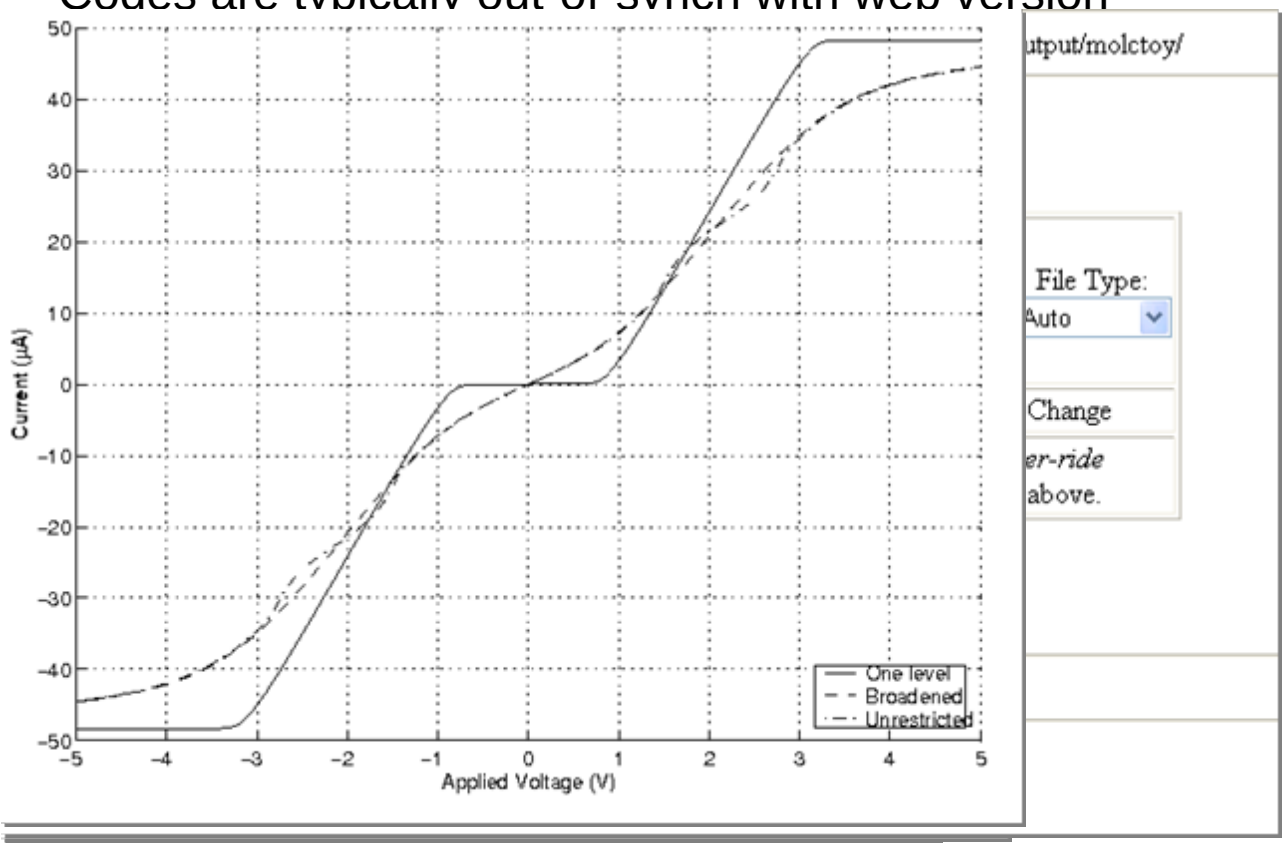


nanoVIS rendering server

Developed by
Wei Qiao, Insoo Woo, David S. Ebert
PURPL Lab, Purdue University

Typical Web-based Simulations

- Started at Purdue 1995 with PUNCH:
  - » Enabled researchers and students to access real simulation codes
  - » traditionally 800 users annually.
- Typical usability is marginal
- Codes are typically out-of-synch with web version



The OLD static GUI

- Form sheet input
- Batch submission
- Output in some file
- Visualize a gif image
- Other output file
- Visualize gif image

Typical Questions:

- What was my input?
- Did I enter things right?

Symptoms of:

- No VISUAL feedback.
- Not interactive.

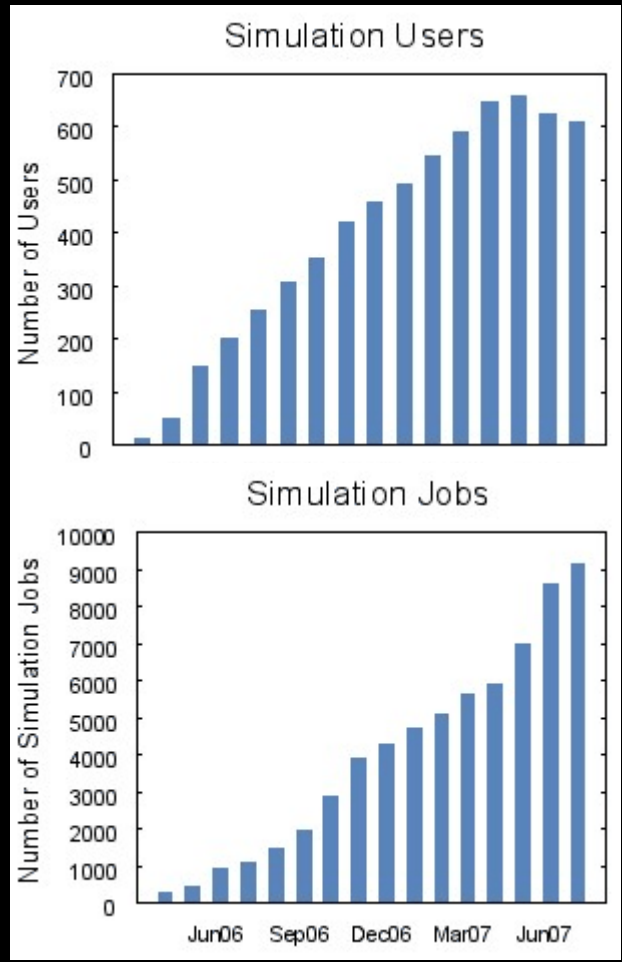
nanowire

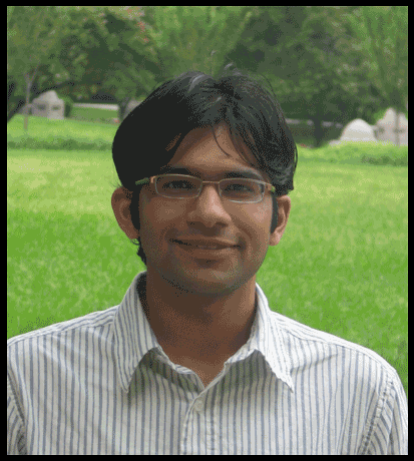
Usage

Released May 19, 2006

610 Users

9,115 Simulations





Saumitra Mehrotra

Univ. of Cincinnati

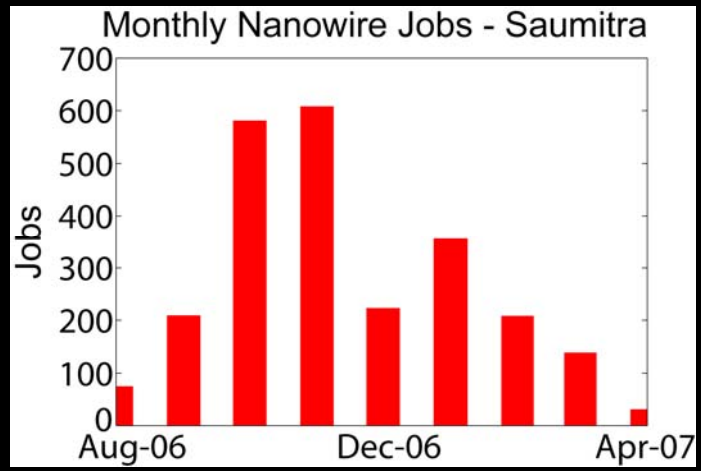
In the past 10 months:

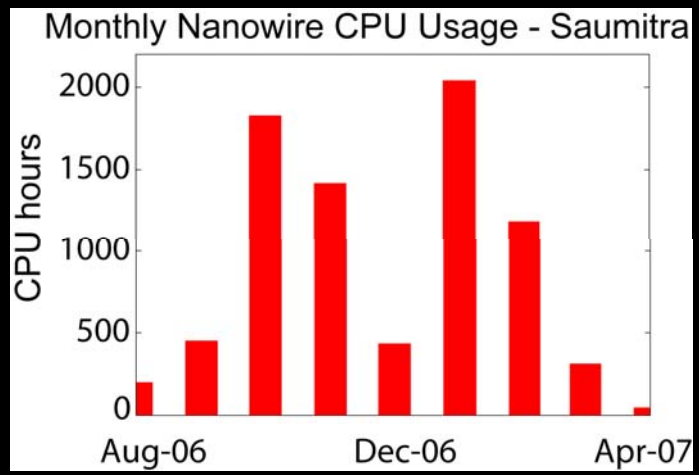
26 tools / 3,327 simulations

- 47 simulations: bandstructure lab
- 240 simulations: FETtoy
- 2,855 simulations: nanowire
- 8,242 nanowire CPU hours

- “and more” content
  134 items, 52 hours

- 96 support tickets
  69 entered manually,
  27 filed automatically by application





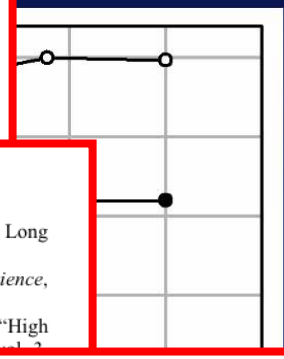
IEEE Workshop on Microelectronics and Electron Devices (WMED), April 20 2007

Process Variation Study for Silicon

Simulation Tool

SiNW FET Vs FinFET – Gate Length Variation

Process Variation Study for Silicon Nanowire Transistors



performance in circuits and superior reproducibility for the SiNW FETs.

Fig. 4 shows the variation in the threshold voltage with change in the gate dielectric thickness. Again, the SiNW FET shows a smaller variation (1.2 mV/A) compared with the FinFET's 5 mV/A. Also of interest is the sensitivity of the devices to the gate length. Shown in Fig. 5 is the threshold

REFERENCES

[1] W.S.Shi et al., "Synthesis of Large Areas of Highly Oriented, Very Long Silicon Nanowires," *Adv. Mater.* 12, 1343, 2000.

[2] D. Ma et al.," Small-Diameter Silicon Nanowire Surfaces," *Science*, 299, p. 1874, 2003.

[3] Y. Cui, Z. Zhong, D. Wang, W. U. Wang, and C. M. Lieber, "High

[7] J. Wang, E. Polizzi, M. Lundstrom, "A three-dimensional quantum simulation of silicon nanowire transistors with the effective-mass approximation," *Journal of Applied Physics* **96**(4), pp. 2192-2203, 2004.

[8] Simulations were performed on http://nanohub.org

[9] J. Wang, E. Polizzi, and M. Lundstrom, "A computational study of ballistic silicon nanowire transistors," in *IEDM Tech. Dig.*, Dec. 8–10, 2003,pp. 695–698.

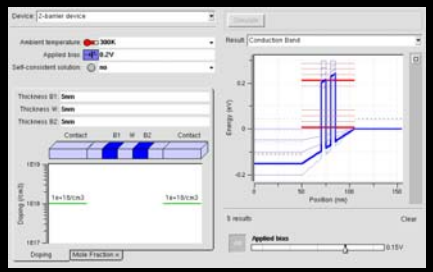
Use in Education

The nanoHUB has proven itself to be an extremely valuable tool for education and research. …We have used the Resonant Tunneling Diode simulator and the MSL simulator on the nanoHUB for homework exercises and mid-term exams. A class survey of the use of the nanoHUB simulation engines had shown that ***the experience is quite positive. The staff at the nanoHUB has been very responsive in supporting our class activities in a professional manner.***

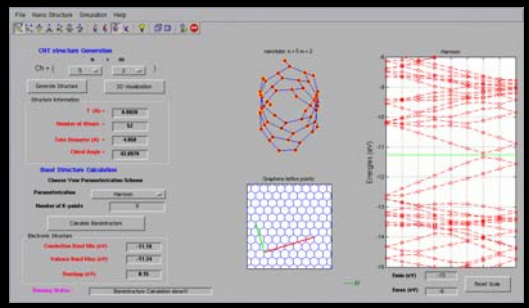
H.-S. Philip Wong

Professor of Electrical Engineering

Stanford University



Resonant Tunneling Diodes



MSL simulator

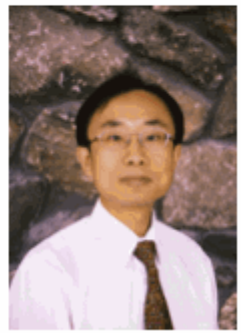
New Contributor

Contributors

H.-S. Philip Wong

Contributions	2
Affiliation	Stanford University
Web Site	http://www.stanford.edu/~hspwong

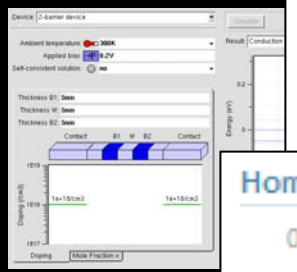
Biog eceived the B.Sc. (Hons.) in 1982 from the University M.S. in 1983 from the State University of New York at he Ph.D. in 1988 from Lehigh University, all in ing. He joined the IBM T. J. Watson Research Center,



H.-S. Philip Wong

Professor of Electrical Engineering

Stanford University



Resonant T
Diodes

Resonant Tunneling Diode Simulation

H.-S. Philip Wong
Stanford University

1. In this problem, we will use software on *nanoHUB.org* to plot the I-V characteristic of a resonant tunneling diode. Visit the following page:
   https://www.nanohub.org/members/tools/rtd_tool_information
   Please use the following parameters:
   a) 2-barrier device
   b) Barrier thickness (Al_xGaAs): 5nm
   c) Well thickness (GaAs): 5 nm
   d) Temperature: 300 K
   e) Doping at contacts: 10^{18}/cm^3
   Plot the I-V characteristic for V=0 – 0.4 volt. What are the values of I_p & I_v?
   p.s. DON'T turn the self-consistent potential on

2. In the previous homework, we have learned how to use the RTD software on *nanoHUB.org*. Design a RTD that gives the largest PVCR (peak-to-valley current ratio). You can adjust any parameter in the simulator, and again, DON'T turn on the self-consistent analysis.
   Explain why and how you choose your parameters to maximize the PVCR.

3. Consider the RTD-based SRAM circuit discussed in class (see *IEEE Transactions on Nanotechnology, Vol. 4, No. 4, p.472 (2005)*). We are going to do some simplified analysis to "design" a RTD SRAM.
   For a typical DRAM the storage capacitance is 35 fF (C_s = 35 fF). Assume the bit line capacitance is 0.2 pF/mm and the bit line is 500 um long. Also assume the leakage current of the storage node is 0.5 pA per cell.
   By using the RTD simulator on *nanoHUB.org*, design a RTD that will result into a working SRAM cell (you may use the results from the homework as a starting point). You have to answer the following questions:
   a) What is the layer structure, i.e. material and thickness of your RTD?
   b) What is the area of the RTD required?
   c) If the area of a typical DRAM cell is $6F^2$ where F = half-pitch of the technology (typically identified as the "technology node"), will the area of your RTD fits on top of the DRAM cell for F = 130 nm, 90 nm, 65 nm, 32 nm, 22 nm technology? Ignore the problem of wiring the RTD for this exercise.
   d) What are the voltages of the two stable points (V_0, V_1) of the storage cell? Show how you determine the V_0, V_1 and whether the cell is stable upon reading the cell (read "0" and "1").
   e) How can you make V_0 and V_1 closer to ground and V_{DD}?

Homework for Resonant Tunneling Diodes

06 Jan, 2006 | Teaching Materials | Contributor(s): H.-S. Philip Wong

This homework assignment was created by H.-S. Philip Wong for EE 218 "Introduction to Nanoelectronics and Nanotechnology" (Stanford University). It includes a couple of simple "warm up" exercises and two design problems, intended to teach students the electronic properties of resonant tunneling ...

Deji Akinwande

Stanford University

In Philip Wong's Fall 2005 class

A Composite Circuit Model for NDR Devices in Random Access Memory Cells

Deji Akinwande, *Member, IEEE*, and H.-S. Philip Wong, *Fellow, IEEE*

***Abstract*—Devices exhibiting negative differential resistance (NDR), such as resonant tunneling diodes and Esaki-type diodes,**

Word Line VDD

C. Validation of Composite Model

Analytical models are not useful if they are inaccurate. In Fig. 4, a graphical comparison between the three sets of composite models and experimental composite data from the NDR device reported in [6] are shown. As another example,

[1]Online, available http://www.nanohub.org, "Resonant tunneling diodes simulator." The "self-consistent solution" option was turned off. Contact/well material = GaAs, barrier material = AlAs, contact doping = $1 \times 10^{19}/\text{cm}^3$, barrier width = 1 nm, well width = 1.5 nm, RTD area = 918 nm^2.

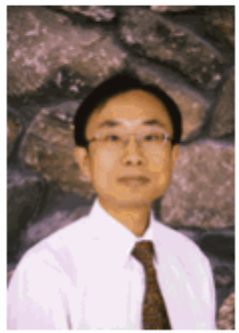
More Contributions

Contributors

H.-S. Philip Wong

Contributions	2
Affiliation	Stanford University
Web Site	http://www.stanford.edu/~hspwong

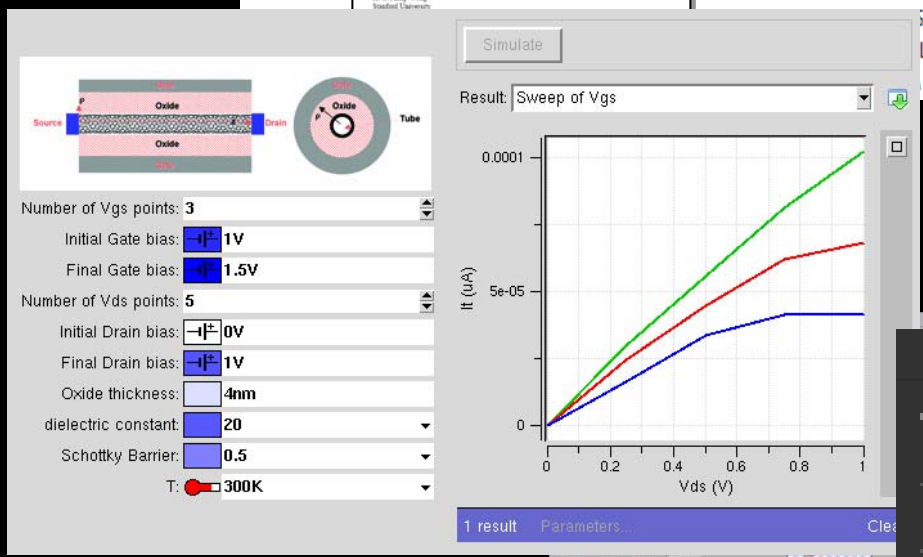
Biog Resonant Tunneling Diode Simulation eceived the B.Sc. (Hons.) in 1982 from the University tate University of New York at Lehigh University, all in T. J. Watson Research Center,



H.-S. Philip Wong

Professor of Electrical Engineering

Stanford University



Schottky-Barrier CNFET
Online March 16, 2007

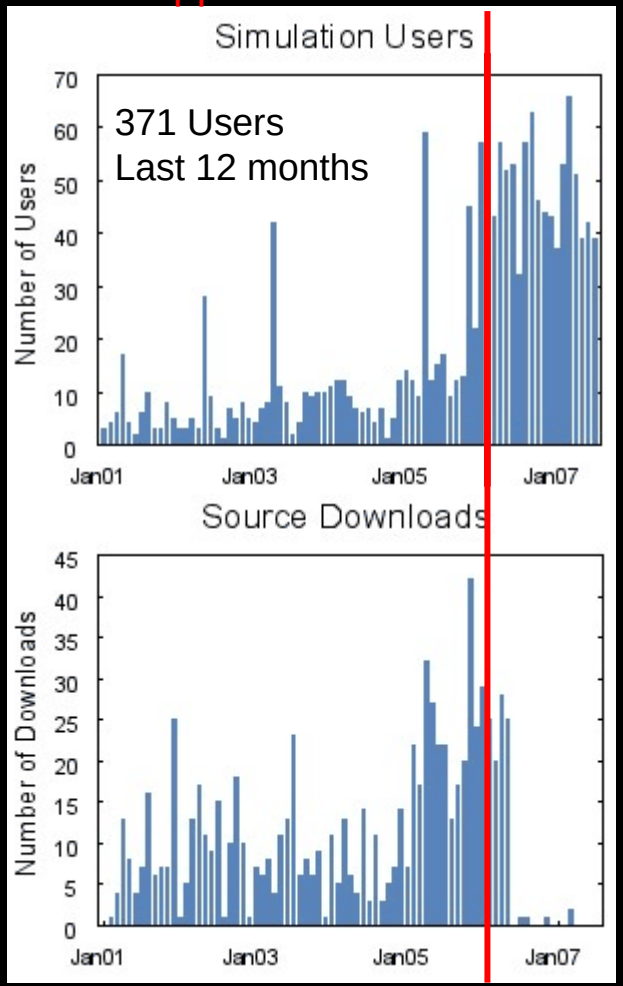
USAGE STATS

Users:	179
Jobs:	1065
Avg. exec. time:	45 secs

Last 12 Months: updated 04 Dec, 2007

Case in point

Rappture version Feb 06



TCAD simulations using SCHRED [15] or ISE, …., were used to support our analysis and compute the inversion carrier profiles in the devices.

Effect of channel positioning on the 1/ f noise in silicon-on-insulator metal-oxide-semiconductor

M von Haartman, M Oestling,
Journal of Applied Physics, 2007 - link.aip.org**...**

- Same behavior across all similar converted tools
- User's don't have to download/install software

nanoHUB online simulation and more — an NCN project

nanoHUB Cyberinfrastructure:

The Engineering

"Under the Hood"

Dr. Michael McLennan
Software Architect

Prof. Gerhard Klimeck
Associate Director of Technology

PURDUE UNIVERSITY

NCN NSF

Cyberinfrastructure for Running Tools

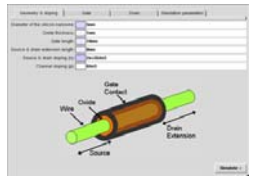
nanoHUB online simulation and more
an NCN project

Content Database

Maxwell's Daemon

Physical Machine

Virtual Machine

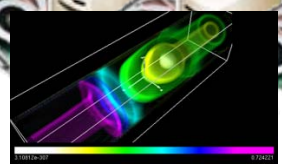


Open Science Grid

nanoHUB cluster

Violin

TeraGrid



Rendering Farm

PURDUE UNIVERSITY

NCN

NSF

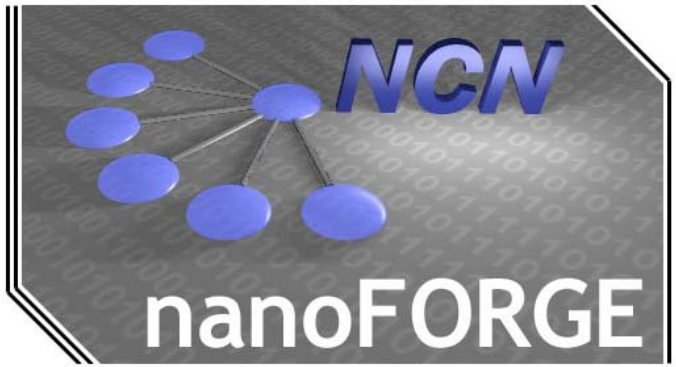
nanoFORGE.org

Open-source AND closed-source code development

201 registered projects

Welcome to nanoFORGE, the project development area of nanoHUB.org. The following pages are maintained by the various owners of each project. Many of these tools are available as Open Source, and you can download the code via Subversion from this site. Some tools are closed source at the request of the authors, and only a restricted development team has access to the code. See each project page for details.

Become a member! Sign up for a free nanoHUB account and use this site to manage your software project.



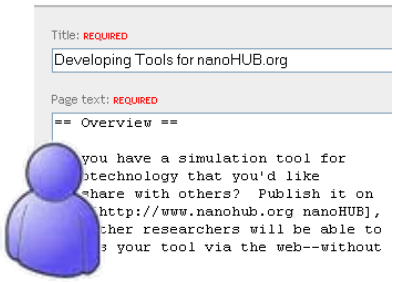
Infrastructure Projects

- hubzero
- lib-gangli
- nanohub
- nanohub-for-kids
- nanohub-support
- ncn
- ncn_students
- nmi
- pharmengine
- rappture
- rappture-runtime
- rkspack
- sysman
- xhub

Applications

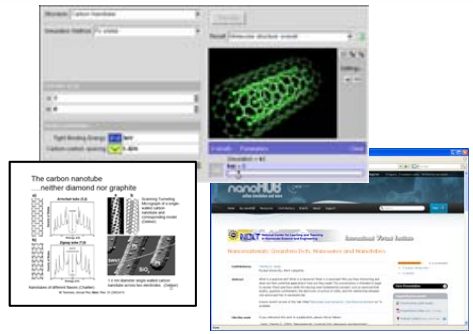
- app-abinit
- app-adept
- app-bandstrlab
- app-beamprop
- app-biomoca
- app-biomolelab
- app-biophet
- app-biotrpnp
- app-blast
- app-brownianmotion
- app-bstr_sc_lab
- app-cacti
- app-cenems
- app-cgtb
- app-chemkinetics
- app-chess
- app-cndo

Other Cyberinfrastructure



Knowledge Articles & Blogs

Tool Development

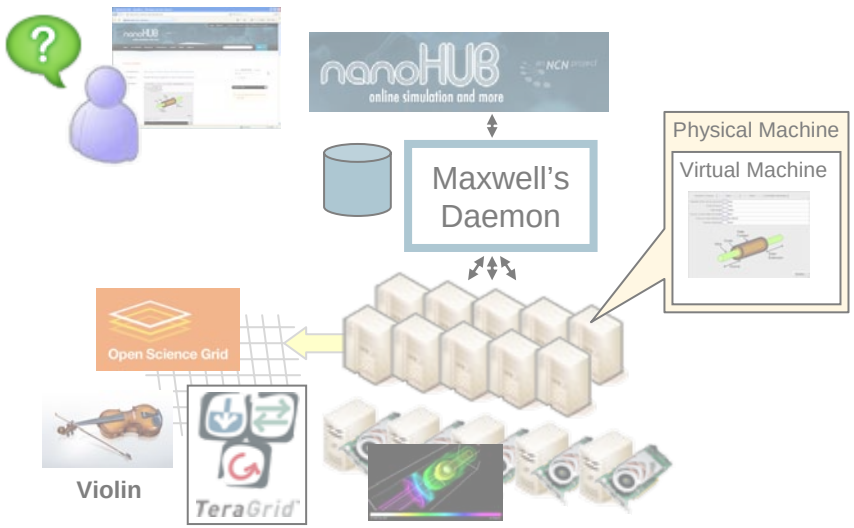


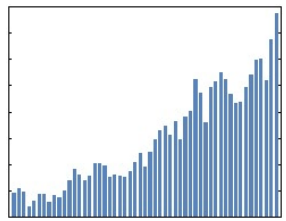
Recommendations

Citations & Digital Object Identifiers

Incentive System

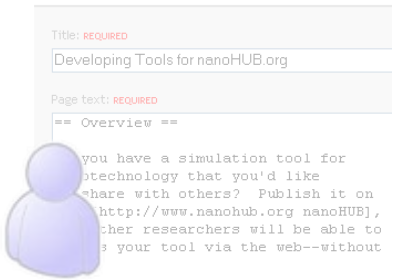
Questions & Answers



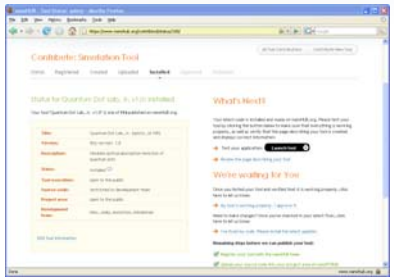


More Statistics

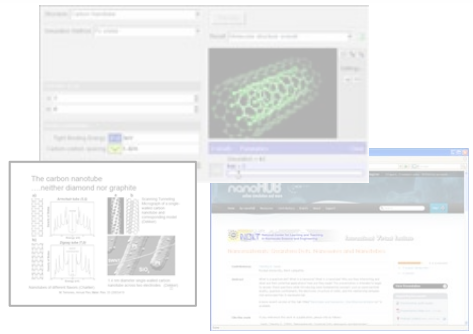
Tool Development Framework



Knowledge
Articles & Blogs



Tool Development



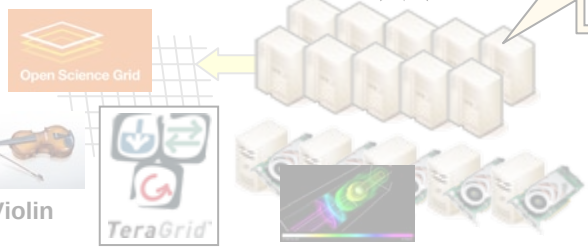
Recommendations

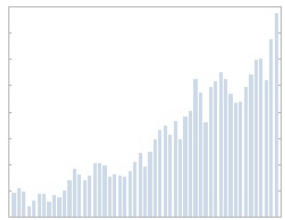
Citations &
Digital Object
Identifiers

\+

Incentive
System

Questions &
Answers





More
Statistics

PURDUE
UNIVERSITY

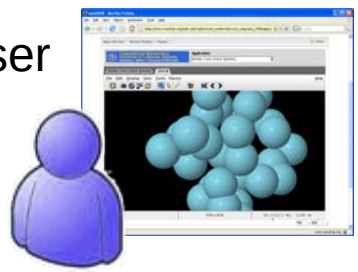
NCN

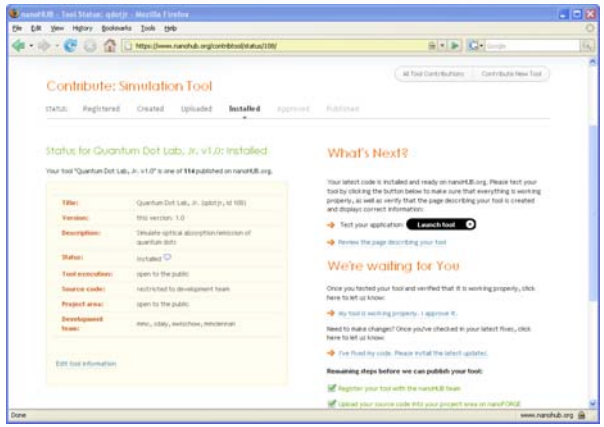
Tool Development Framework

Tool Developer

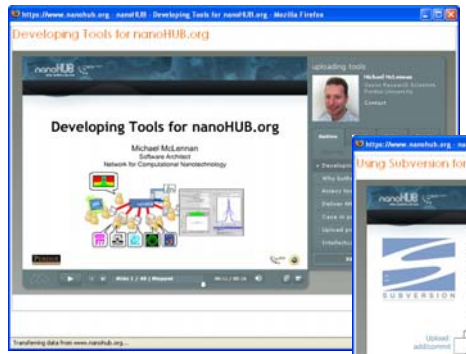
- Registered
- Created
- Uploaded
- Installed
- Approved
- Published

End User



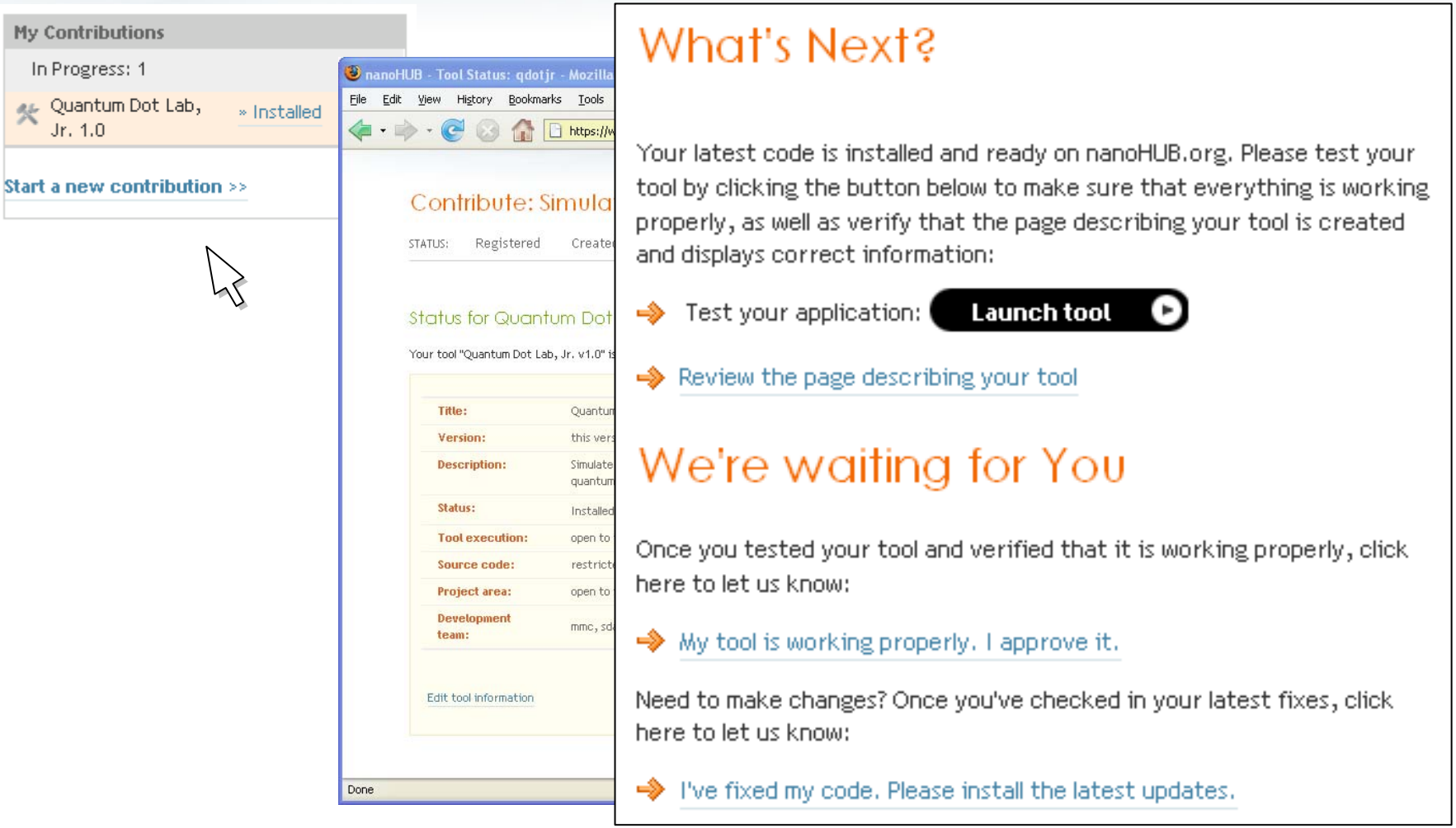


Web-based Publishing System



Summer School at UIUC
Online seminars

Web-based Publishing System

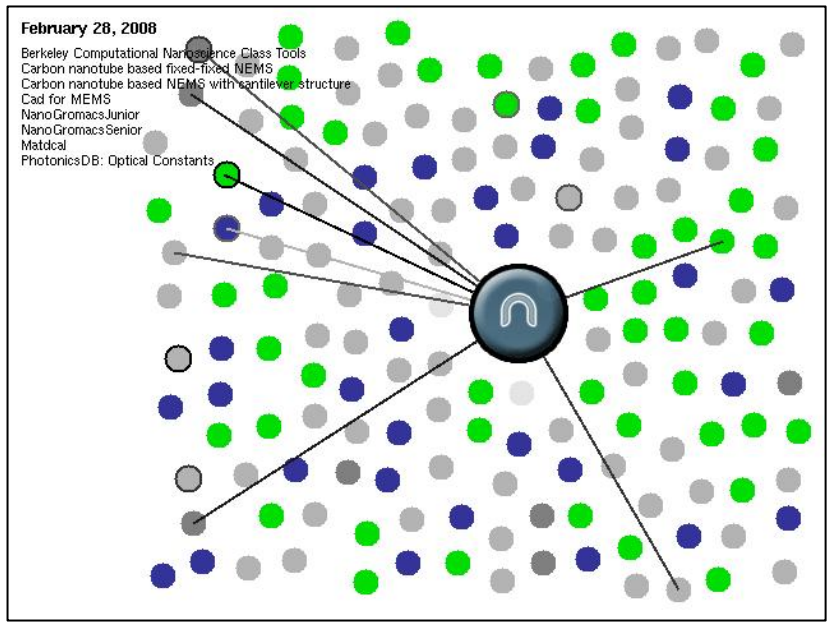


Usage since April 2007

199 Projects

During the past year…
166 Active Projects

125 Active Developers
- #1 - drichards
- #2 - joeringg
- #3 - ssahmed
- #4 - saumitra
- #5 - paul_nano_tran



State changes they made:	506
State changes we helped with:	431
TOTAL:	937

Time Development for One Tool >>

Time Development for All Tools >>

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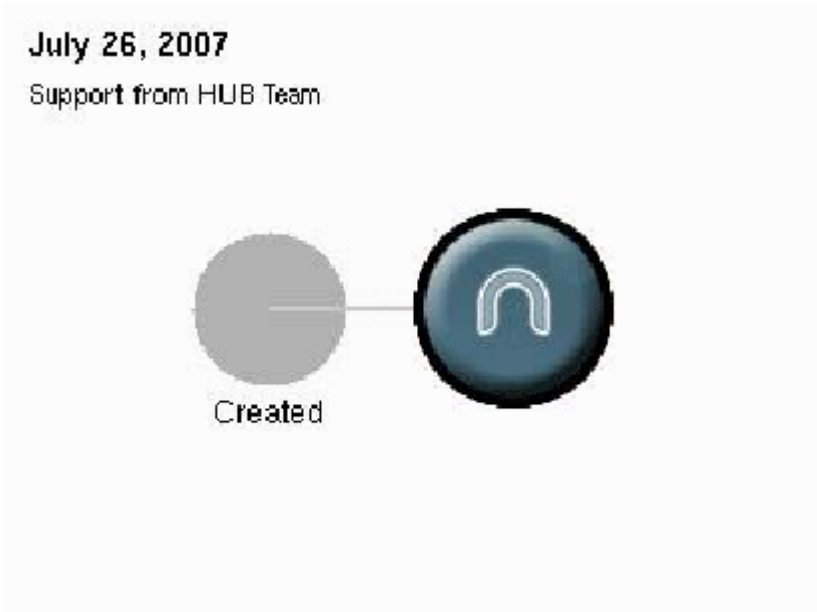

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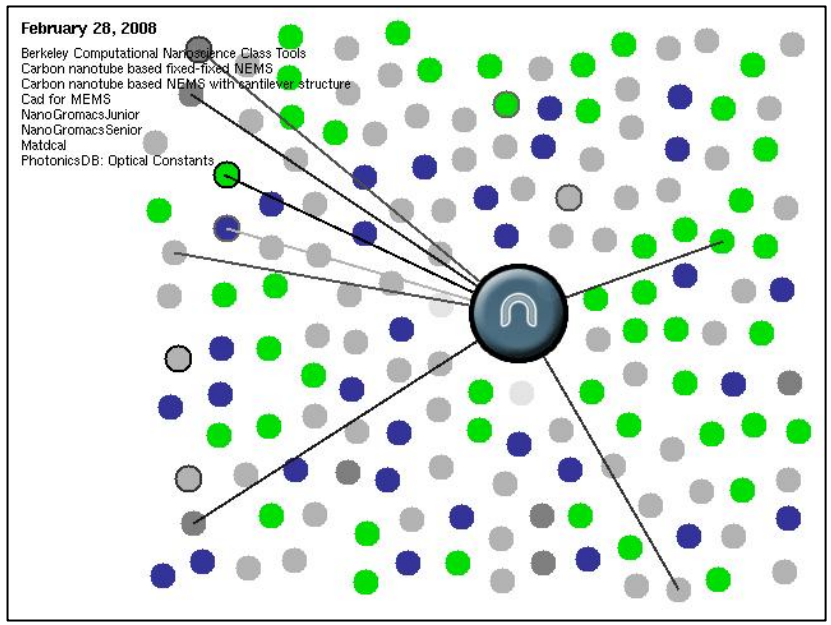

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- #4 - saumitra
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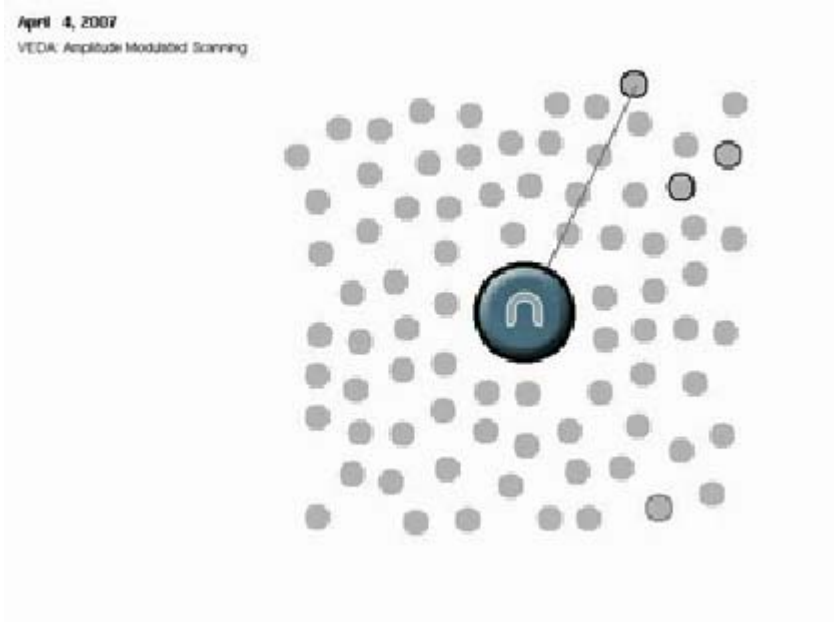
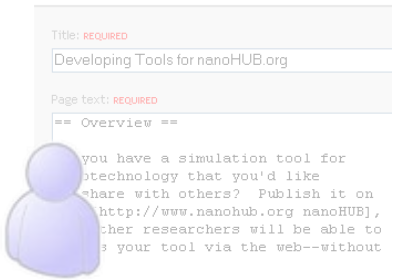


State changes they made:	506
State changes we helped with:	431
TOTAL:	937

Time Development for One Tool >>

Time Development for All Tools >>

Recommendation Engine



Knowledge Articles & Blogs

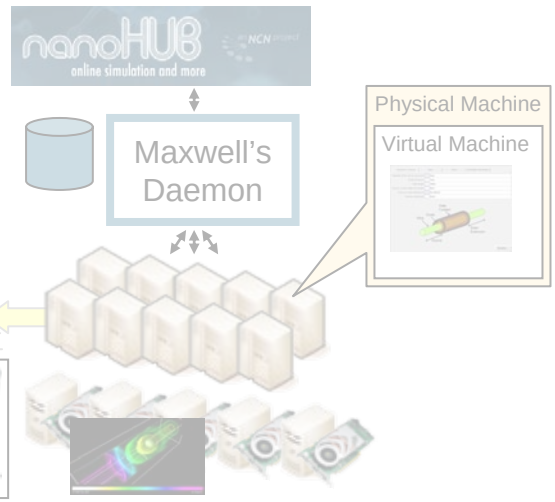
Tool Development

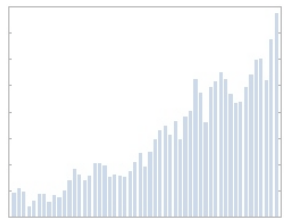
Recommendations

Citations & Digital Object Identifiers

\+ Incentive System

Questions & Answers



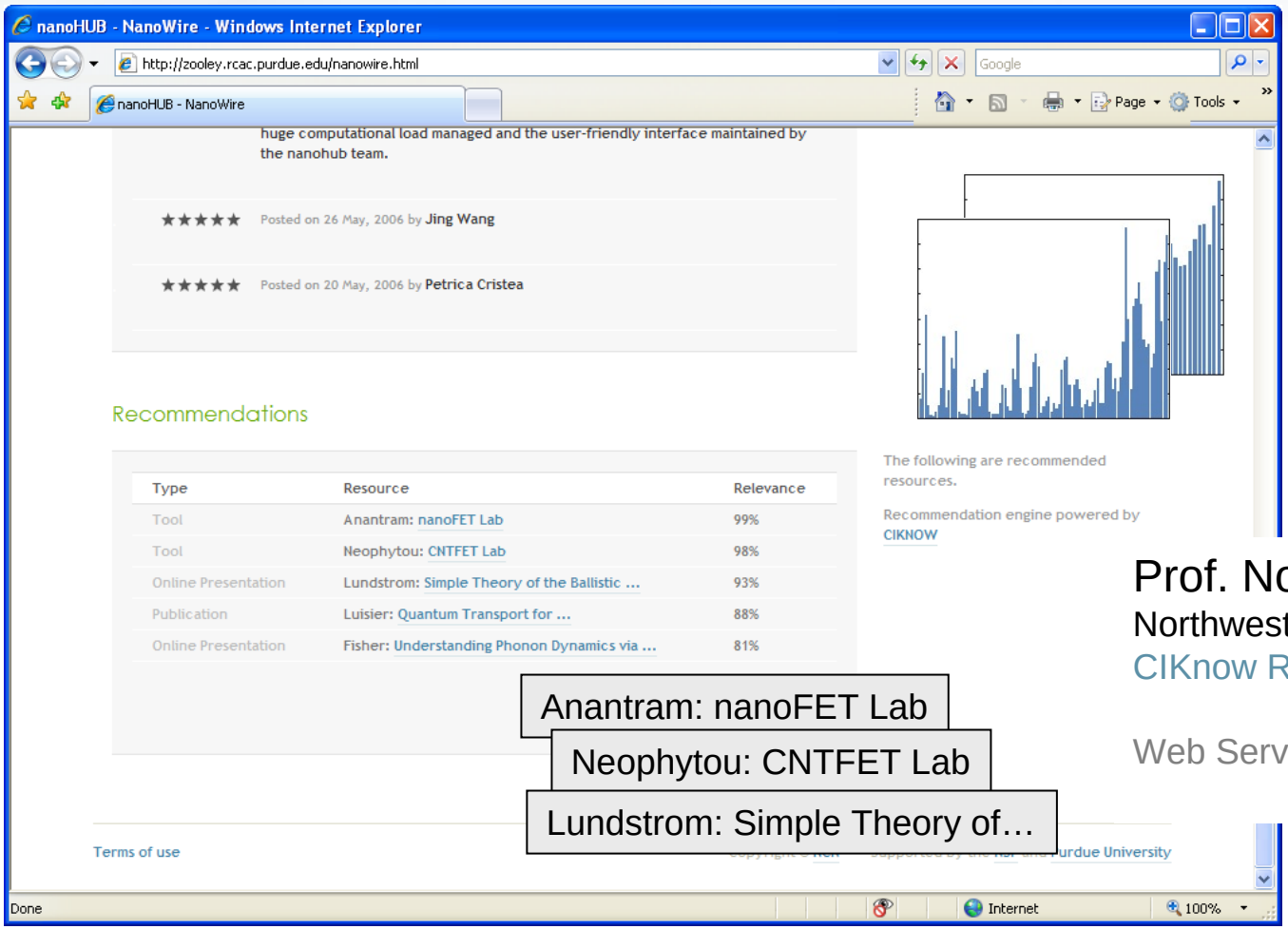


More Statistics

PURDUE UNIVERSITY

nanoHUB online simulation and more — an NCN project

People who used this tool also used...



Anantram: nanoFET Lab

Neophytou: CNTFET Lab

Lundstrom: Simple Theory of…

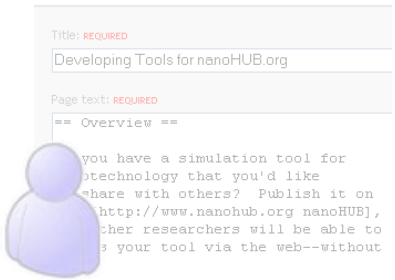
Prof. Noshir Contractor
Northwestern University
CIKnow Recommendation Engine

Web Service

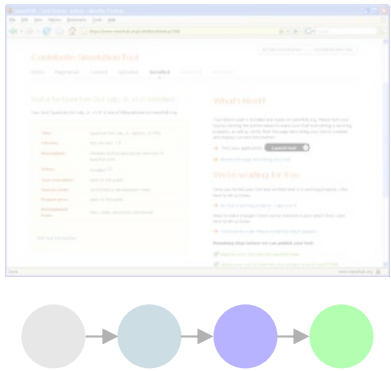
PURDUE UNIVERSITY

NCN NSF

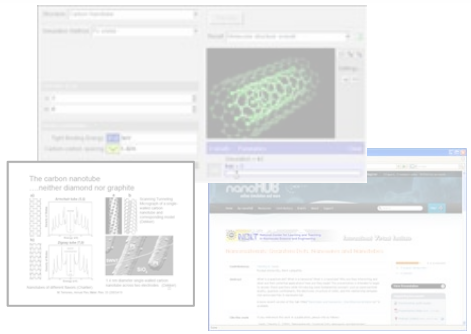
Citations and Digital Object Identifiers



Knowledge Articles & Blogs



Tool Development

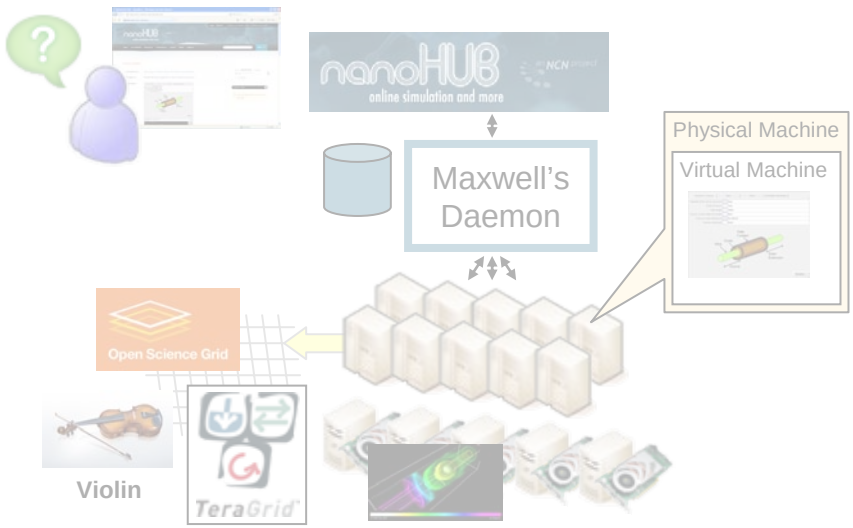


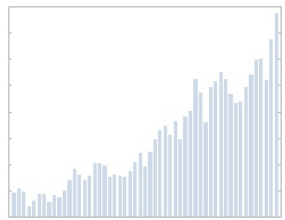
Recommendations

Citations & Digital Object Identifiers

Incentive System

Questions & Answers





More Statistics

PURDUE UNIVERSITY

NCN

Adding Digital Object Identifiers to Tools

Each tool includes citation instructions:

If you reference this work in a publication, please cite as follows:

Ren, Zhibin; Goasguen, Sebastien; Matsudaira, Akira; Ahmed, Shaikh S.; Cantley, Kurtis (2006), "nanoMOS 3.0", 10254/nanohub-r1305.2.
BibTex | EndNote

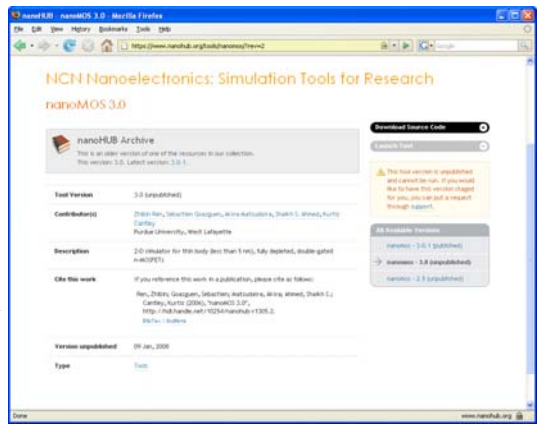
Purdue Library System

nanoHUB resource/version

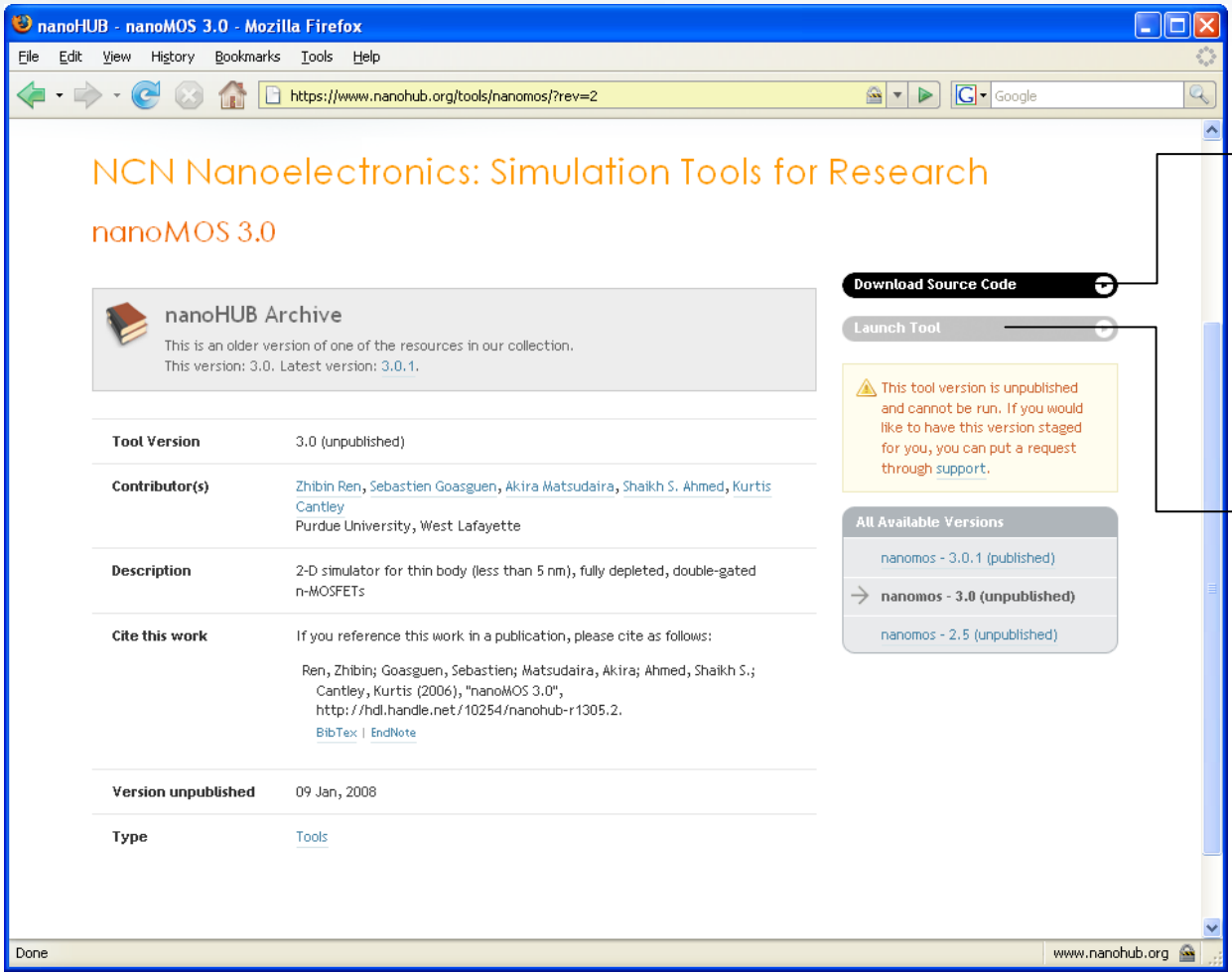
`http://hdl.handle.net/10254/nanohub-r1305.2`

Handle System®
Unique Persistent Identifiers for Internet Resources

→ PURDUE UNIVERSITY LIBRARIES →

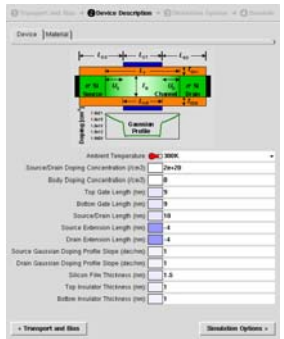


Archived Versions at nanoHUB

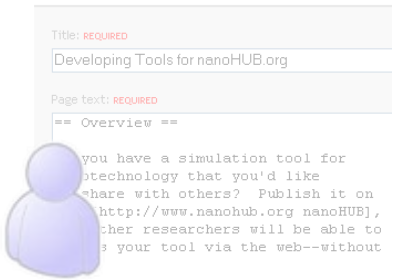


Source code bundle for each published Version.

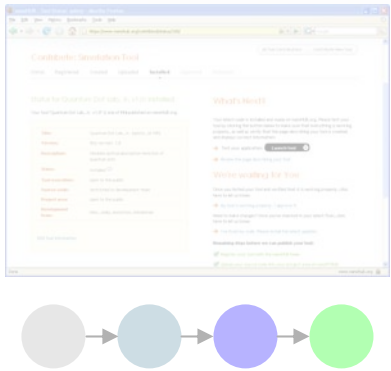
Some versions remain online. Others can be restored upon request.



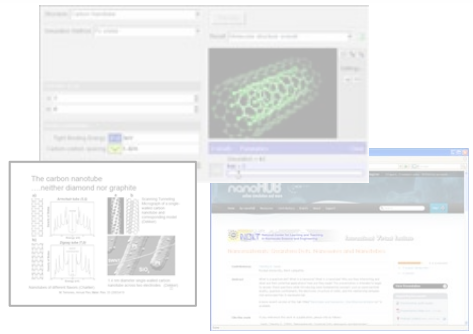
Incentive System for Questions & Answers



Knowledge Articles & Blogs



Tool Development

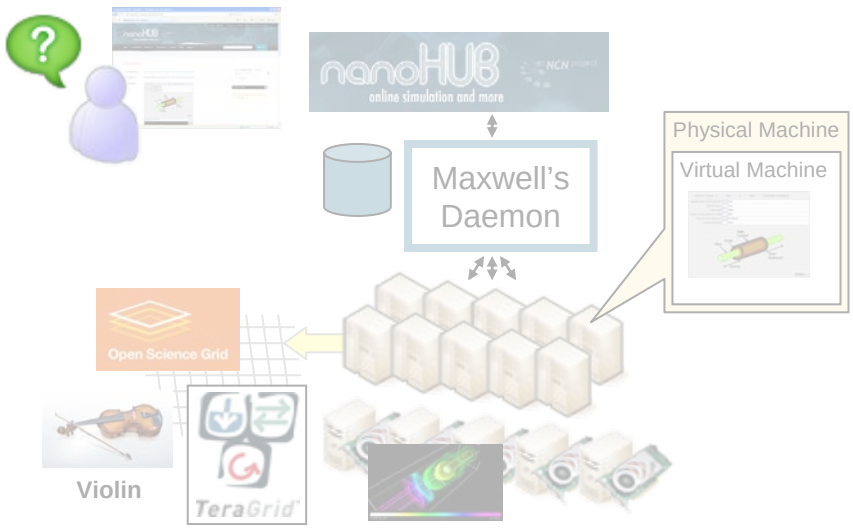


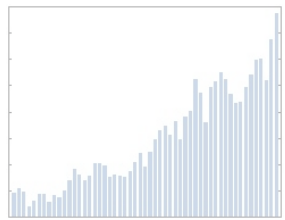
Recommendations

Citations & Digital Object Identifiers

\+ Incentive System

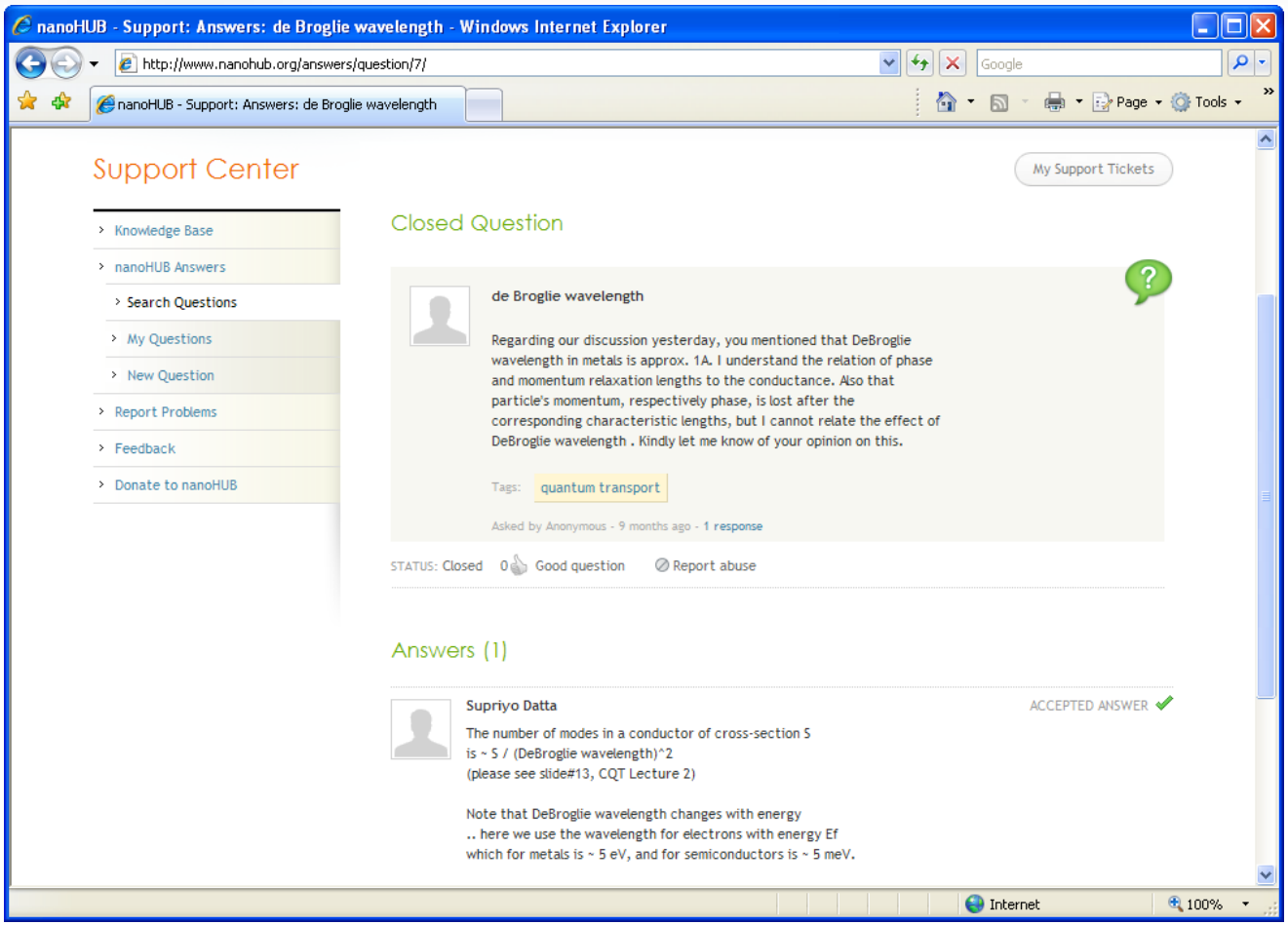
Questions & Answers





More Statistics

Questions & Answers Forum



48 Questions since July 2007:

27 … 0 answers
21 … 1 answer
0 … 2 answers

Incentive System

Let the community help judge:

Reward for each question/answer:

When question is closed…

50-70 points based on:
- Votes for good question
- Votes for good answers
- Number of answers

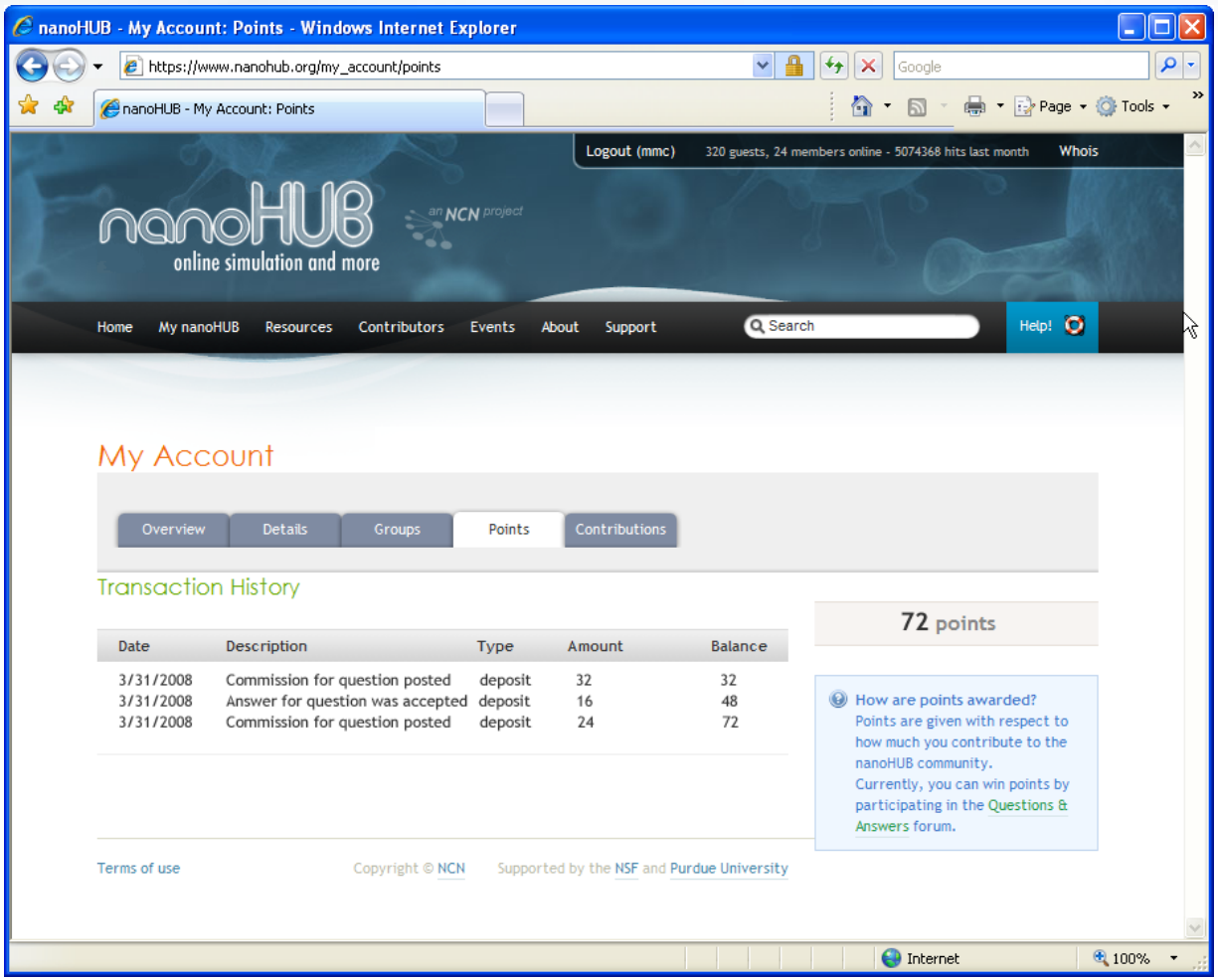
Additional bounty for selected answer

Each month after that…

20% of total question value

Split between parties:
- 33% questioner
- 33% best answer
- 33% all good answers

Accounting

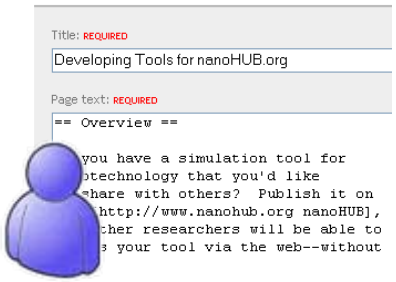


New Accounting Information

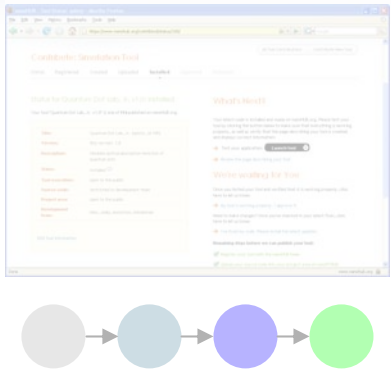
Spend points on:

- questions
- nanoHUB store (coming soon)
- premium services (coming soon)

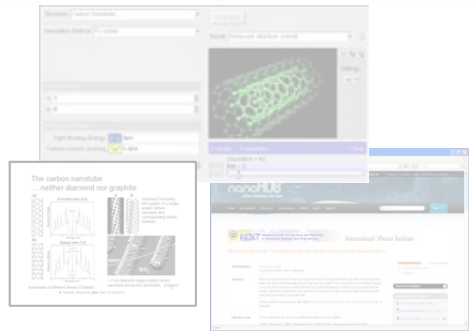
Knowledge Articles & Blogs



Knowledge Articles & Blogs



Tool Development

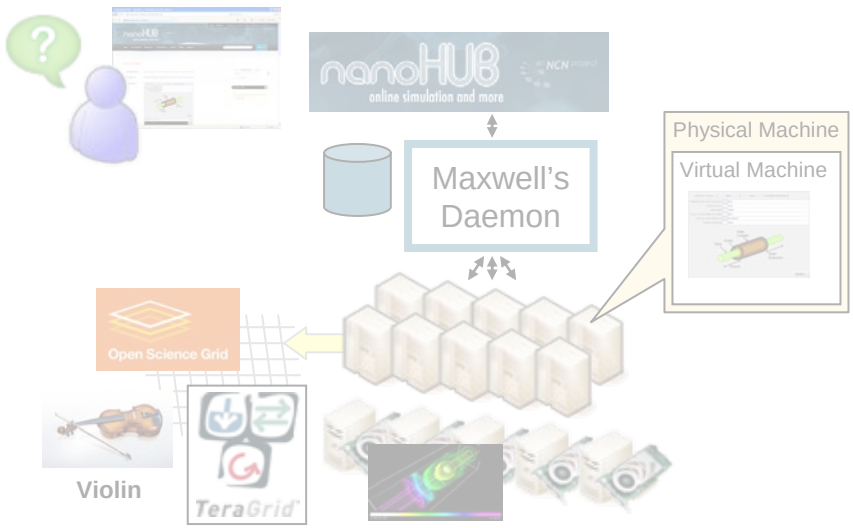


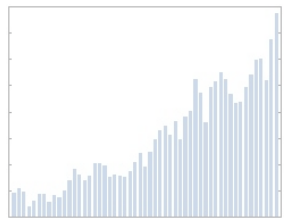
Recommendations

Citations & Digital Object Identifiers

Incentive System

Questions & Answers





More Statistics

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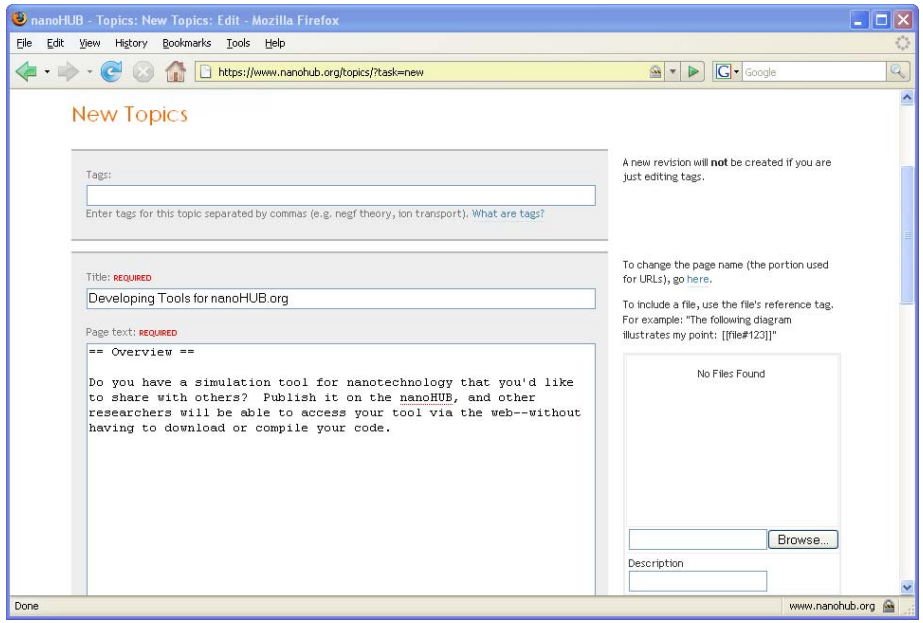
NCN

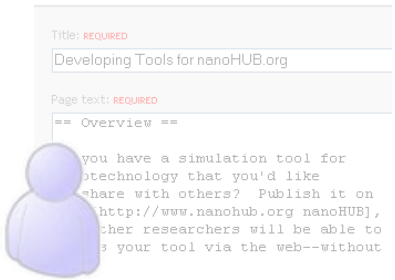
"Topic" Pages

Cross between a wiki and a blog

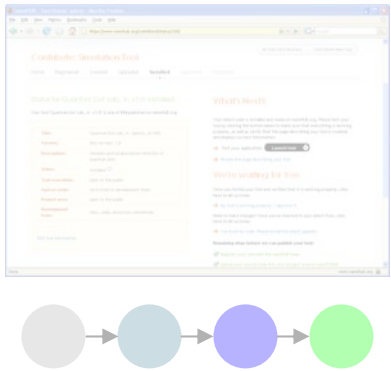
- Similar to Google's "knol"
- Uses wiki mark-up
- Add equations in LaTeX format
- Embed references to hub resources
- Complete revision history
- Well-defined list of authors
- Others can add comments
- Others can suggest changes
- Tags categorize pages



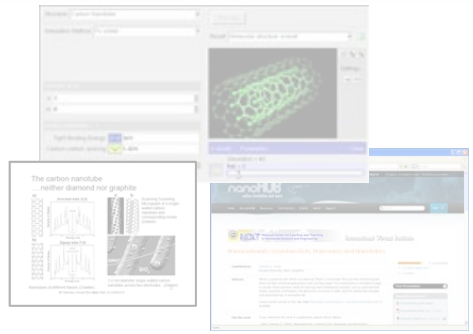
More Statistics



Knowledge Articles & Blogs



Tool Development

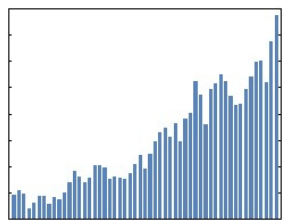


Recommendations

Citations & Digital Object Identifiers

Incentive System

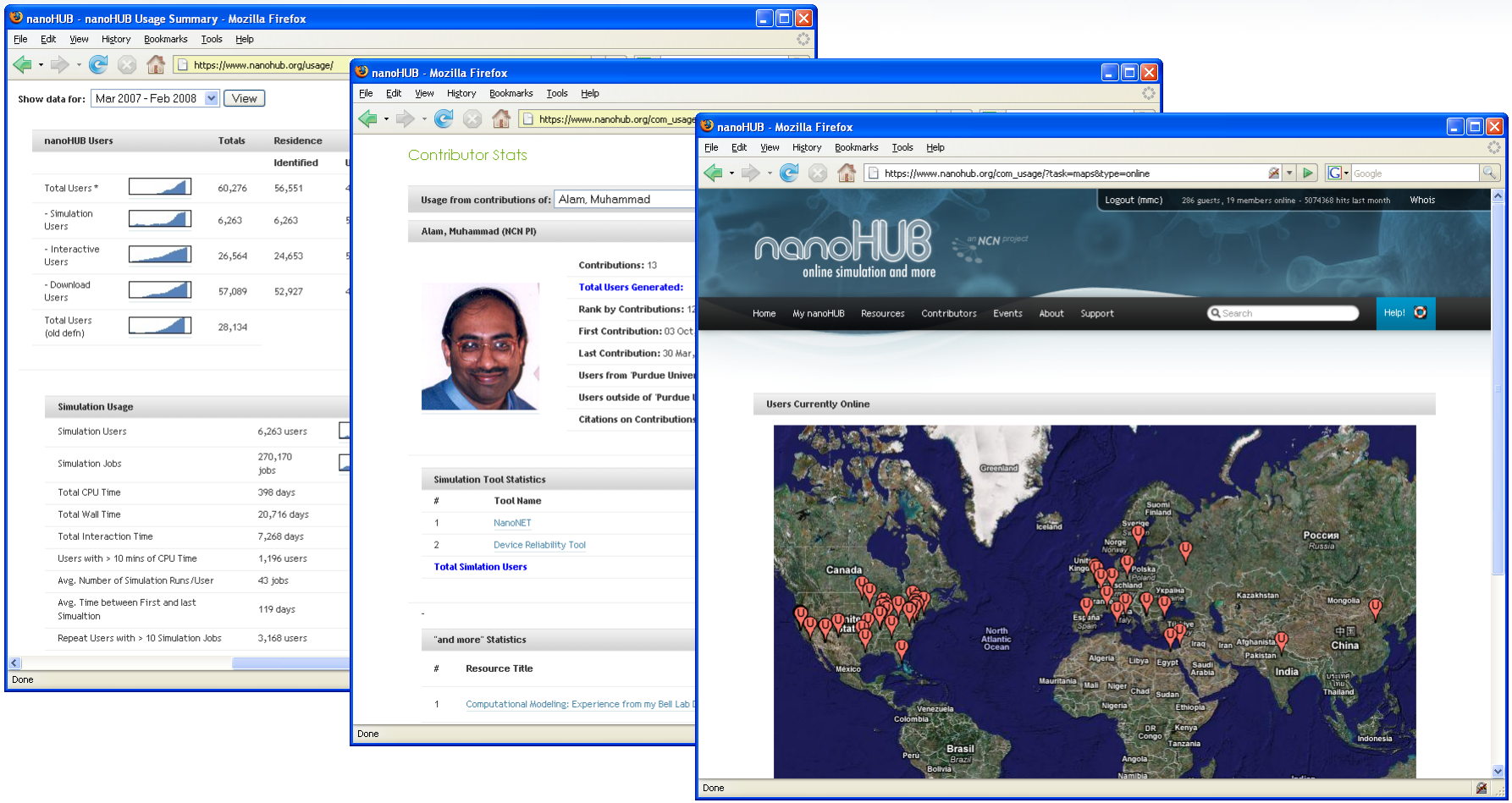
Questions & Answers



More Statistics

nanoHUB
online simulation and more
an NCN project

New Ways to Browse Usage Measures



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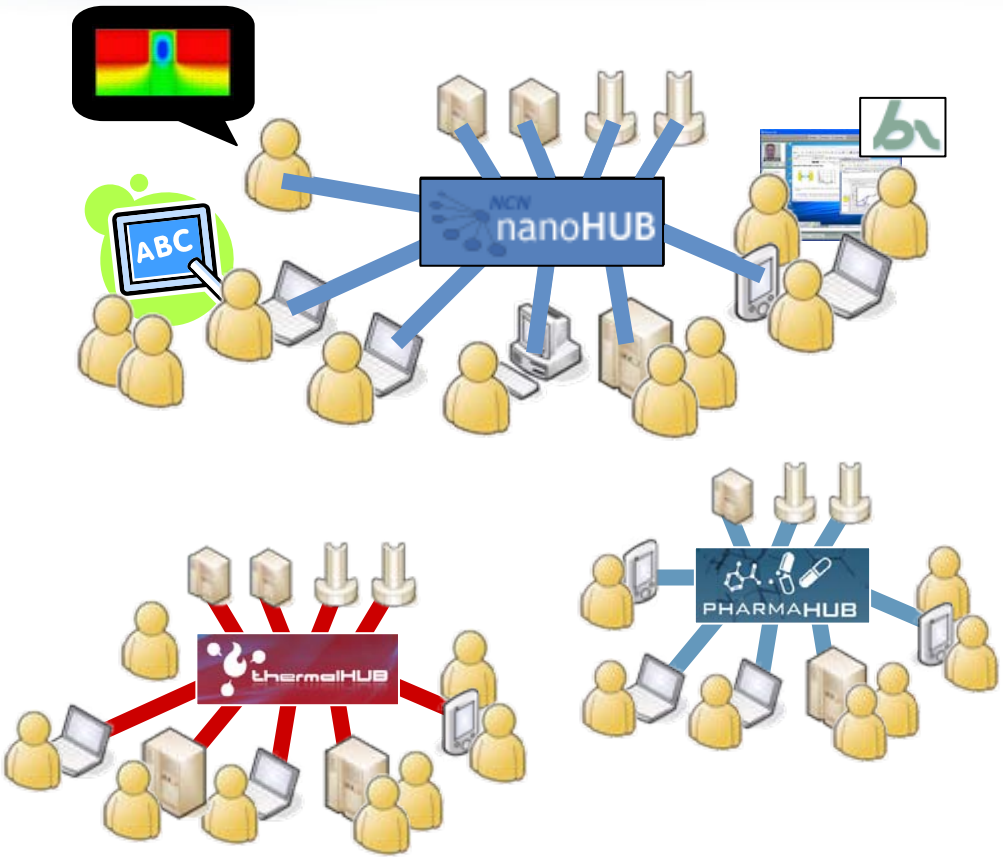
NCN

NSF

General Framework



HUB0

PURDUE UNIVERSITY

http://hubzero.org

- Linux/Apache/MySQL/PHP
- LDAP authentication
- Joomla Content Mgmt
- Hub website components
- Maxwell's Daemon
- Rappture Toolkit

New Hubs Online Now

GlobalHUB.org – Dan Hirleman, ME at Purdue
global engineering education
online since 12/17/2007

pharmaHUB.org – Rex Reklaitis, CE at Purdue
pharmaceutical product development and manufacturing
online since 12/11/2007

thermalHUB.org – Tim Fisher, ME at Purdue
heat transfer
online since 12/6/2007

IndianaCTSI.org – Anantha Shekhar, IU School of Medicine, Connie Weaver at Purdue
accelerating clinical and translational research in healthcare
online since 10/1/2007

nanohub.org – Mark Lundstrom, ECE at Purdue
the granddaddy of all hubs focused on nanotechnology
online since 2002

Future Directions

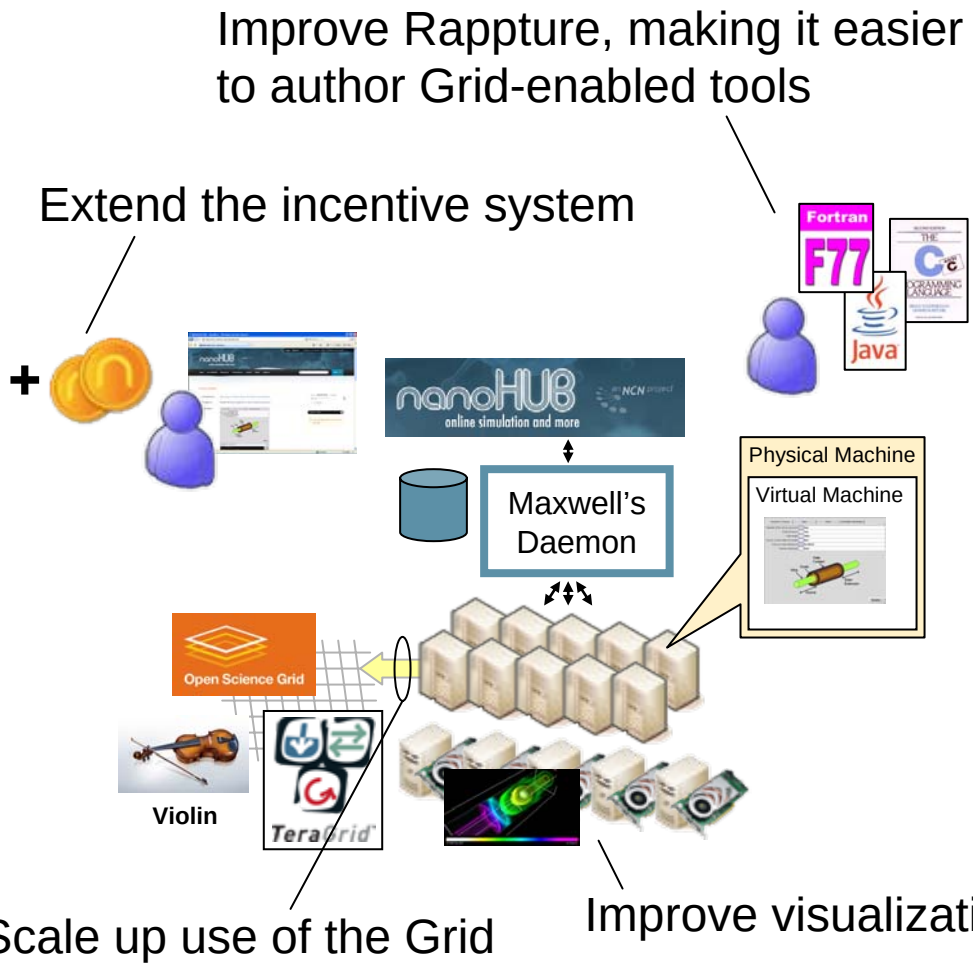
HUB0

PURDUE UNIVERSITY

http://hubzero.org

Hub Development Pipeline:

- 3 hubs under development
- 17 hubs with funding proposed
- 10 hubs being discussed

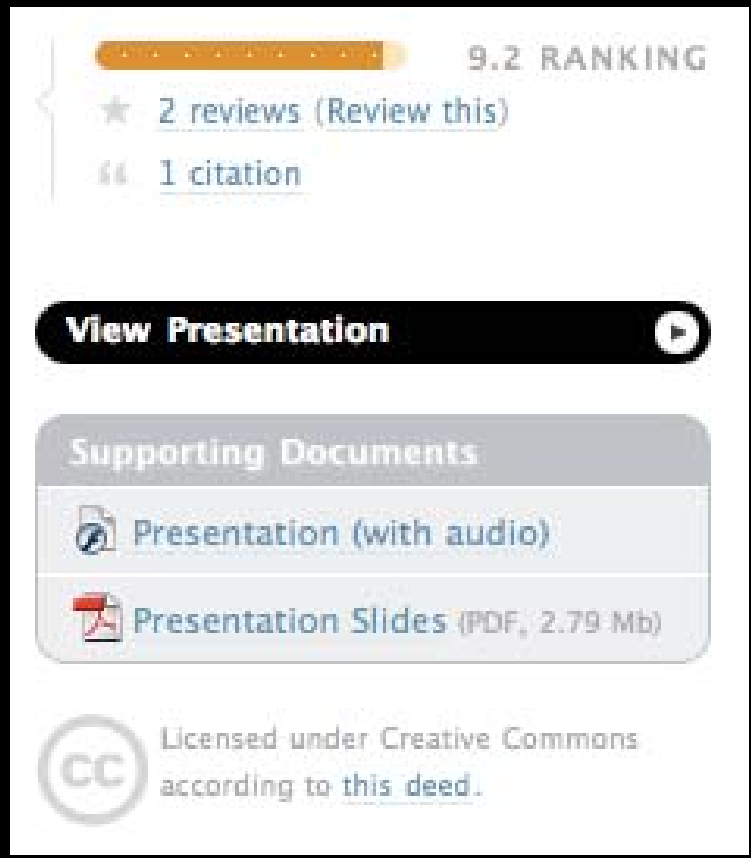


980 resources

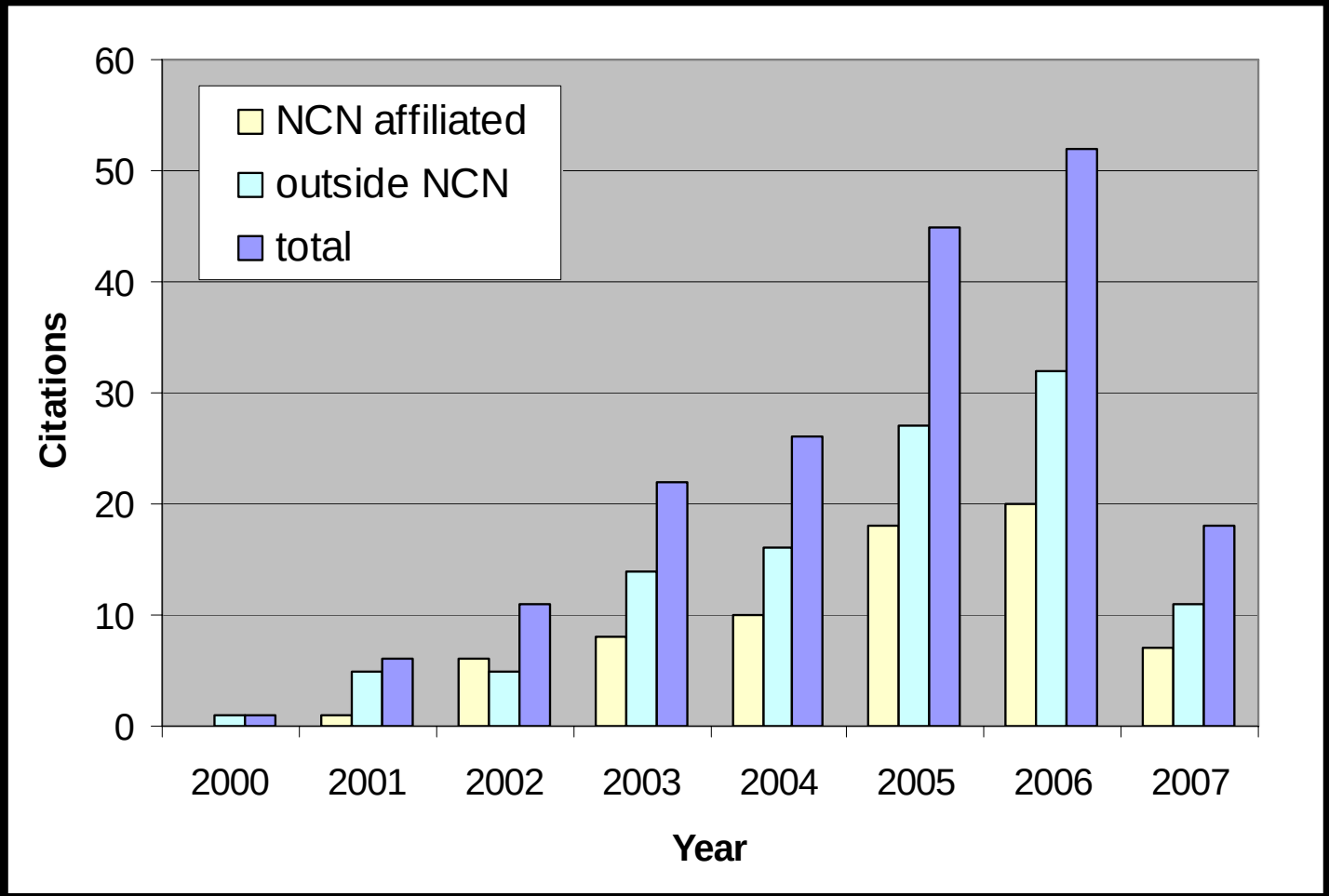
340 added
April 07-March08

Most licenses:

Creative Commons



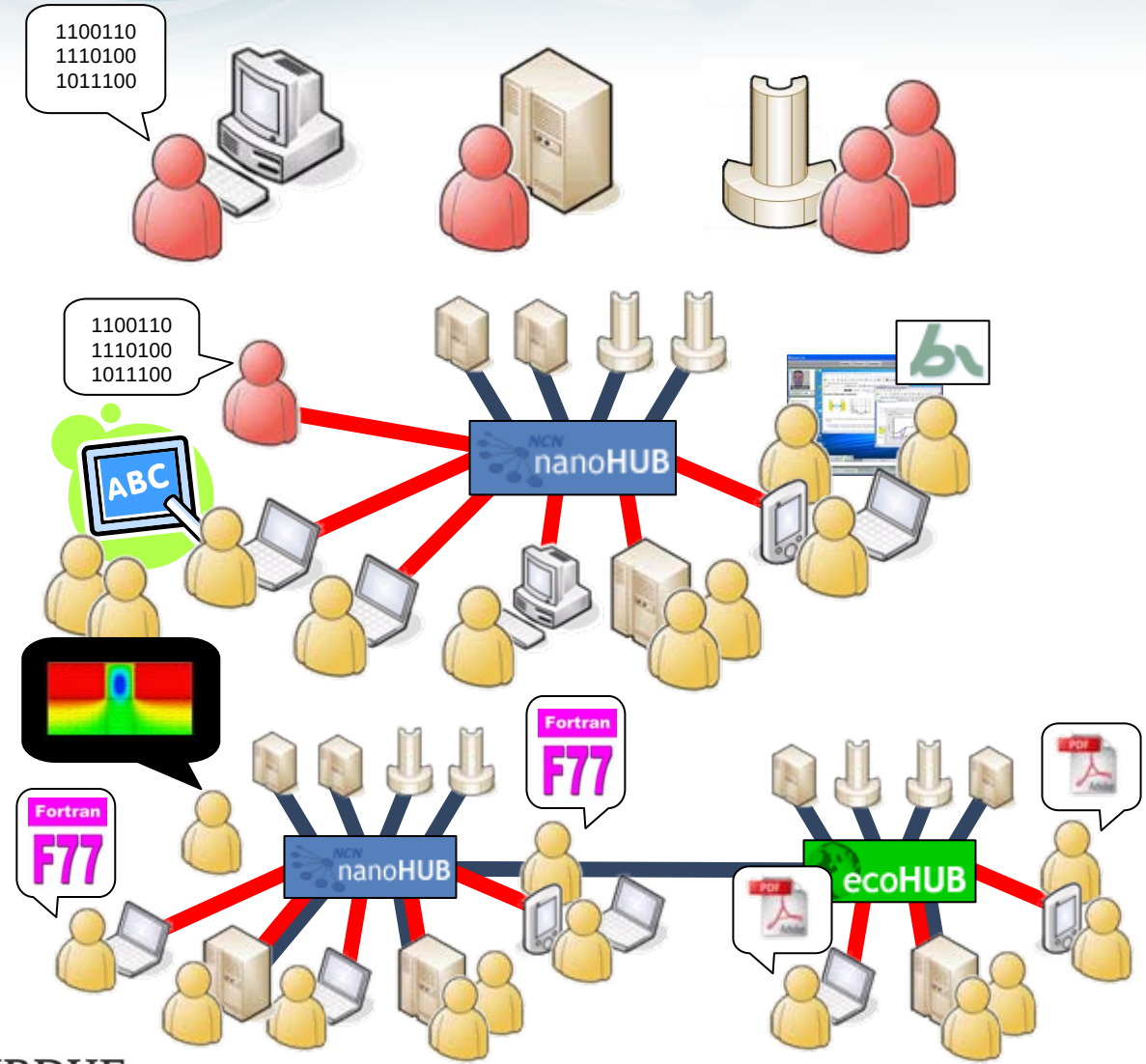
nanoHUB Citations



187
total

114
60%
non-NCN

Evolution of Scientific Computing



Scientific & HPC Computing

few users with specialized knowledge

Science Gateways

cyberinfrastructure, more users

Cyber Communities

ecosystem, users support each other

Who's using this?

3.5 million hits last month

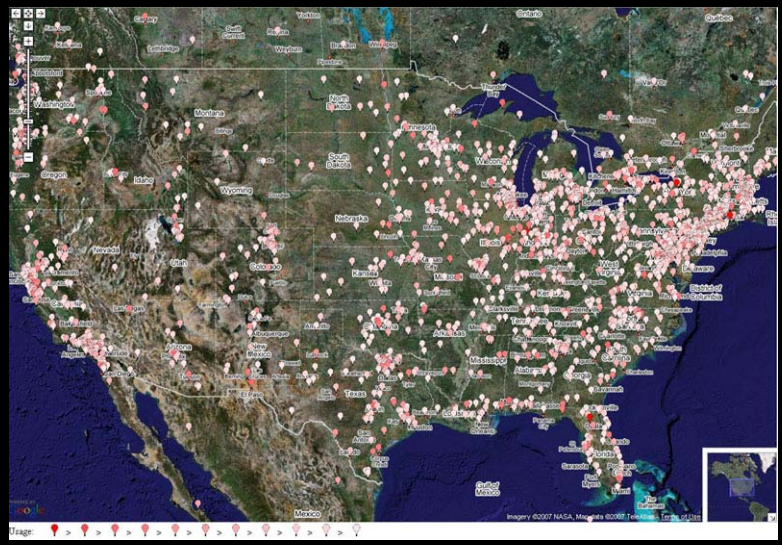
Over 1 million visits last 12 months

218,656 simulation jobs last 12 months

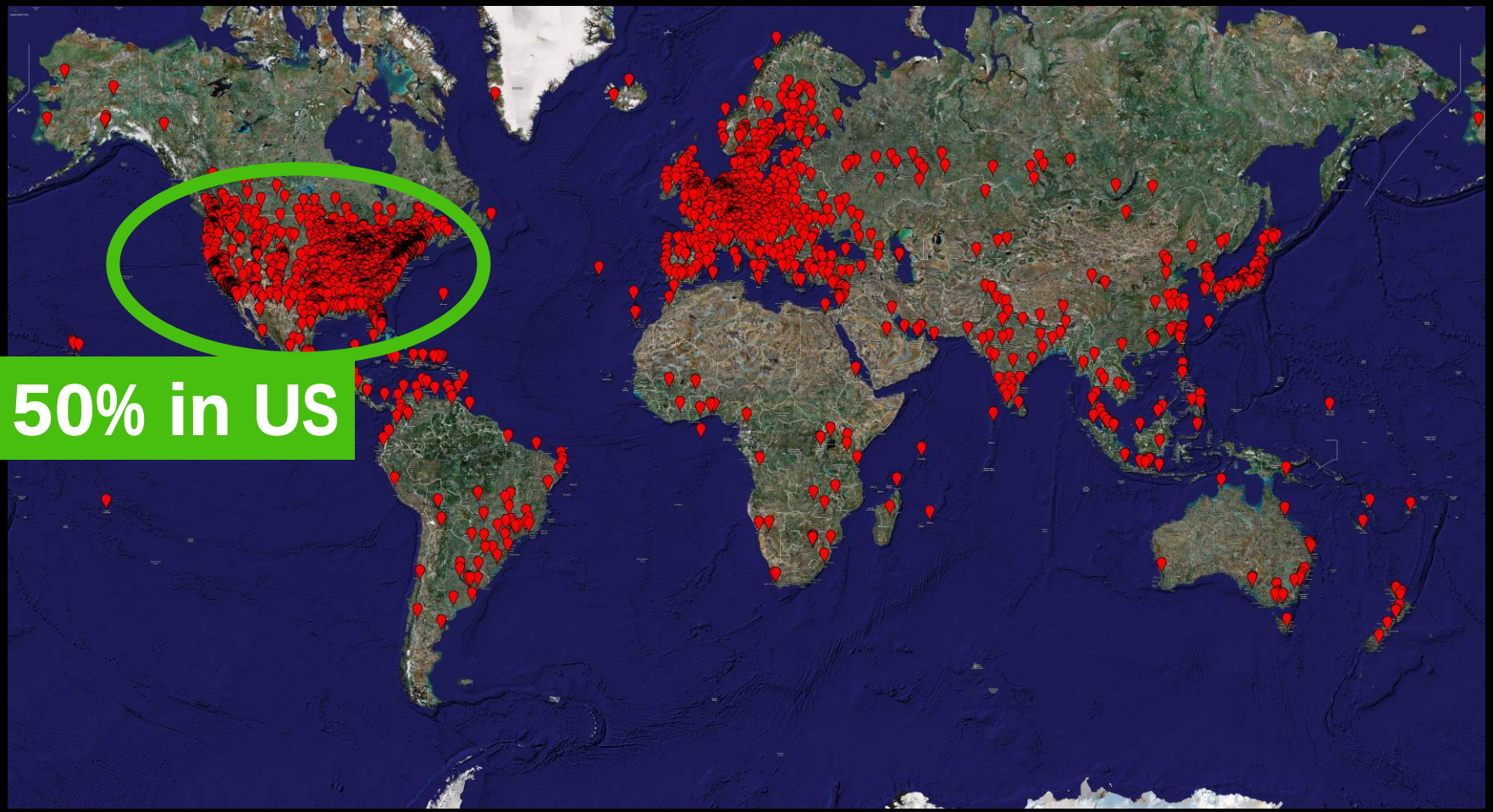
In U.S.: all Top 50 Engineering Schools

14.3% of .edu domains are users

3.7% of .edu ran simulations



A global following



Publishing's Value Proposition to the Community

- In Isaac Newton's day researchers communicated their ideas and results to the community via exchange of letters
- Evolved to the Journals, Proceedings we use today
- Value proposition to authors (contributors):
  - »Community recognition
  - »Citations by others in the community
  - »Promotion of career
- Value proposition to readers (users):
  - »Access to vetted content

HUBzero's Value Proposition to the Community

- HUBzero generalizes the concept of publishing
- Value to authors (contributors):
  - »Share more than ideas and results – share tools, educational materials, and data (can imagine)
  - »Citations by others in the community
  - »Wider use of tools accelerates research, learning, and career (with attitude and culture change)
  - »Promotion of career (with culture change)
- Value to users:
  - »Access to vetted (with community participation) content
  - »Ability to vet simulation-based research

nanoHUB impact by a graduate students

Neophytou, Neophytos

Contributions: 2

Total Simulation Users Served: 1,798

Rank by Contributions: 85 / 480

First Contribution: 19 May, 2006

Last Contribution: 09 Feb, 2007

Citations on Contributions: 7

Simulation Tool Statistics

#	Tool Name	Users served in last 12 months	Total users served	Citations	Published On
1	CNTFET Lab	381	436	4	09 Feb, 2007
2	Bandstructure Lab	887	1,518	3	19 May, 2006
	Total Simlation Users	1,163	1,798		

Any employer will love to see a student with impact!
Industry as well as academia!

nanoHUB online simulation and more — an NCN project

nanoHUB impact by an undergraduate student

Any employer will love to see a student with impact! Industry as well as academia!

Matsudaira, Akira

Contributions: 5

Total Simulation Users Served: 3,526

Rank by Contributions: 43 / 480

First Contribution: 09 Feb, 2006

Last Contribution: 14 Dec, 2006

Citations on Contributions: 109

Simulation Tool Statistics

#	Tool Name	Users served in last 12 months	Total users served	Citations	Published On
1	CNTbands 2.0	663	777	2	14 Dec, 2006
2	nanoMOS	379	981	39	19 May, 2006
3	MOSCap	387	655	-	06 Apr, 2006
4	FETToy	535	1,366	6	14 Feb, 2006
5	Schred	533	1,208	62	09 Feb, 2006
	Total Simlation Users	**1,782**	**3,526**		

nanoHUB online simulation and more — an NCN project

nanoHUB impact by a post-doc

Ahmed, Shaikh

Contributions: 10

Total Simulation Users Served: 3,947

Rank by Contributions: 16 / 480

First Contribution: 09 Feb, 2006

Last Contribution: 14 Jan, 2008

Citations on Contributions: 111

Simulation Tool Statistics

#	Tool Name	Users served in last 12 months	Total users served	Citations	Published On
1	QuaMC 2D Lab	134	154	-	23 Feb, 2007
2	CNTFET Lab	381	436	4	09 Feb, 2007
3	nanoFET Lab	269	322	-	09 Feb, 2007
4	nanoMOS	379	981	39	19 May, 2006
5	MOSCap	387	655	-	06 Apr, 2006
6	MOSFET	786	1,383	-	30 Mar, 2006
7	FETToy	535	1,366	6	14 Feb, 2006
8	Schred	533	1,208	62	09 Feb, 2006
	Total Simlation Users	**2,017**	**3,947**		

nanoHUB impact by a faculty member

Datta, Supriyo (NCN PI)

Contributions: 132
Total Simulation Users Served: 2,005
Total "and more " Users Served: 16,917
Rank by Contributions: 1 / 480
First Contribution: 27 Nov, 2002
Last Contribution: 25 Feb, 2008
Citations on Contributions: 8

Recipient of 2008 IEEE Leon K. Kirchmayer Graduate Teaching Award

Simulation Tool Statistics

#	Tool Name	Users served in last 12 months	Total users served	Citations	Published On
1	FETToy	535	1,366	6	14 Feb, 2006
2	MolCToy	165	847	-	08 Jun, 2005
	Total Simlation Users	**654**	**2,005**		

"and more" Statistics

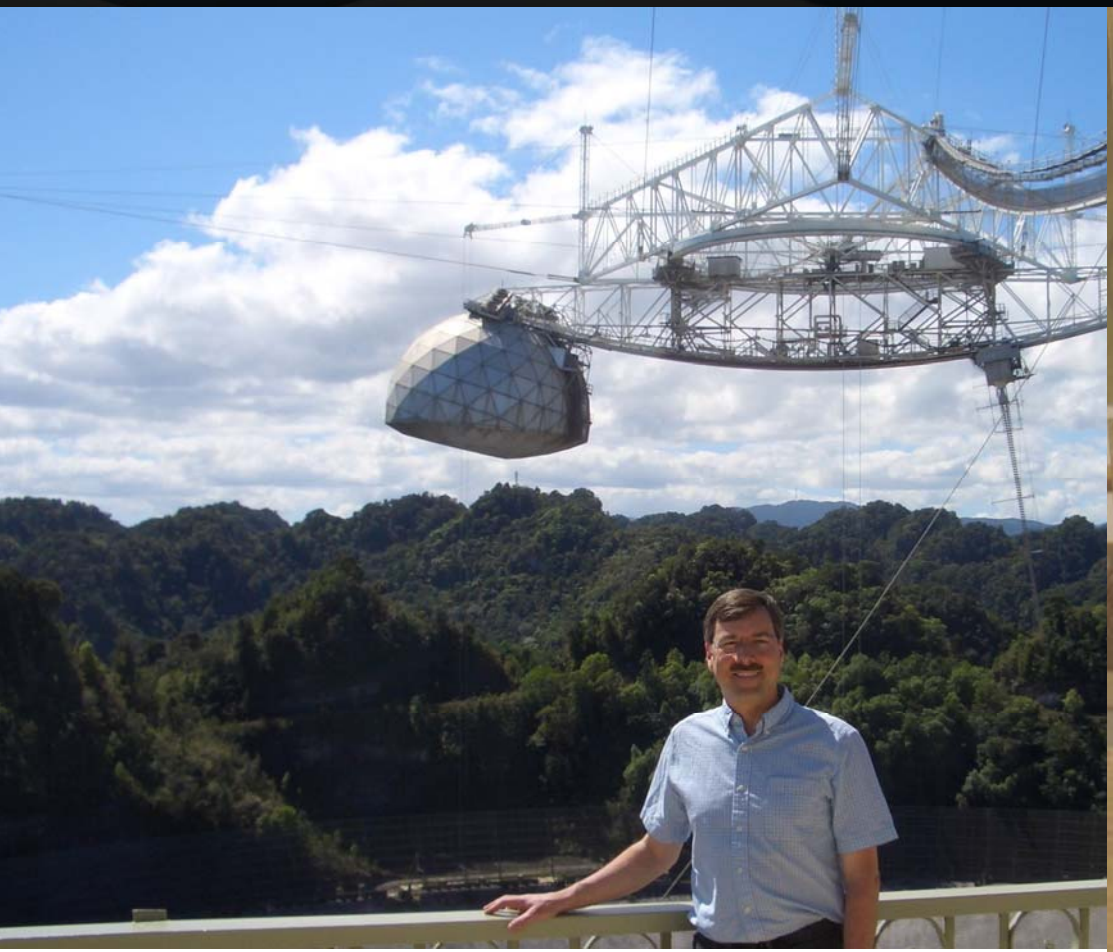
#	Resource Title	Users served in last 12 months	Total users served	Citations	Published On
1	MCW07 Physics of Contact Induced Current Asymmetry in Transport Through Molecules (Online Presentations)	3	3	-	25 Feb, 2008
130	Theory of Ballistic Nanotransistors (Publications)	25	174	-	27 Nov, 2002
	Total "and more" Users	**9,999**	**16,917**		

nanoHUB Assessment

- Assessment -- metrics, nuggets
- Scholarly studies
- Diane Beaudoin -- assessment
- Sean Brophy -- simulation as a learning tool
- George Bodner -- creating classroom environments optimal for learning
- David Radcliffe -- interdisciplinary research methods in engineering education; design thinking and engineering knowledge creation

Dr. Diane Beaudoin

Sustainability



Arecibo Observatory

Sustainability

- **Provision of compute cycles**
  - »Partner with TACC, ORNL, and NCSA
  - »Partner with software vendors
- **Provision of content**
  - »Partner with publishers
  - »Partner with professional societies
  - »Virtual economy for users and contributors
- **Support and development personnel**
  - »HUB automation
  - »Shared cyberinfrastructure and development