nanoHUB
online simulation and more
an NCN project

nanoHUB.org - Future Cyberinfrastructure serving over 75,000 users today

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

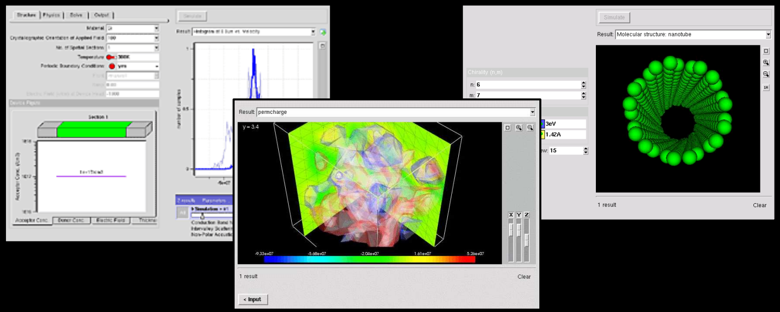
September 24, 2008
IEEE Symposium on Massive Storage Systems and Technologies (MSST)

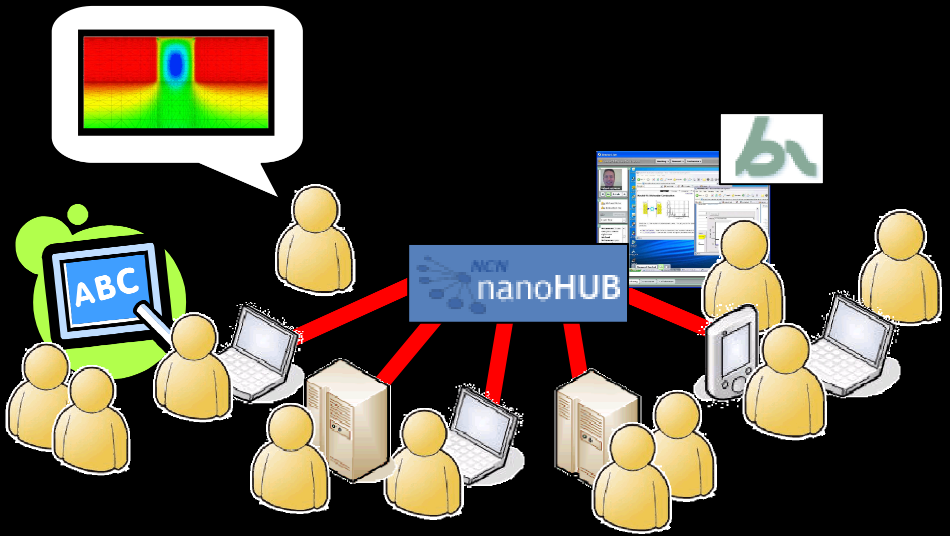
PURDUE
UNIVERSITY

NCN NSF

nanoHUB.org

Online simulation… *…and more!*





What is it?

[*Live Demo>>*]

[*PPT Demo>>*]

[*Short Video>>*]

Impact ?
Scalability ?
Future ?

Free Account

(just confirm your email address)

free!

Interactive Visualization

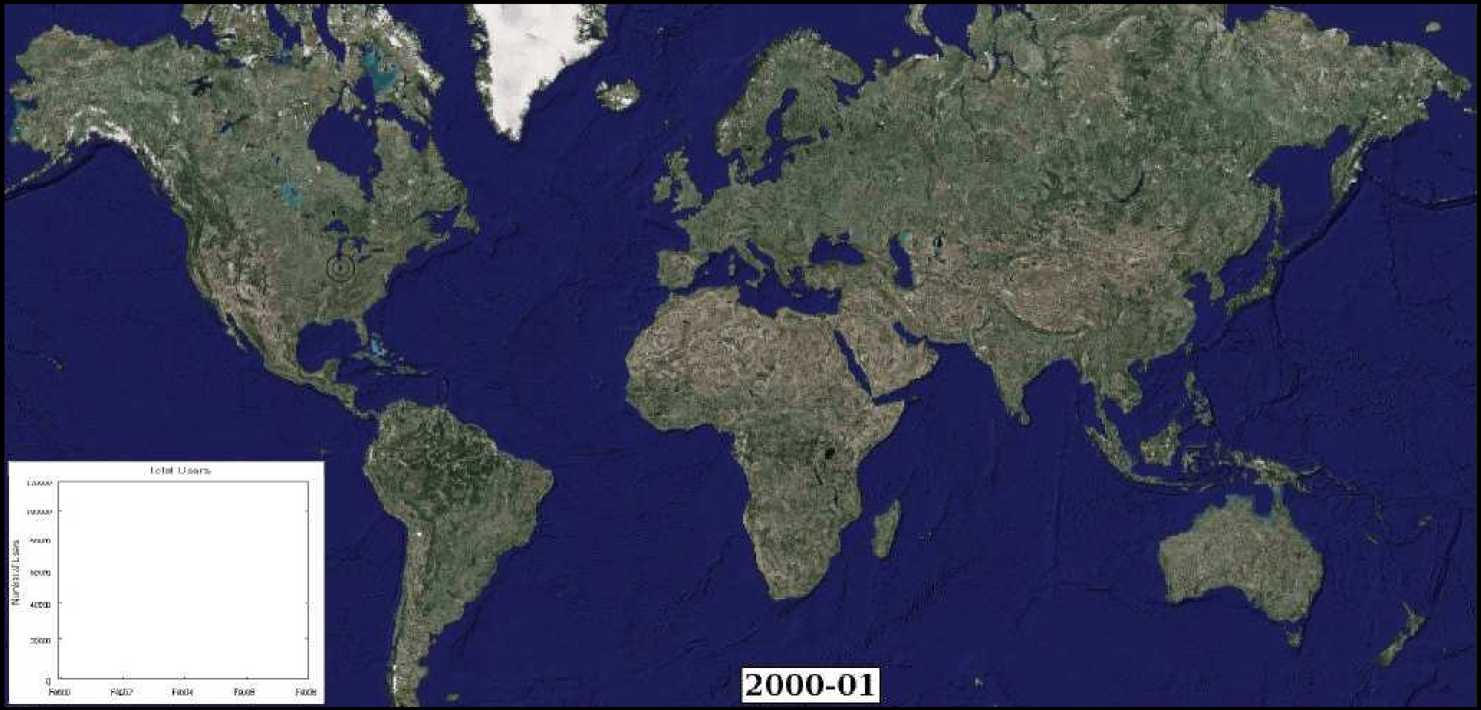
integrated seamlessly

VoLQD
NanoVis

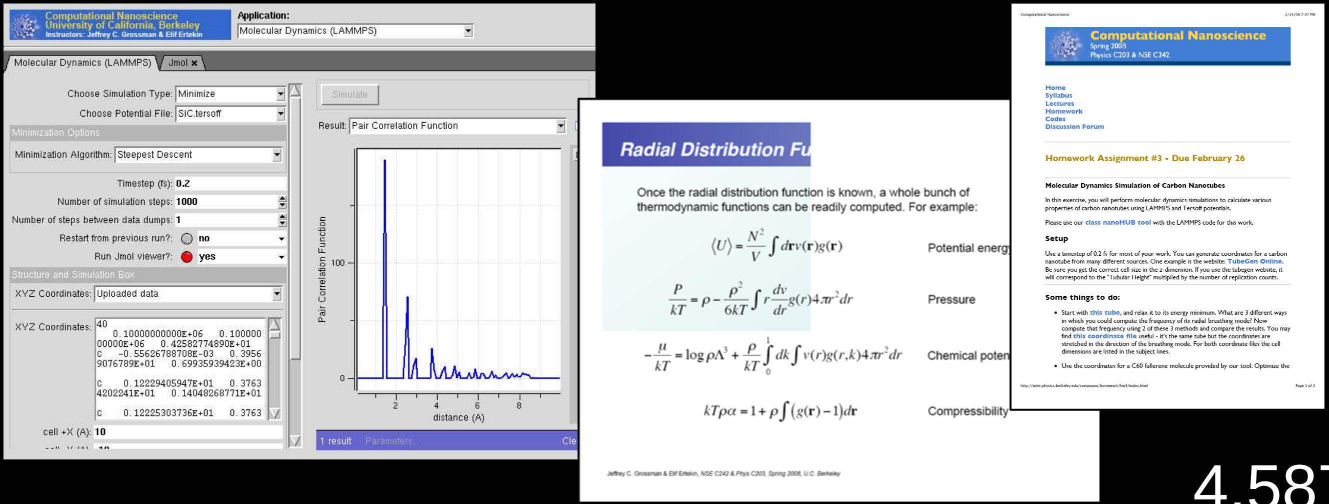
nanoVIS rendering server
Developed by
Wei Qiao, Insoo Woo, David S. Ebert
PURPL Lab, Purdue University

Worldwide Community

7.2 million hits last month
>75,000 unique users last 12 months
Users at all US Top 50 Engineering Schools
14% of all US .edu domains
Users from 172 countries



UC Berkeley Usage



Application: Molecular Dynamics (LAMMPS)

Choose Simulation Type: Minimize

Choose Potential File: SiC.tersoff

Minimization Algorithm: Steepest Descent

Timestep (fs): 0.2

Number of simulation steps: 1000

Number of steps between data dumps: 1

Restart from previous run?: ○ no

Run Jmol viewer?: ● yes

XYZ Coordinates: Uploaded data

XYZ Coordinates:

```
40
    0.10000000000E+06    0.100000
00000E+06    0.42582774890E+01
C    -0.55626788708E-03    0.3956
9076789E+01    0.69935939423E+00

C     0.12229405947E+01    0.3763
4202241E+01    0.14048268771E+01

C     0.12225303736E+01    0.3763
```

cell +X (A): 10

Result: Pair Correlation Function

Radial Distribution Fu

Once the radial distribution function is known, a whole bunch of thermodynamic functions can be readily computed. For example:

$$\langle U \rangle = \frac{N^2}{V} \int d\mathbf{r}\, v(\mathbf{r}) g(\mathbf{r})$$ Potential energ

$$\frac{P}{kT} = \rho - \frac{\rho^2}{6kT} \int r \frac{dv}{dr} g(r) 4\pi r^2 dr$$ Pressure

$$-\frac{\mu}{kT} = \log \rho \Lambda^3 + \frac{\rho}{kT} \int_0^1 dk \int v(r) g(r,k) 4\pi r^2 dr$$ Chemical poten

$$kT\rho\alpha = 1 + \rho \int \left(g(\mathbf{r}) - 1 \right) d\mathbf{r}$$ Compressibility

Jeffrey C. Grossman & Elif Ertekin, NSE C242 & Phys C203, Spring 2008, U.C. Berkeley

Computational Nanoscience 2/14/08 7:07 PM

Computational Nanoscience
Spring 2008
Physics C203 & NSE C242

Home
Syllabus
Lectures
Homework
Codes
Discussion Forum

Homework Assignment #3 - Due February 26

Molecular Dynamics Simulation of Carbon Nanotubes

In this exercise, you will perform molecular dynamics simulations to calculate various properties of carbon nanotubes using LAMMPS and Tersoff potentials.

Please use our **class nanoHUB tool** with the LAMMPS code for this work.

Setup

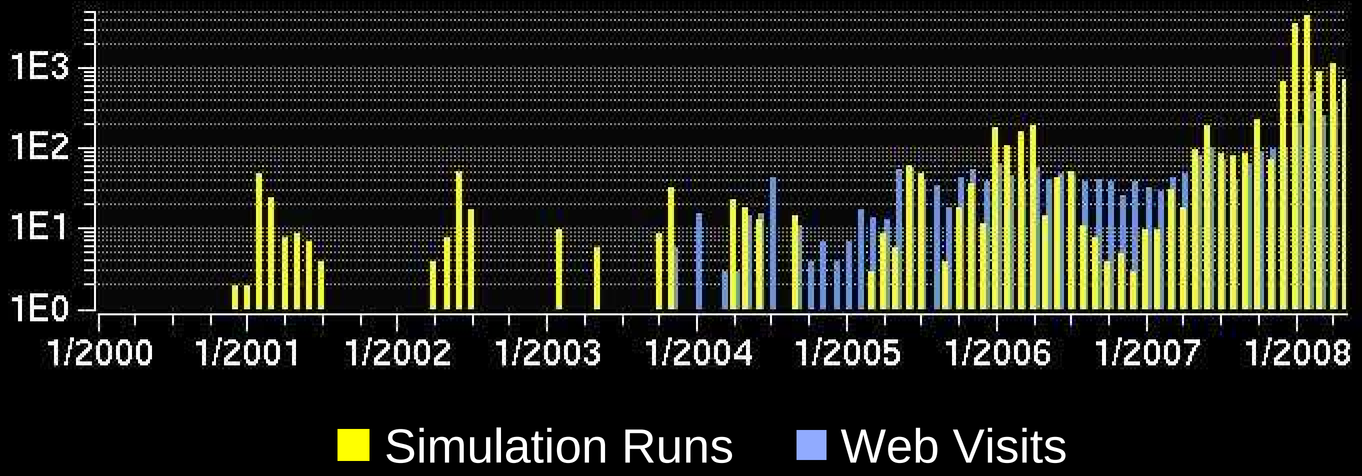
Use a timestep of 0.2 fs for most of your work. You can generate coordinates for a carbon nanotube from many different sources. One example is the website: **TubeGen Online**. Be sure you get the correct cell size in the z-dimension. If you use the tubegen website, it will correspond to the "Tubular Height" multiplied by the number of replication counts.

Some things to do:

- Start with **this tube**, and relax it to its energy minimum. What are 3 different ways in which you could compute the frequency of its radial breathing mode? Now compute that frequency using 2 of these 3 methods and compare the results. You may find **this coordinate file** useful - it's the same tube but the coordinates are stretched in the direction of the breathing mode. For both coordinate files the cell dimensions are listed in the subject lines.
- Use the coordinates for a C60 fullerene molecule provided by our tool. Optimize the

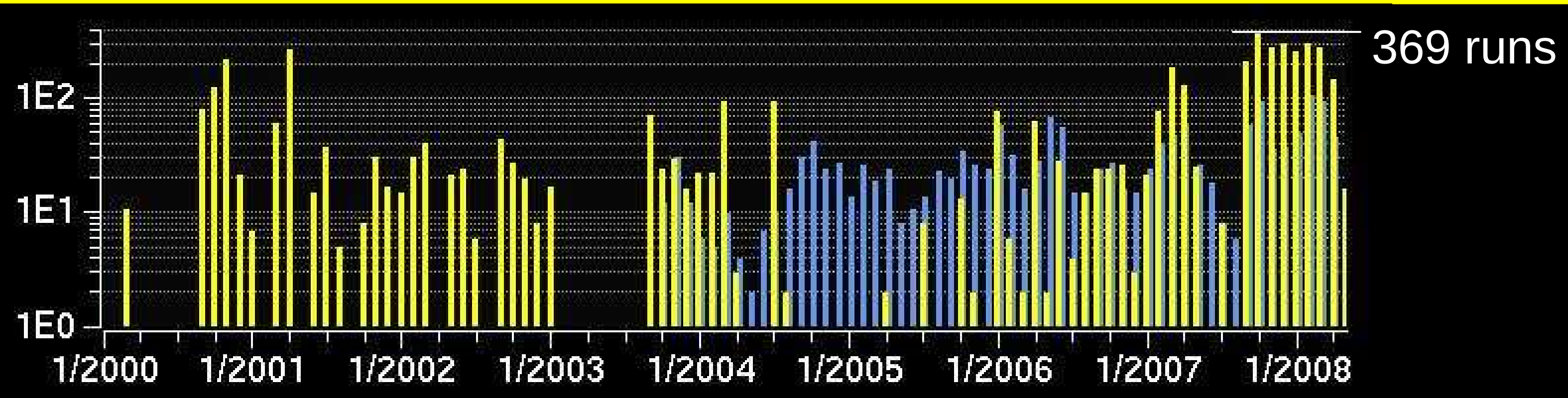
http://mint.physics.berkeley.edu/compnano/homework/hw3/index.html Page 1 of 2

4,587 runs!



44 classes at 18 institutions

Spring 2008	Arizona St.	EEE/CSE 101	Introductory Engineering Design	Vasileska
Spring 2008	Arizona St.	EEE352	Properties of Electronic Materials	Ferry
Spring 2008	Arizona St.	EE533	Semiconductor Transport	Vasileska



Spring 2							
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Spring 2008	Portland State	ECE511	Solid State Electronics	Pejcinovic		1	
Spring 2008	Portland State	ECE516	IC Technologies	Natter		1	
Spring 2008	Purdue	ECE305	Semiconductor Devices	Melloch	1		
Spring 2008	Purdue	ECE305	Semiconductor Devices	Woodall	1		
Spring 2008	Purdue	ECE606	Solid State Devices	Alam		1	
Spring 2008	Purdue	MSE382	Mechanical Response of Materials	Strachan	1		
Spring 2008	South. Ill/Carbondale	ECE593	Advanced Topics in ECE	Ahmed		1	
Spring 2008	UC Berkeley	PHYC203/NSEC242	Computational Nanoscience	Grossman/Ertekin	1		

Spring 2008	UC Berkeley	PHYC203/NSEC242	Computational Nanoscience	Grossman/Ertekin

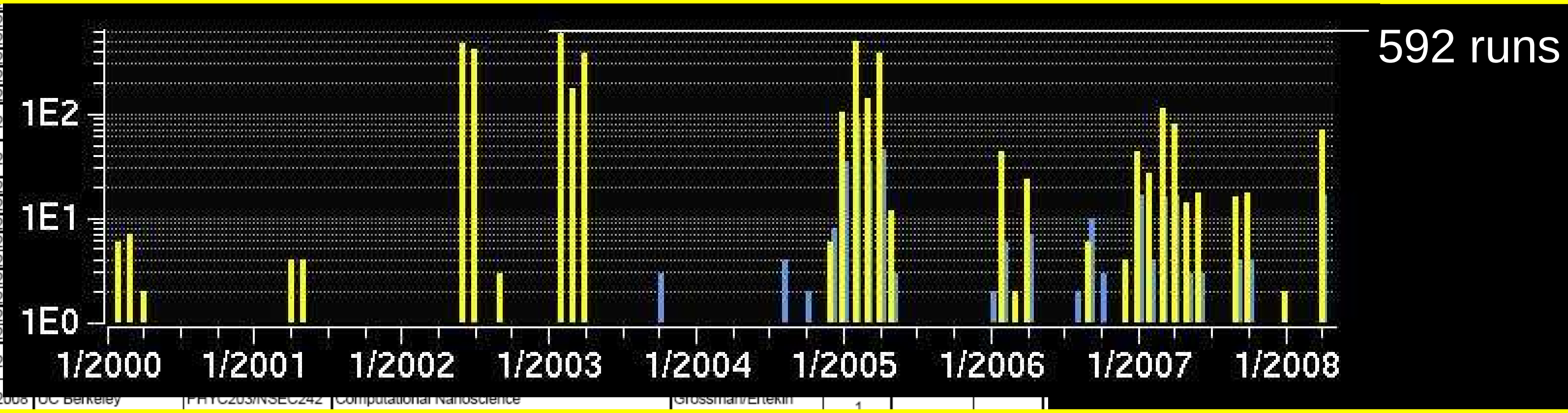
Table 1.4 in annual report

44 classes at 18 institutions

Spring 2008	Arizona St.	EEE/CSE 101	Introductory Engineering Design	Vasileska
Spring 2008	Arizona St.	EEE352	Properties of Electronic Materials	Ferry
Spring 2008	Arizona St.	EE533	Semiconductor Transport	Vasileska

Spring 2008	Arizona St.	EE533	Semiconductor Transport	Vasileska		1	
Spring 2008	Ball State	PHY466	Condensed Matter Physics	Cosby	1		
Spring 2008	Cornell	M&AE 656(6560)	Nanoscale Energy Transport and Conversion			1	

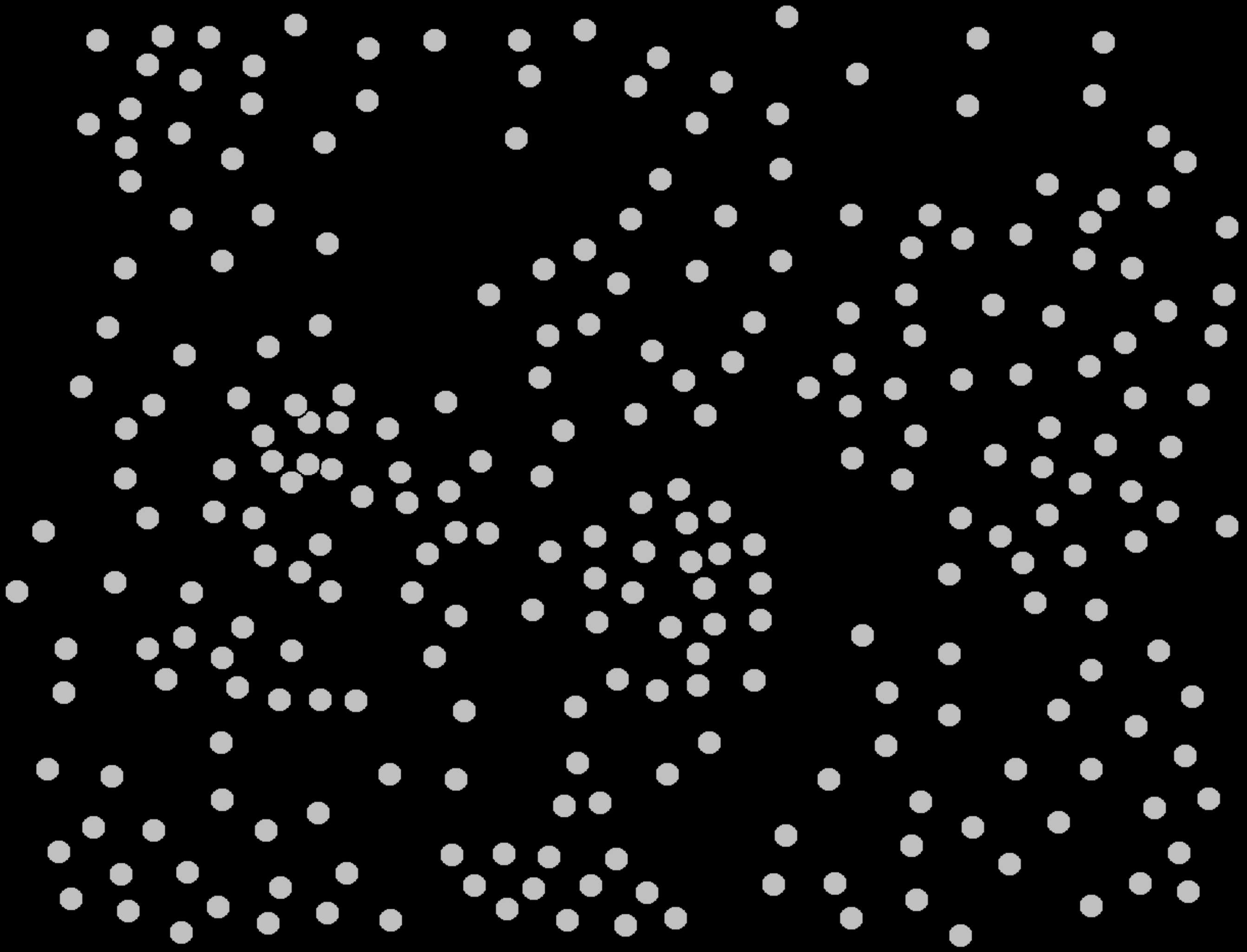
Spring 2008	Ball State	PHY466	Condensed Matter Physics	Cosby



Spring 2008	UC Berkeley	PHYC203/NSEC242	Computational Nanoscience	Grossman/Ertekin

Table 1.4 in annual report

265 Citations



265 Citations

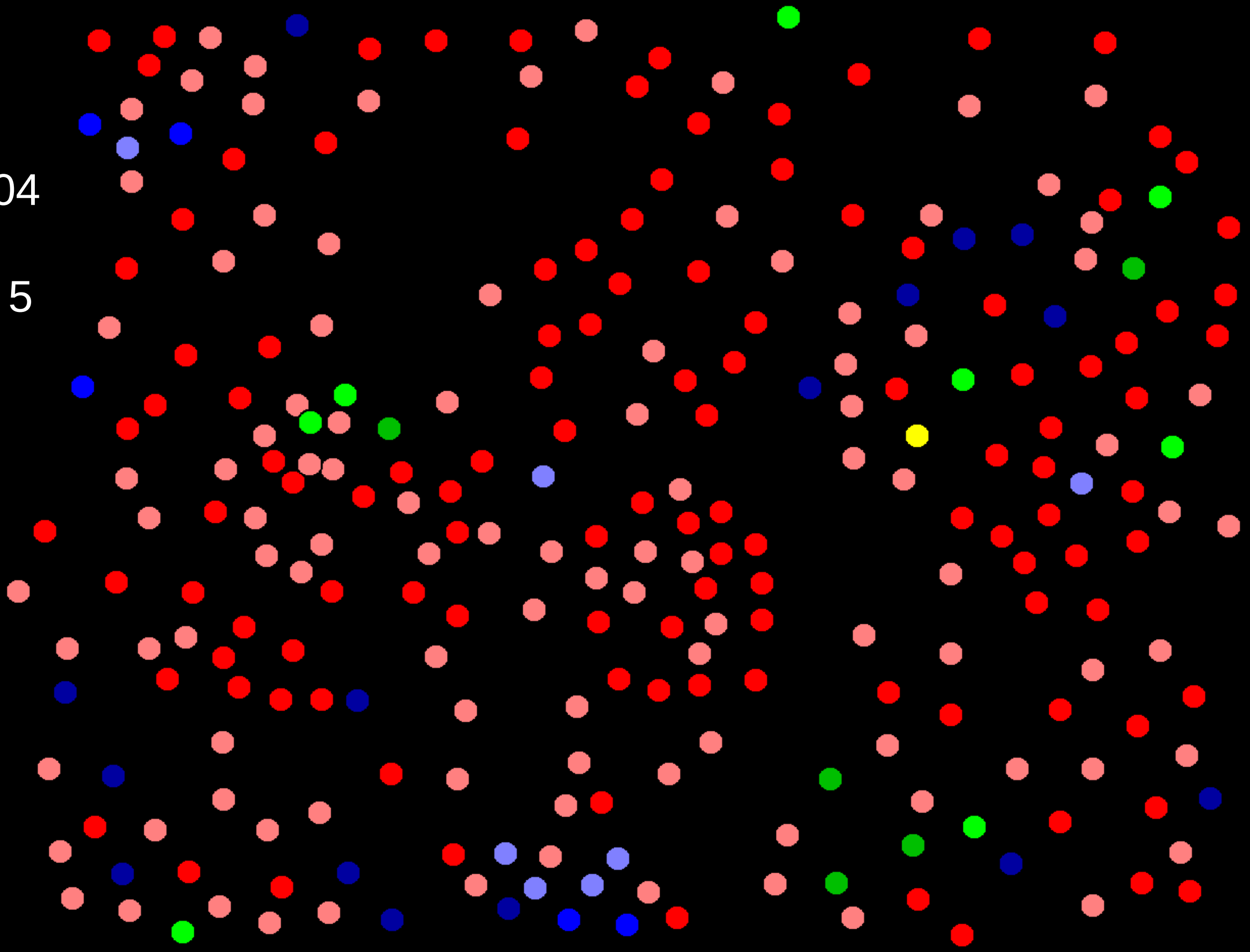
Published Where?

- ● **Journals** 119
- ● **Proceedings** 104
- ● **Ph.D. thesis** 8
- ● **Masters thesis** 5
- ● **Books** 1

89%

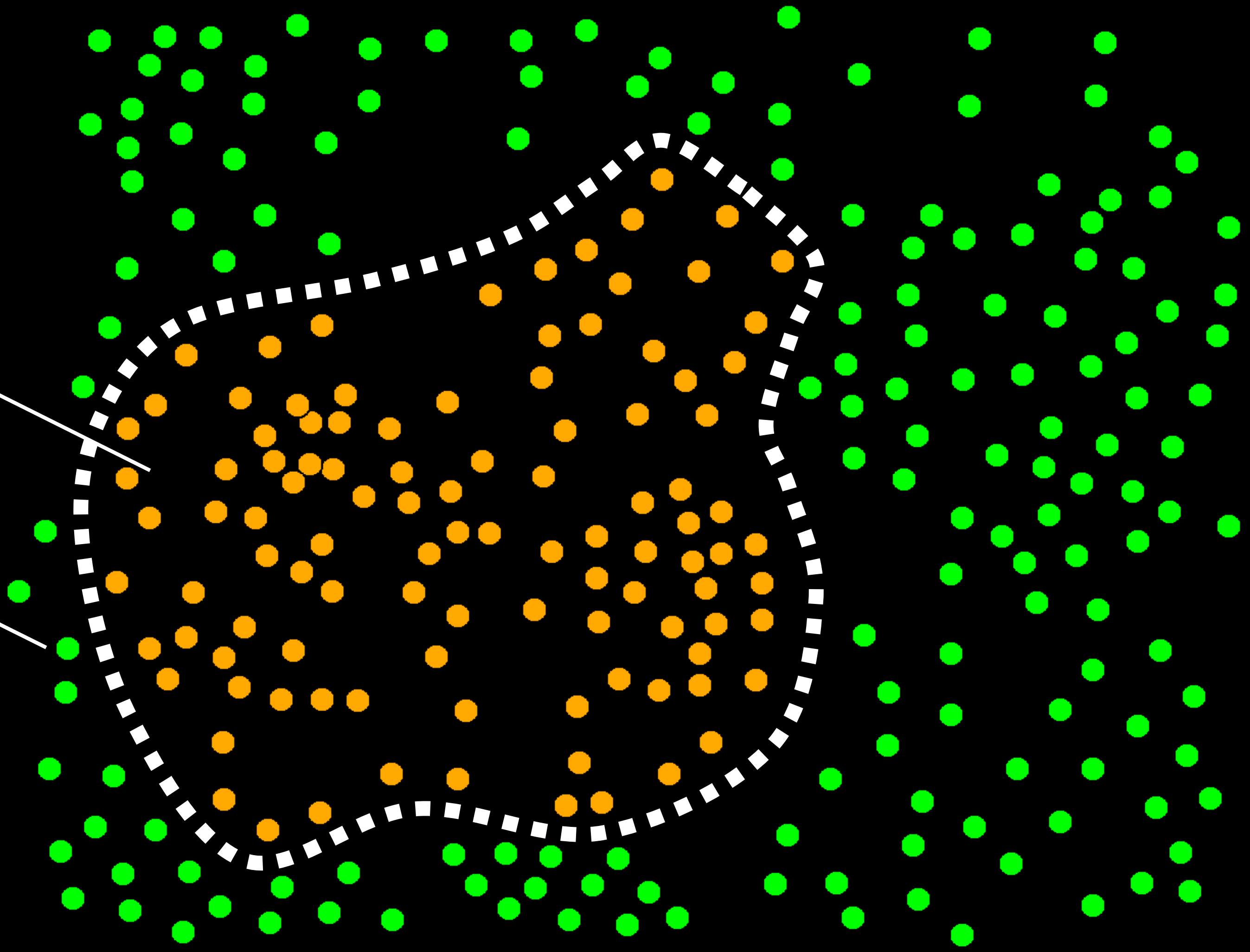
- ● **Conferences** 8
- ● **Magazines** 5
- ● **TechReps** 15

11%



265 Citations

Who?

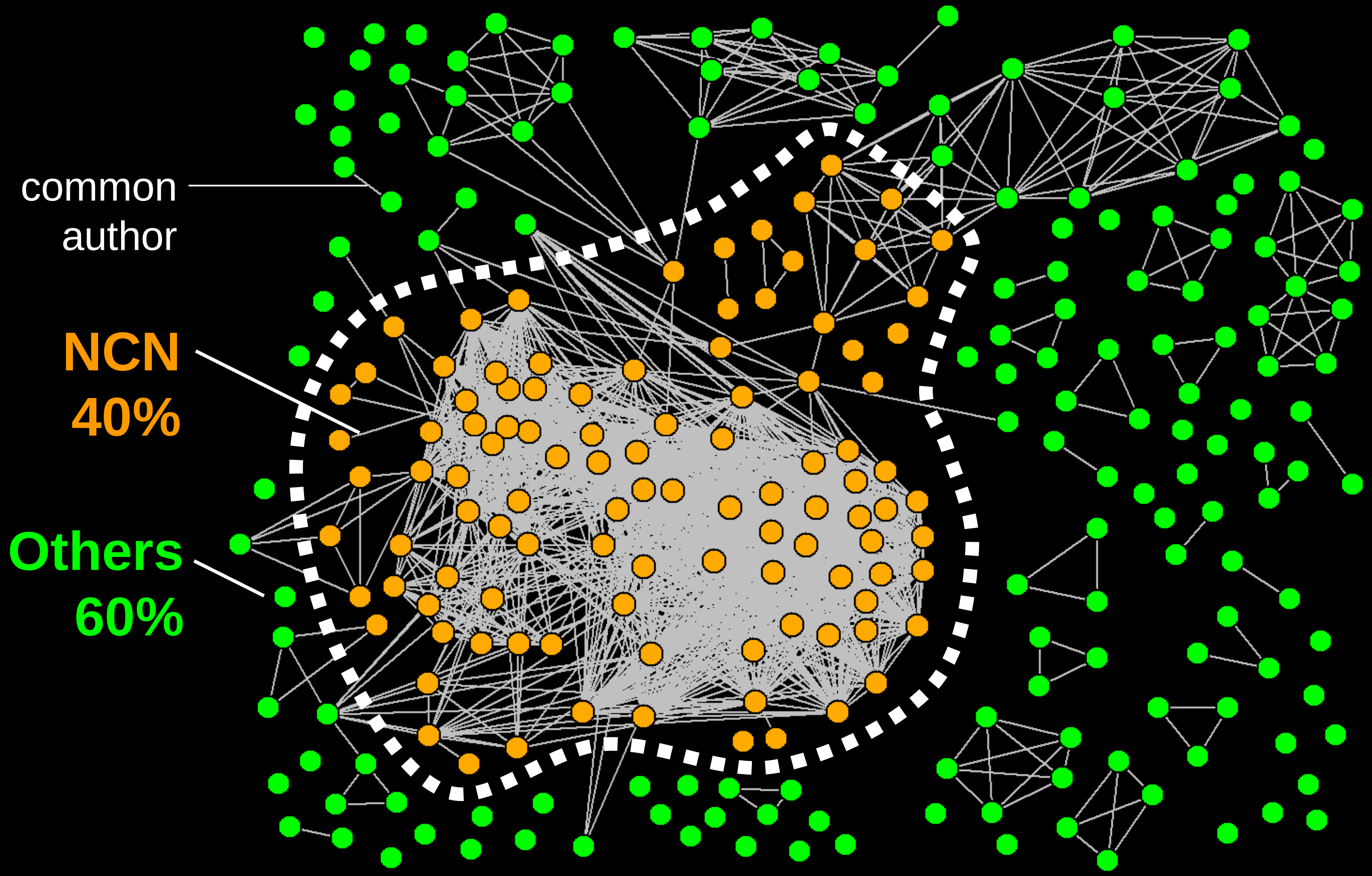


NCN
40%

Others
60%

265 Citations

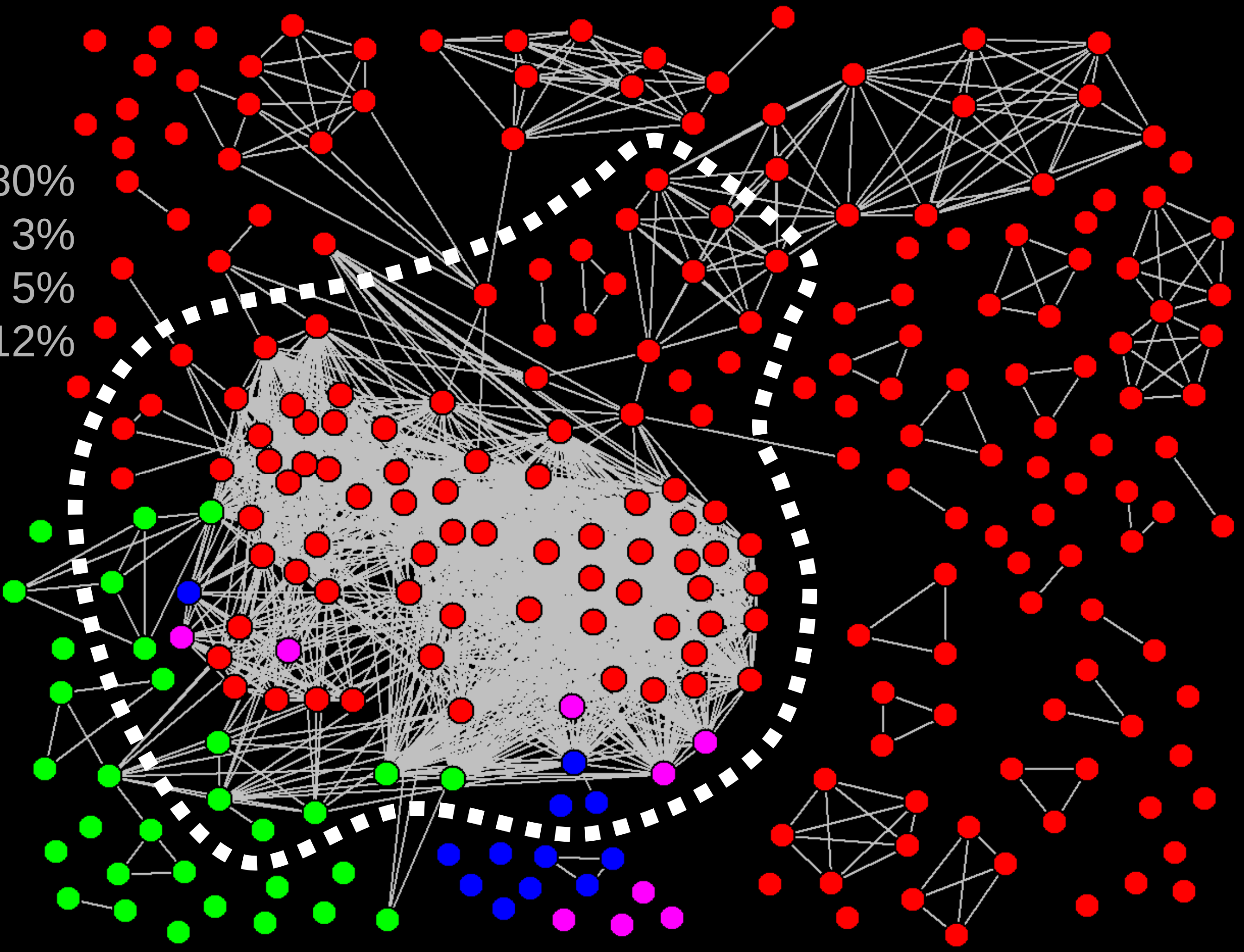
Who? With Whom?



265 Citations

Cited for what?

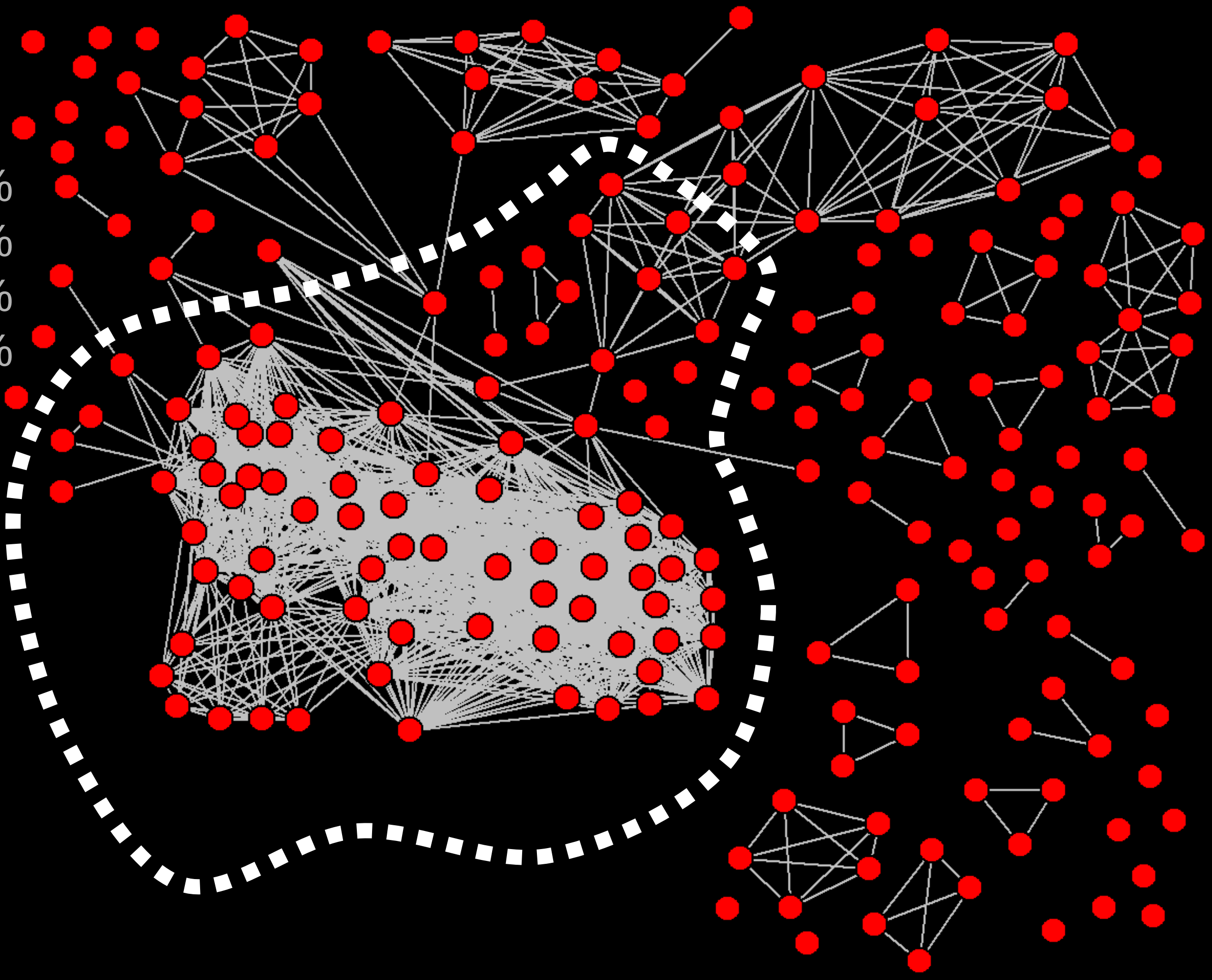
🔴	Research	213	80%
🟣	Res/Edu	9	3%
🔵	Education	12	5%
🟢	Cyberinfr	31	12%



Focus on Research

213 Citations

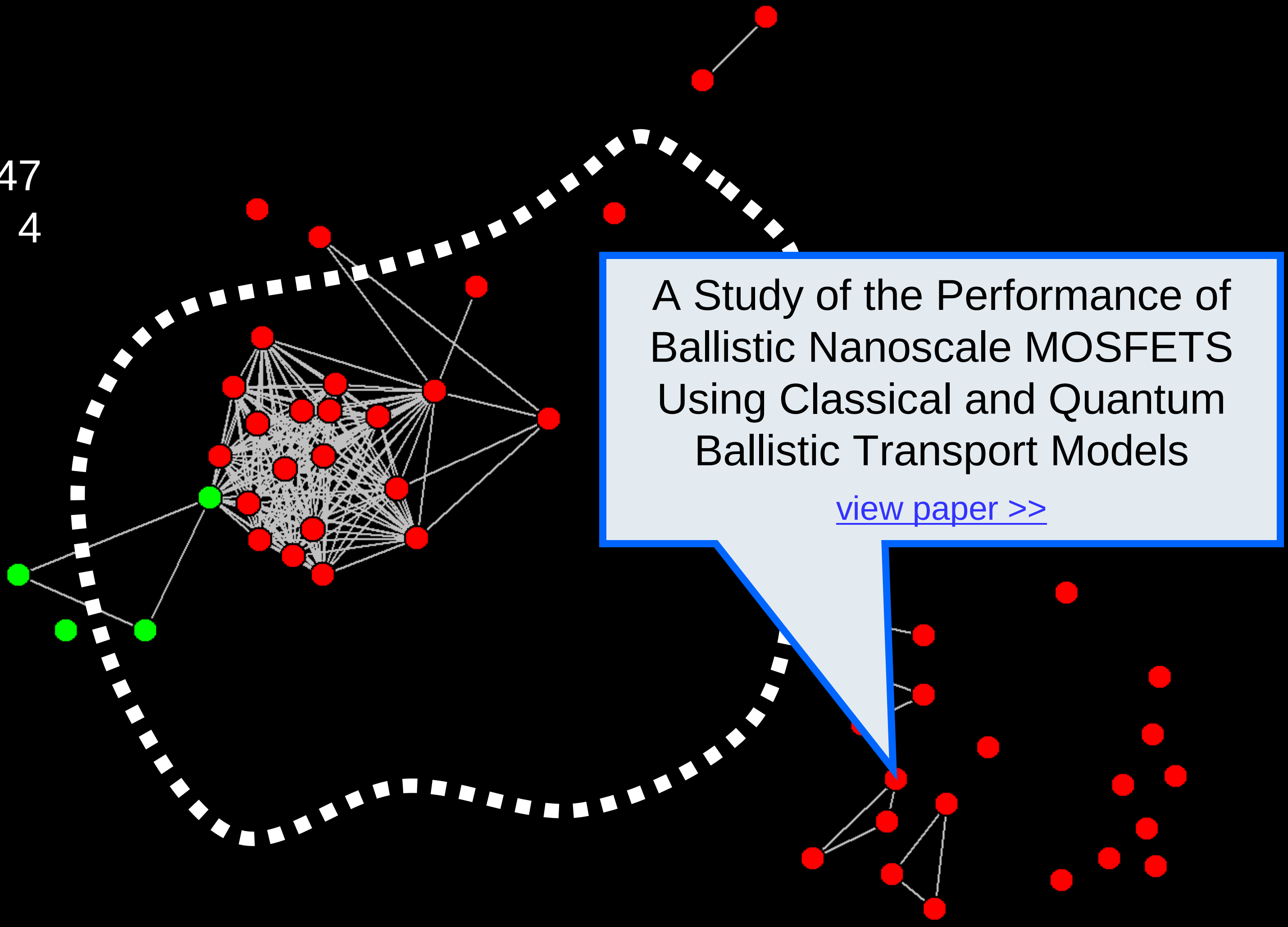
●	Research	213	80%
●	Res/Edu	9	3%
●	Education	12	5%
●	Cyberinfr	31	12%



Focus on nanoMOS

51 Citations

🔴	Research	47
🟢	Cyberinfr	4



A Study of the Performance of Ballistic Nanoscale MOSFETS Using Classical and Quantum Ballistic Transport Models

view paper >>

A Study of the Performance of Ballistic Nanoscale MOSFETS Using Classical and Quantum Ballistic Transport Models

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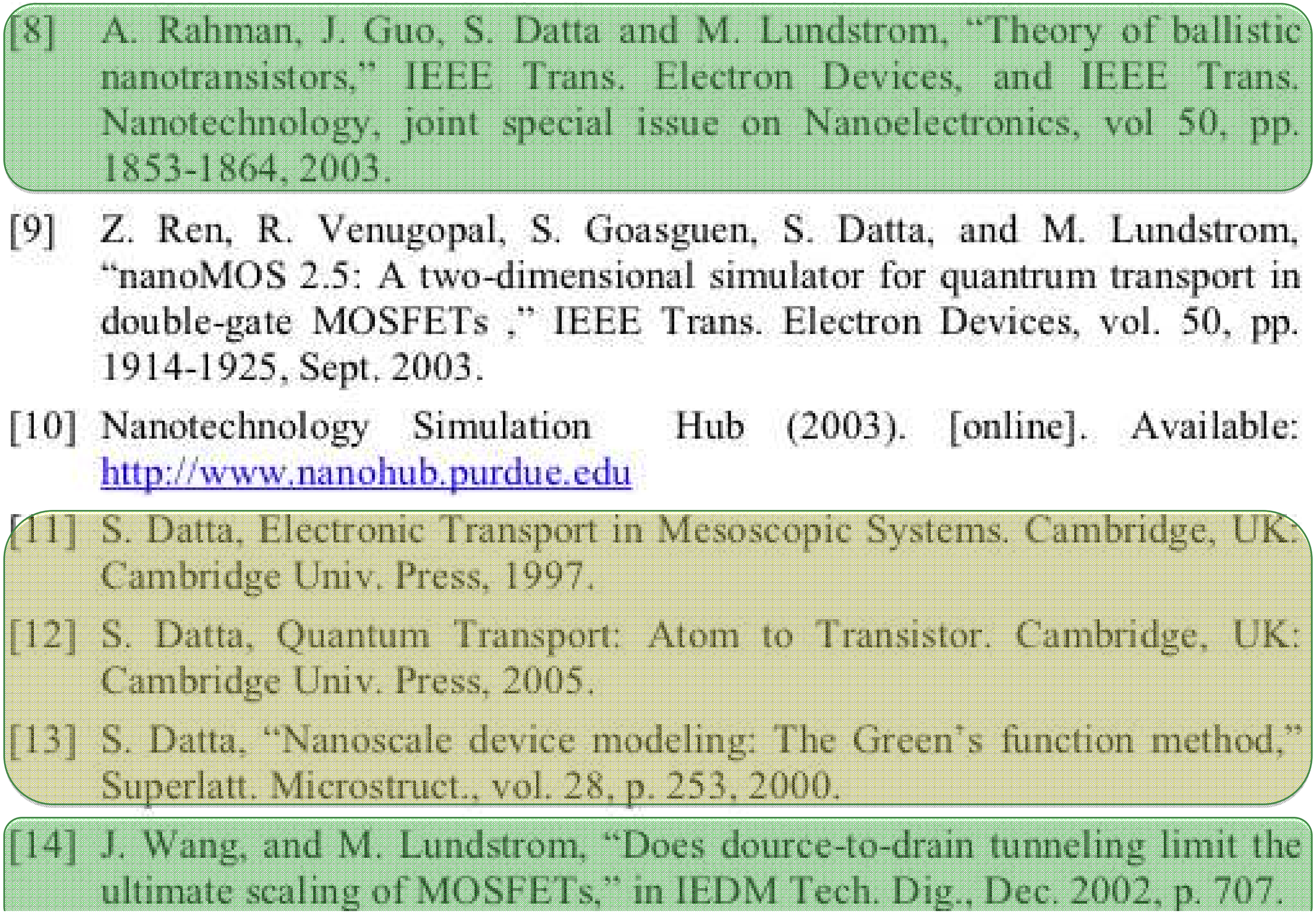

[8] A. Rahman, J. Guo, S. Datta and M. Lundstrom, "Theory of ballistic nanotransistors," IEEE Trans. Electron Devices, and IEEE Trans. Nanotechnology, joint special issue on Nanoelectronics, vol 50, pp. 1853-1864, 2003.

[9] Z. Ren, R. Venugopal, S. Goasguen, S. Datta, and M. Lundstrom, "nanoMOS 2.5: A two-dimensional simulator for quantrum transport in double-gate MOSFETs ," IEEE Trans. Electron Devices, vol. 50, pp. 1914-1925, Sept. 2003.

[10] Nanotechnology Simulation Hub (2003). [online]. Available: http://www.nanohub.purdue.edu

[11] S. Datta, Electronic Transport in Mesoscopic Systems. Cambridge, UK: Cambridge Univ. Press, 1997.

[12] S. Datta, Quantum Transport: Atom to Transistor. Cambridge, UK: Cambridge Univ. Press, 2005.

[13] S. Datta, "Nanoscale device modeling: The Green's function method," Superlatt. Microstruct., vol. 28, p. 253, 2000.

[14] J. Wang, and M. Lundstrom, "Does dource-to-drain tunneling limit the ultimate scaling of MOSFETs," in IEDM Tech. Dig., Dec. 2002, p. 707.

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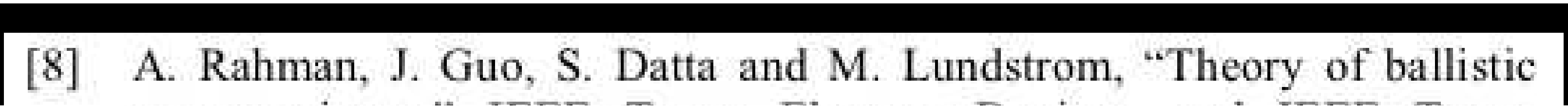
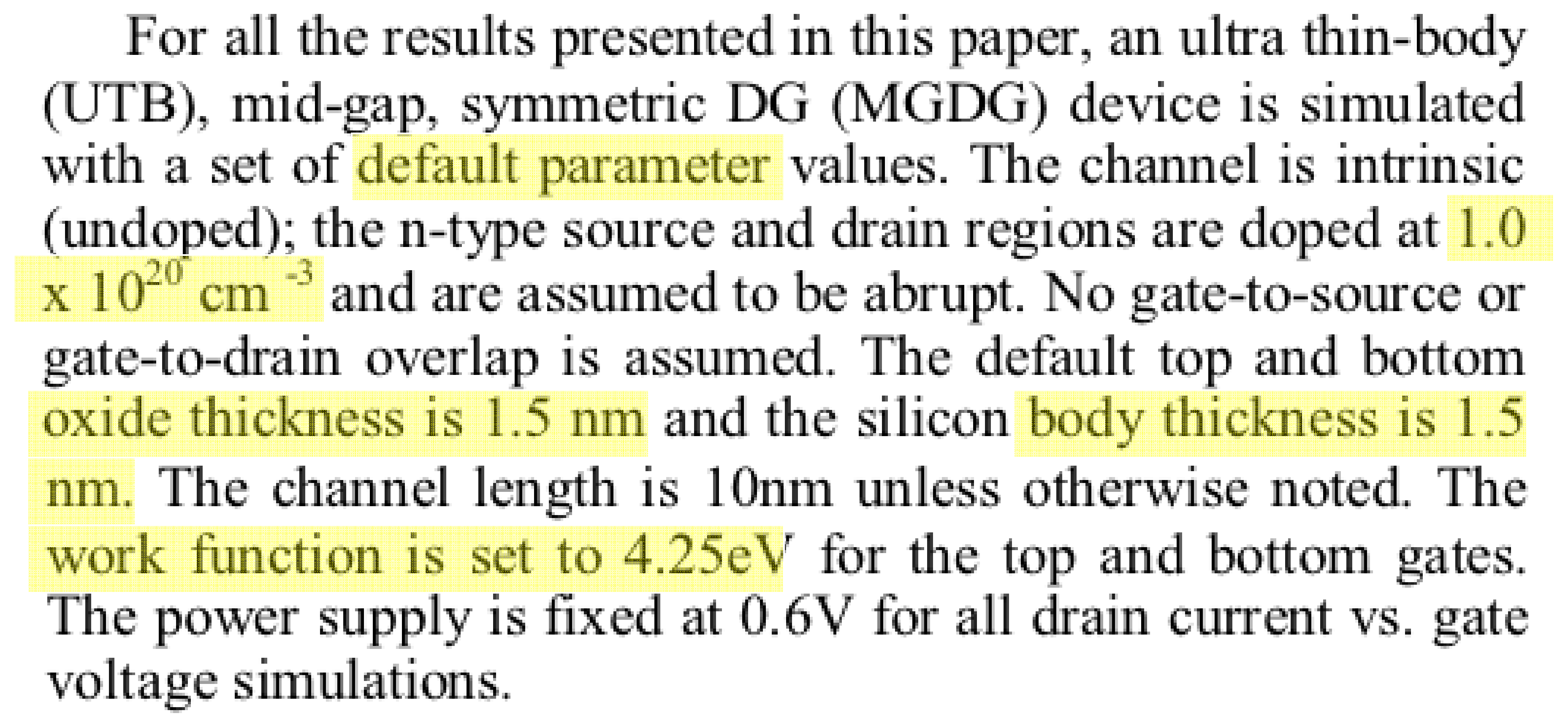
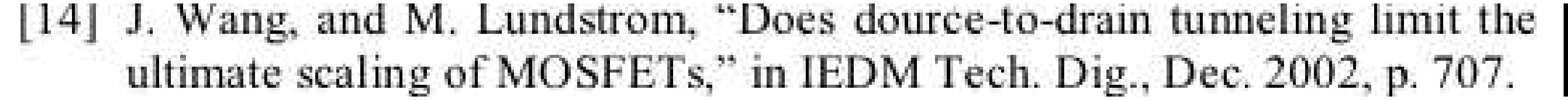
A Study of the Performance of Ballistic Nanoscale MOSFETS Using Classical and Quantum Ballistic Transport Models



[8] A. Rahman, J. Guo, S. Datta and M. Lundstrom, "Theory of ballistic

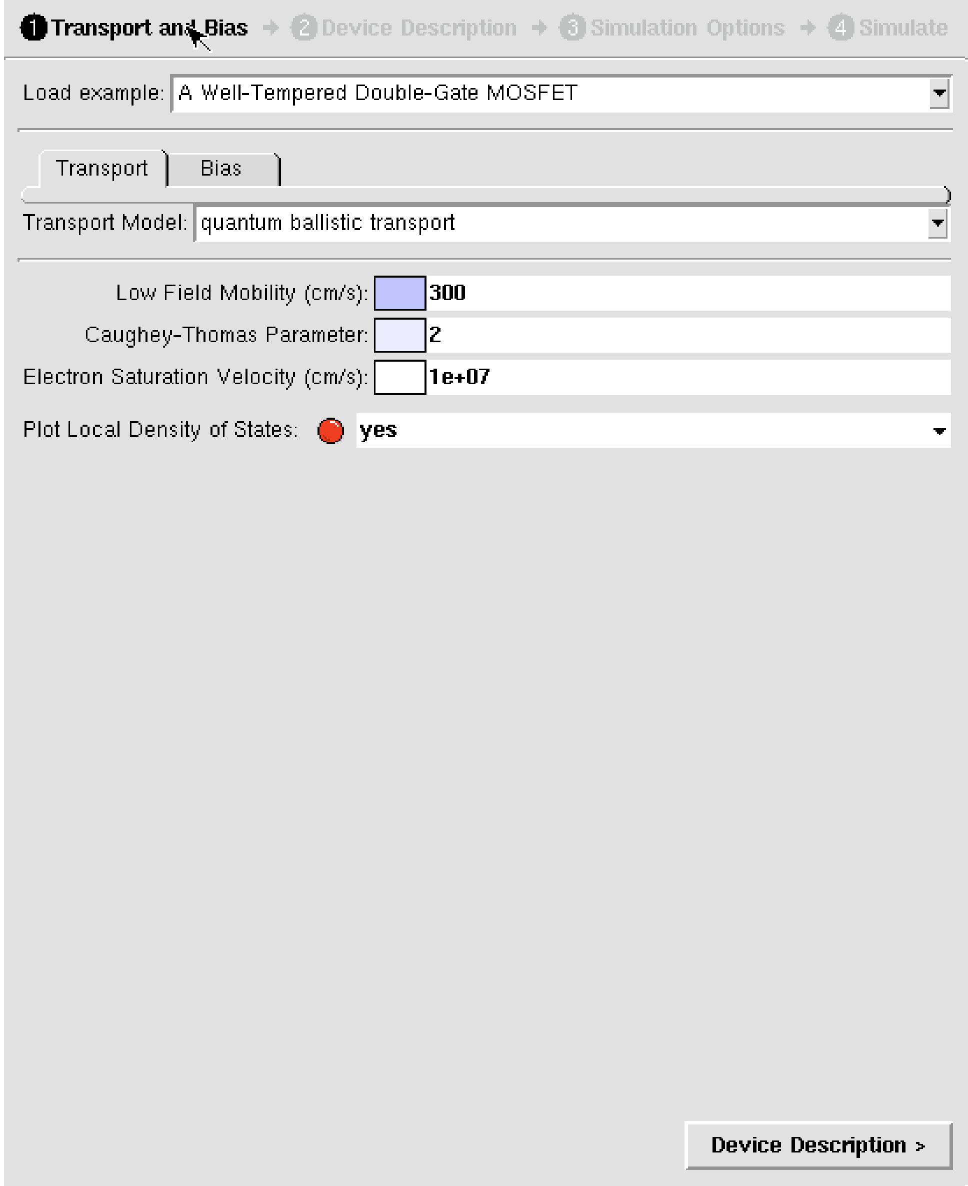


For all the results presented in this paper, an ultra thin-body (UTB), mid-gap, symmetric DG (MGDG) device is simulated with a set of default parameter values. The channel is intrinsic (undoped); the n-type source and drain regions are doped at $1.0 \times 10^{20}\ \mathrm{cm}^{-3}$ and are assumed to be abrupt. No gate-to-source or gate-to-drain overlap is assumed. The default top and bottom oxide thickness is 1.5 nm and the silicon body thickness is 1.5 nm. The channel length is 10nm unless otherwise noted. The work function is set to 4.25eV for the top and bottom gates. The power supply is fixed at 0.6V for all drain current vs. gate voltage simulations.



[14] J. Wang, and M. Lundstrom, "Does dource-to-drain tunneling limit the ultimate scaling of MOSFETs," in IEDM Tech. Dig., Dec. 2002, p. 707.

nanoMOS: Transport Model / Bias



Load example: A Well-Tempered Double-Gate MOSFET

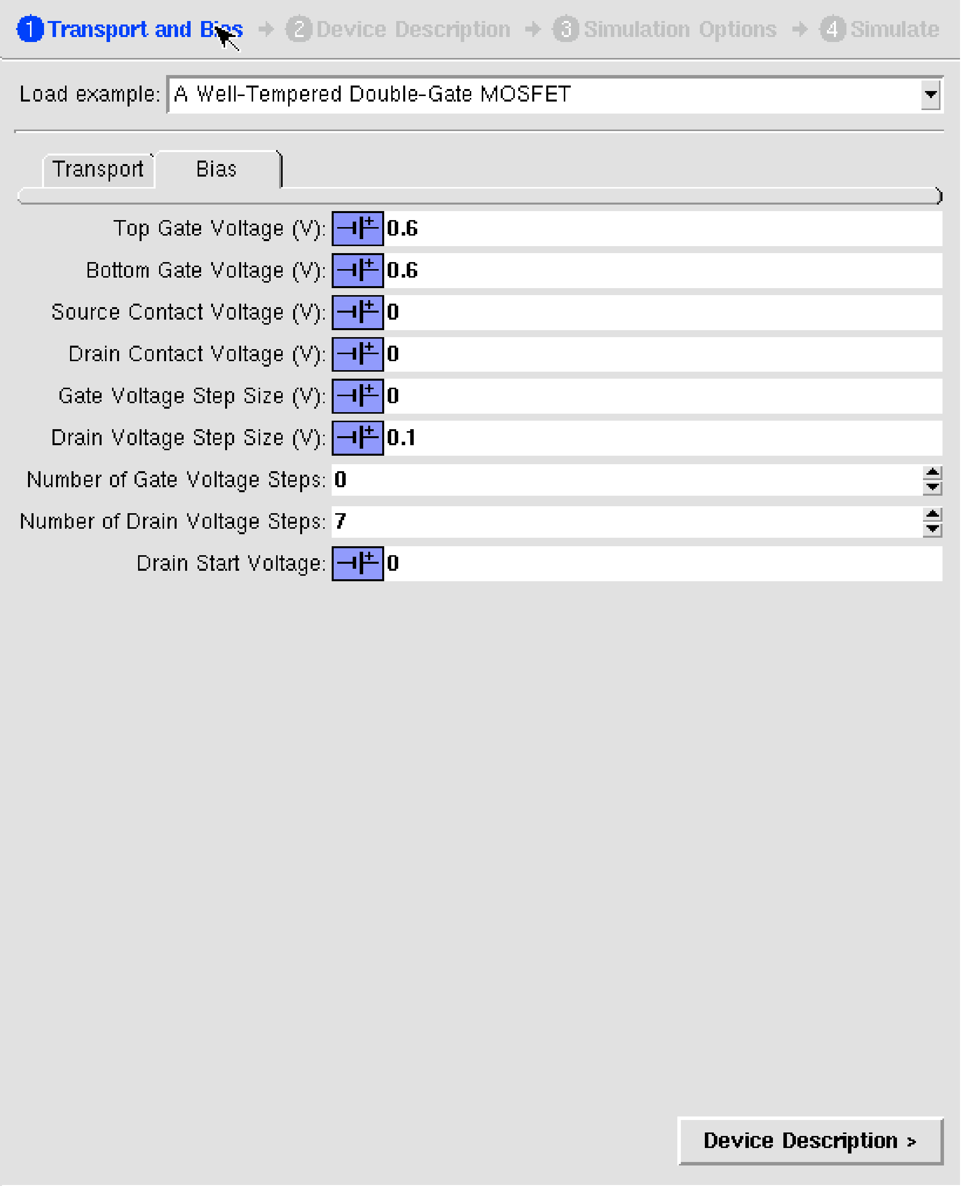
Transport Model: quantum ballistic transport

Low Field Mobility (cm/s): 300

Caughey-Thomas Parameter: 2

Electron Saturation Velocity (cm/s): 1e+07

Plot Local Density of States: ● yes



Load example: A Well-Tempered Double-Gate MOSFET

Top Gate Voltage (V): 0.6

Bottom Gate Voltage (V): 0.6

Source Contact Voltage (V): 0

Drain Contact Voltage (V): 0

Gate Voltage Step Size (V): 0

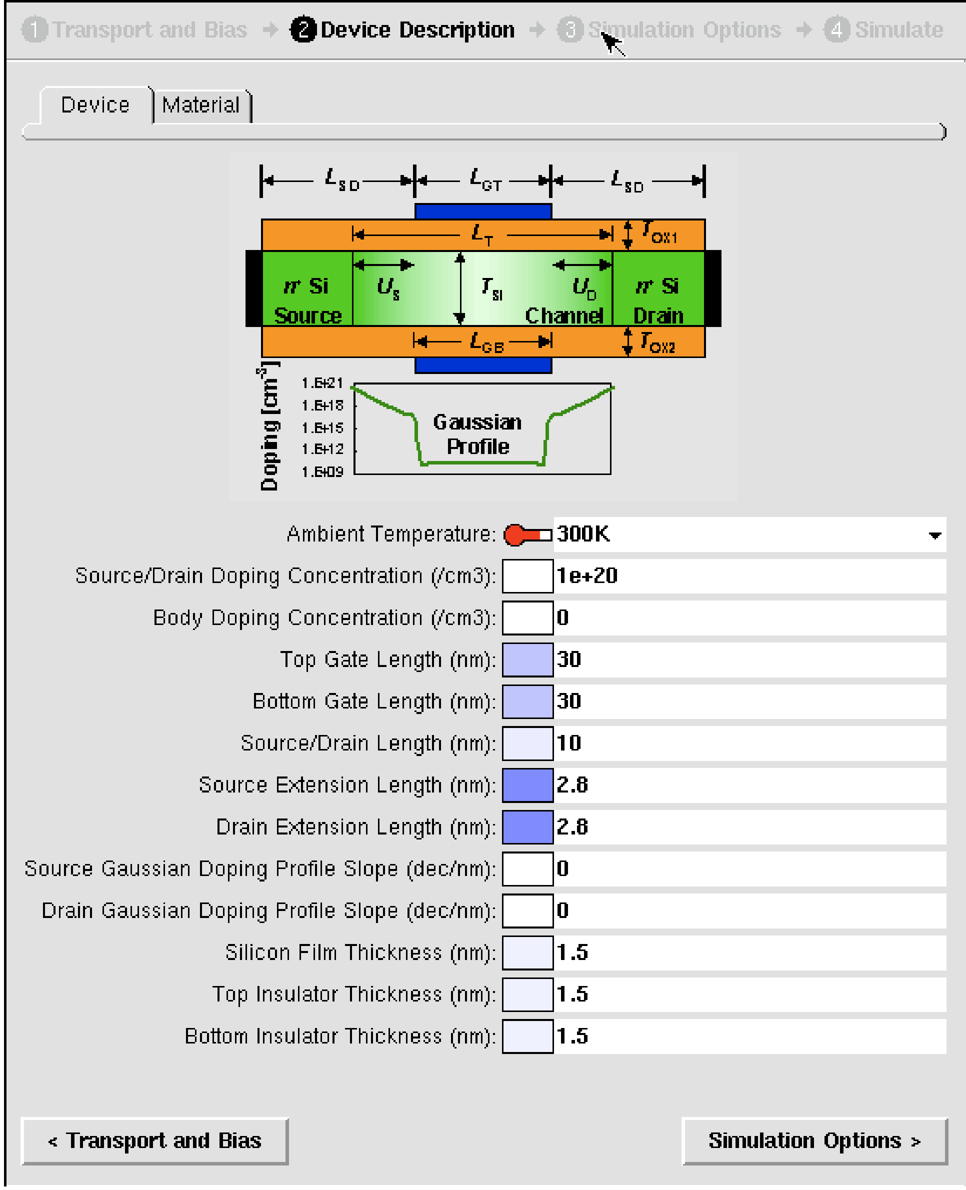
Drain Voltage Step Size (V): 0.1

Number of Gate Voltage Steps: 0

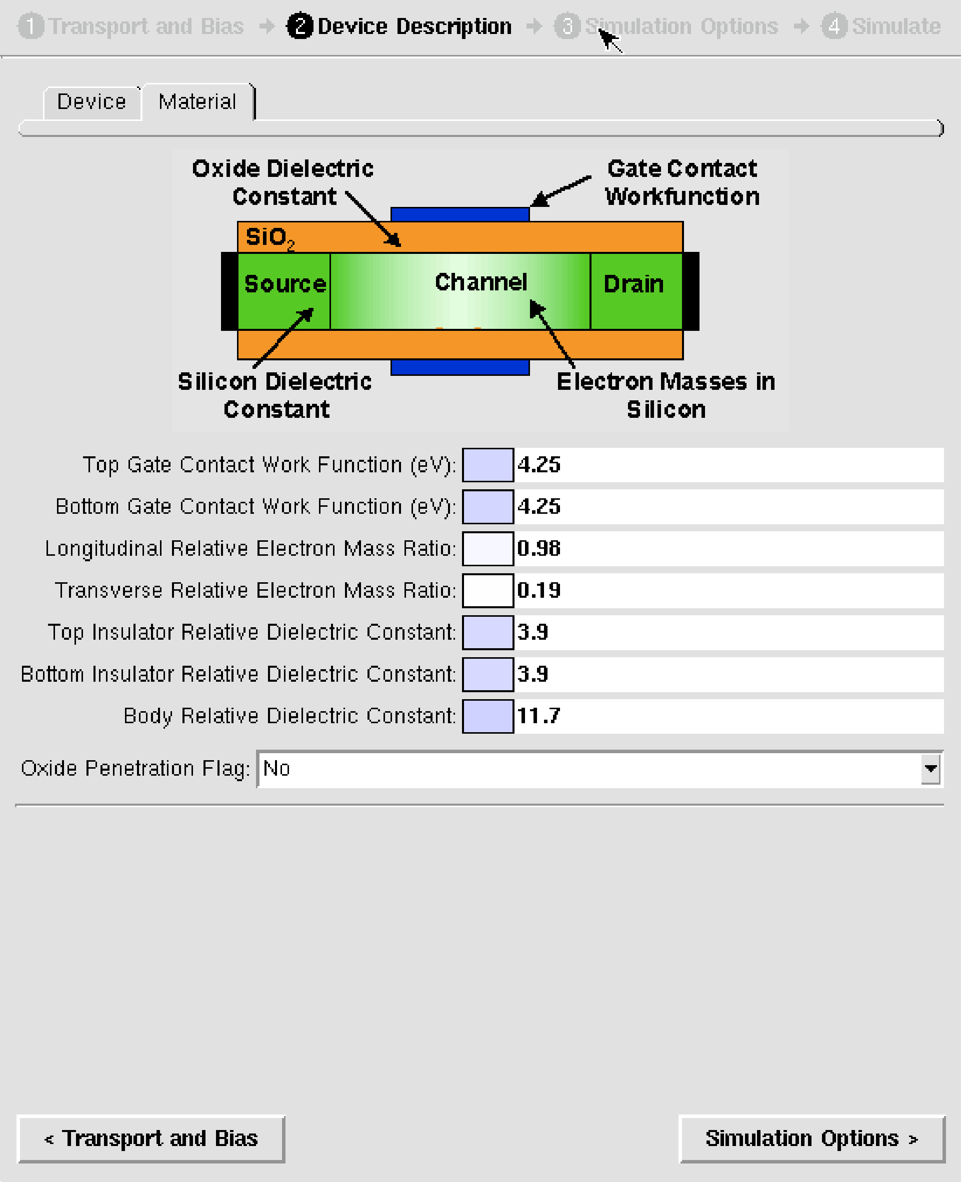
Number of Drain Voltage Steps: 7

Drain Start Voltage: 0

nanoMOS: Device / Materials Specs

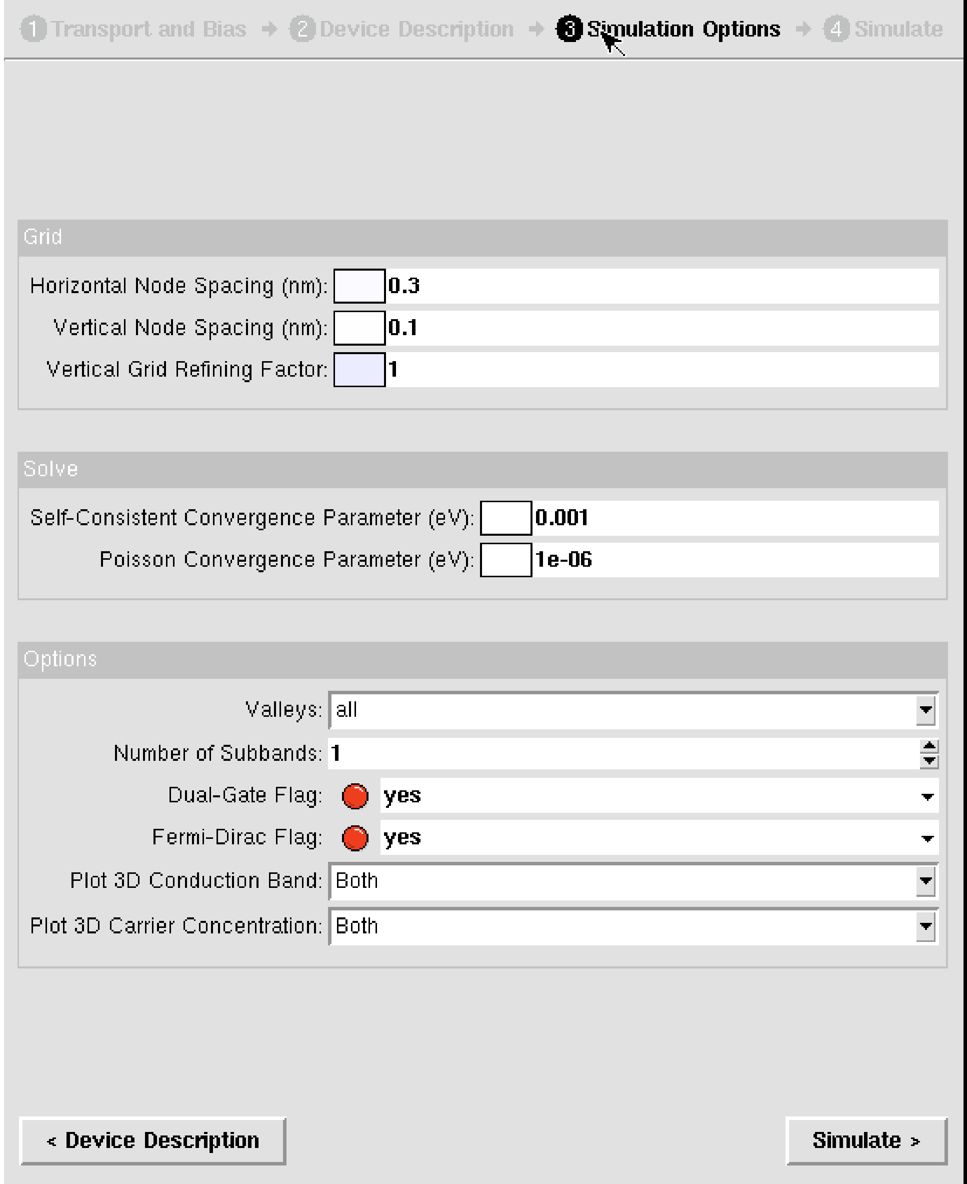


Ambient Temperature: 300K
Source/Drain Doping Concentration (/cm3): 1e+20
Body Doping Concentration (/cm3): 0
Top Gate Length (nm): 30
Bottom Gate Length (nm): 30
Source/Drain Length (nm): 10
Source Extension Length (nm): 2.8
Drain Extension Length (nm): 2.8
Source Gaussian Doping Profile Slope (dec/nm): 0
Drain Gaussian Doping Profile Slope (dec/nm): 0
Silicon Film Thickness (nm): 1.5
Top Insulator Thickness (nm): 1.5
Bottom Insulator Thickness (nm): 1.5



Top Gate Contact Work Function (eV): 4.25
Bottom Gate Contact Work Function (eV): 4.25
Longitudinal Relative Electron Mass Ratio: 0.98
Transverse Relative Electron Mass Ratio: 0.19
Top Insulator Relative Dielectric Constant: 3.9
Bottom Insulator Relative Dielectric Constant: 3.9
Body Relative Dielectric Constant: 11.7
Oxide Penetration Flag: No

nanoMOS: Algorithm Details



Grid

Horizontal Node Spacing (nm): 0.3

Vertical Node Spacing (nm): 0.1

Vertical Grid Refining Factor: 1

Solve

Self-Consistent Convergence Parameter (eV): 0.001

Poisson Convergence Parameter (eV): 1e-06

Options

Valleys: all

Number of Subbands: 1

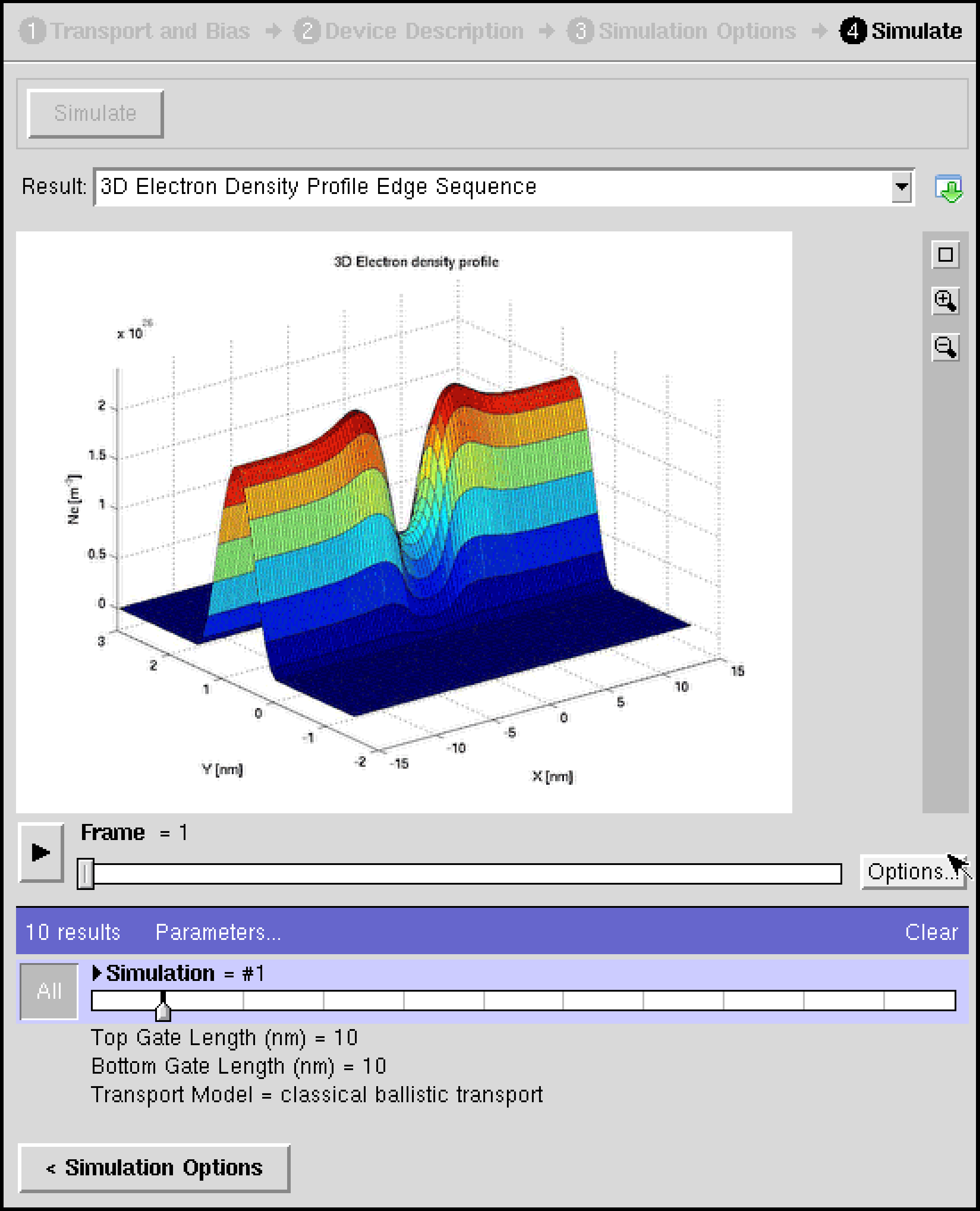
Dual-Gate Flag: ● yes

Fermi-Dirac Flag: ● yes

Plot 3D Conduction Band: Both

Plot 3D Carrier Concentration: Both

Gate Dependence of the Electron Density



Result: 3D Electron Density Profile Edge Sequence

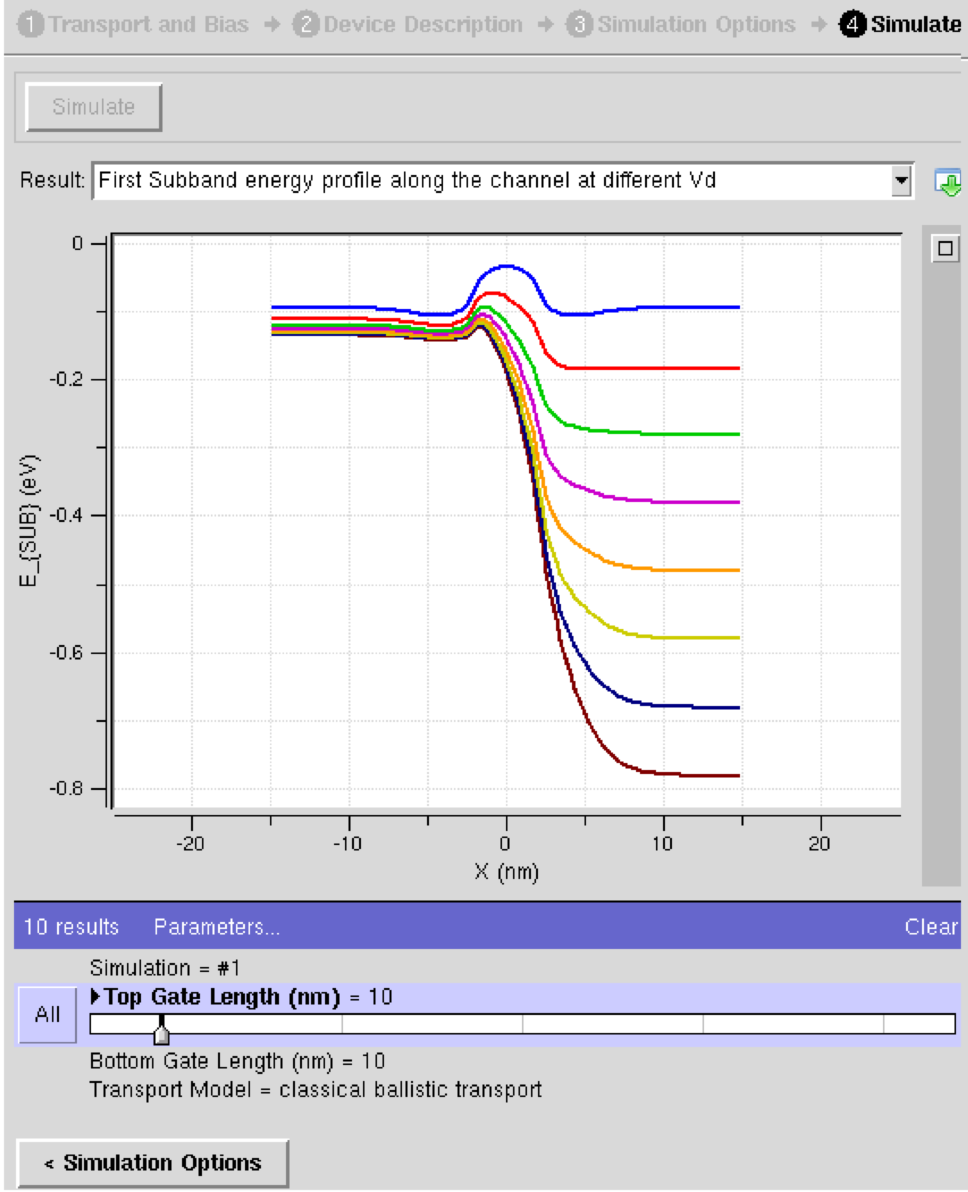
Frame = 1

10 results

Simulation = #1

Top Gate Length (nm) = 10
Bottom Gate Length (nm) = 10
Transport Model = classical ballistic transport

Gate Length Dependence



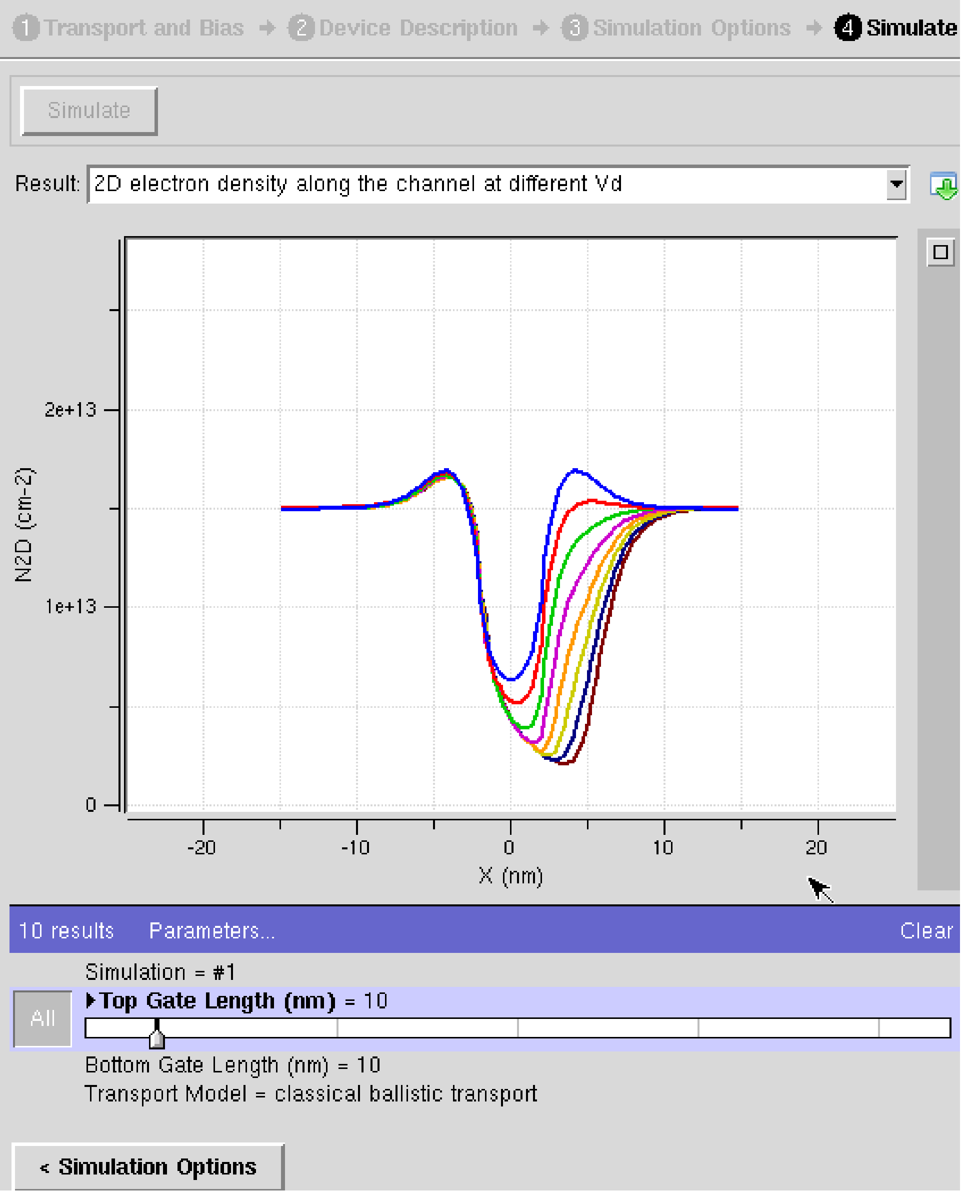
Result: First Subband energy profile along the channel at different Vd

Simulation = #1

Top Gate Length (nm) = 10

Bottom Gate Length (nm) = 10

Transport Model = classical ballistic transport



Result: 2D electron density along the channel at different Vd

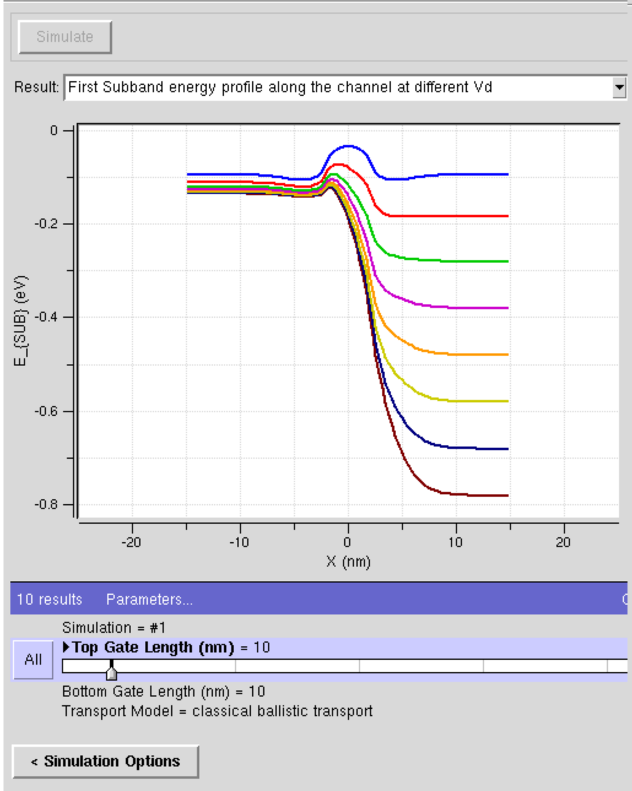
Simulation = #1

Top Gate Length (nm) = 10

Bottom Gate Length (nm) = 10

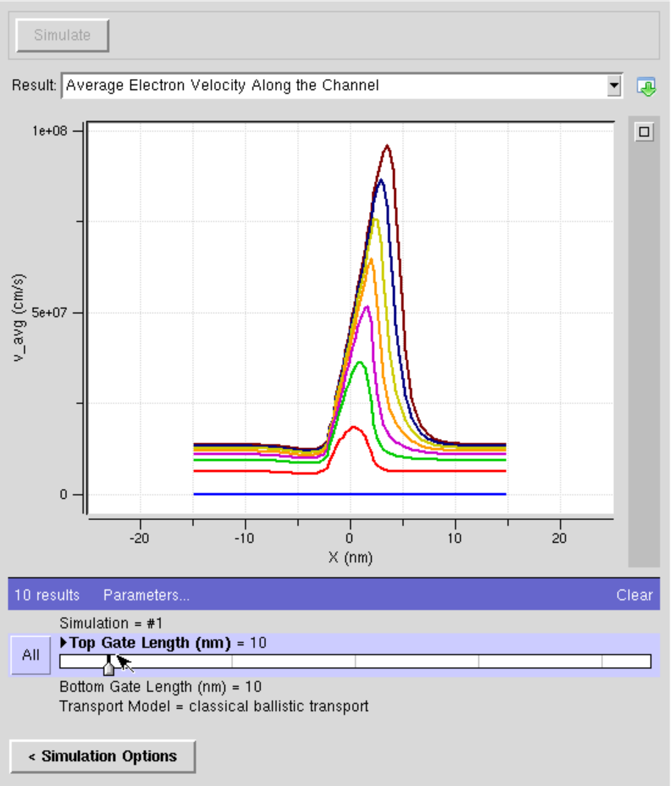
Transport Model = classical ballistic transport

Gate Length Dependence



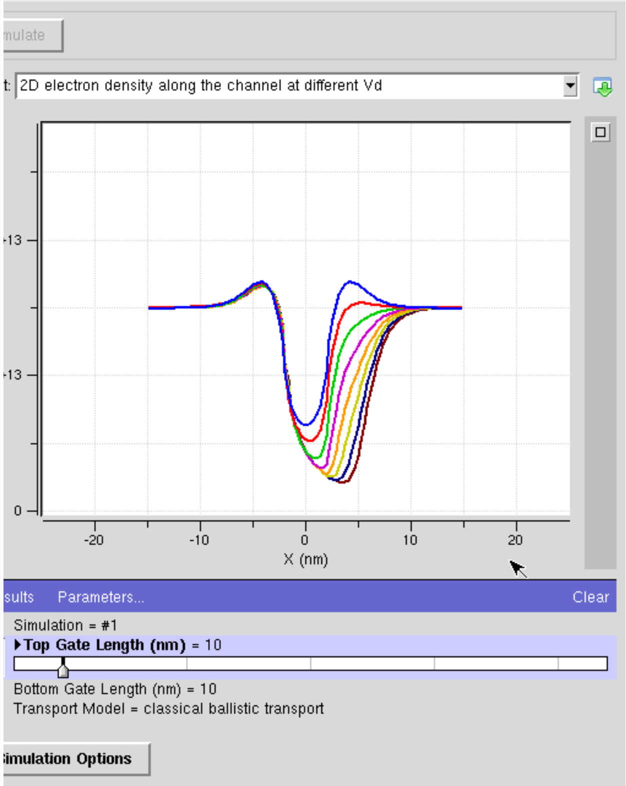
Result: First Subband energy profile along the channel at different Vd

Simulation = #1
Top Gate Length (nm) = 10
Bottom Gate Length (nm) = 10
Transport Model = classical ballistic transport



Result: Average Electron Velocity Along the Channel

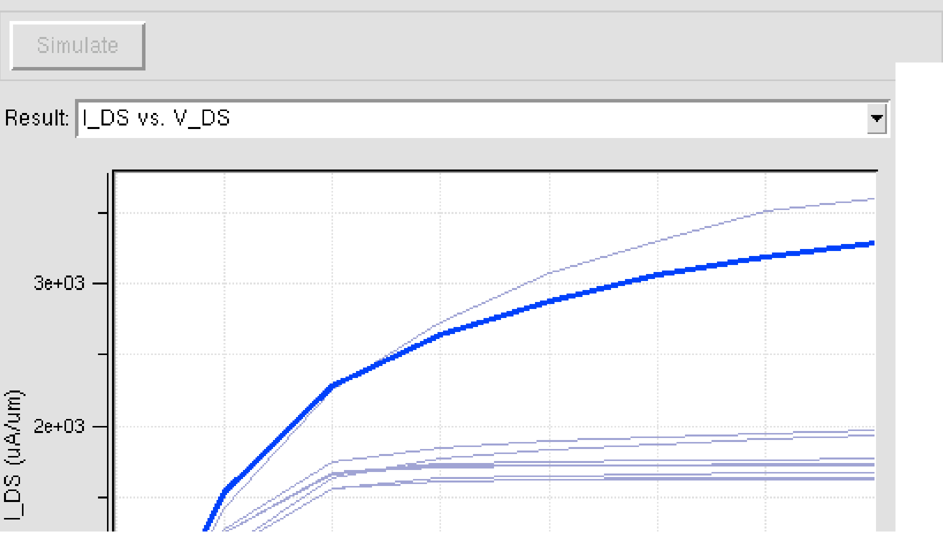
Simulation = #1
Top Gate Length (nm) = 10
Bottom Gate Length (nm) = 10
Transport Model = classical ballistic transport

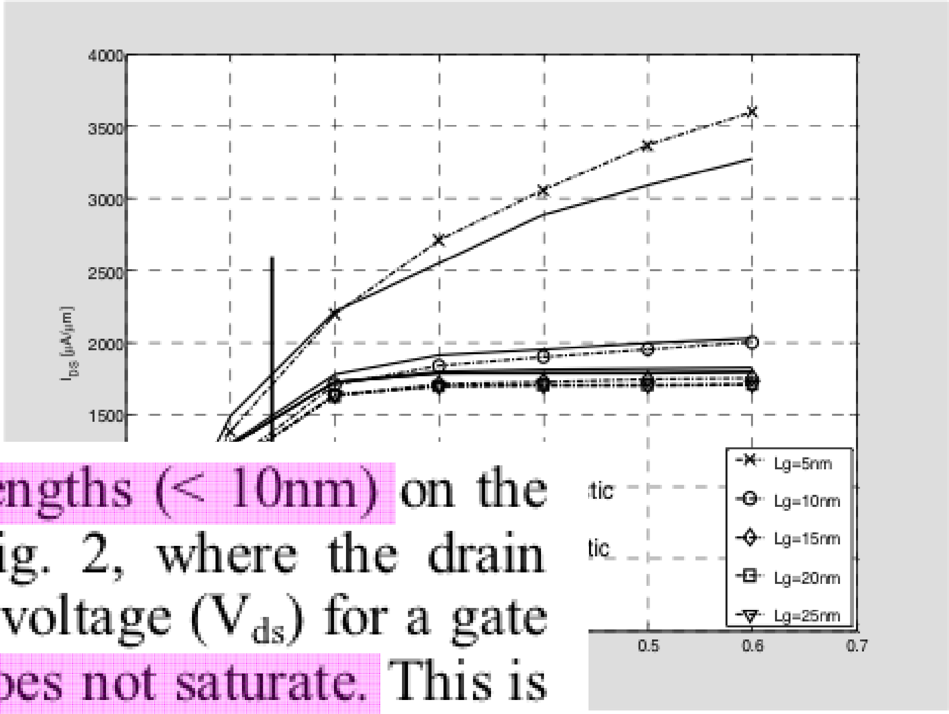


t: 2D electron density along the channel at different Vd

Simulation = #1
Top Gate Length (nm) = 10
Bottom Gate Length (nm) = 10
Transport Model = classical ballistic transport

A Study of the Performance of Ballistic Nanoscale MOSFETS Using Classical and Quantum Ballistic Transport Models



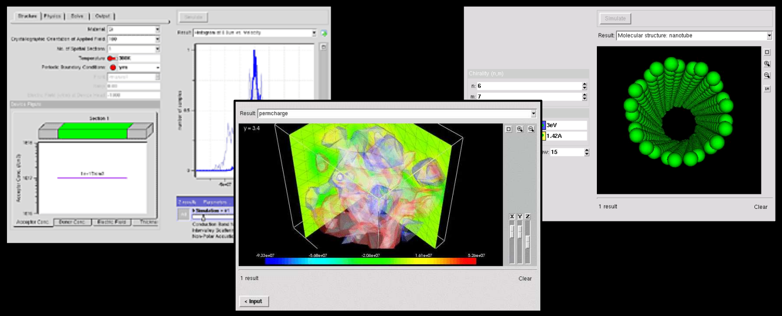


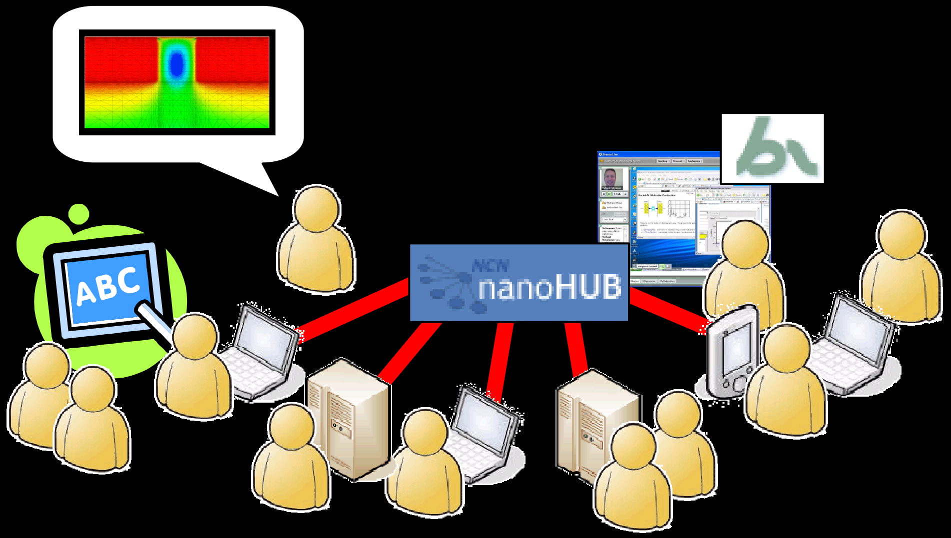
5nm and 20nm at V_{gs}=0.6V.

The impact of ultra-short channel lengths (< 10nm) on the saturation current is also visible in Fig. 2, where the drain current is plotted as a function of drain voltage (V_{ds}) for a gate voltage of 0.6V. For L_g=5nm, the I_{ds} does not saturate. This is because the channel potential along with the density of states (DOS) is pulled down in energy as the V_{ds} is increased making the DOS always available in the channel. To minimize this problem, the gate control of the channel must be enhanced by thinning the gate insulator. An interesting observation is that

nanoHUB.org

Online simulation… *…and more!*





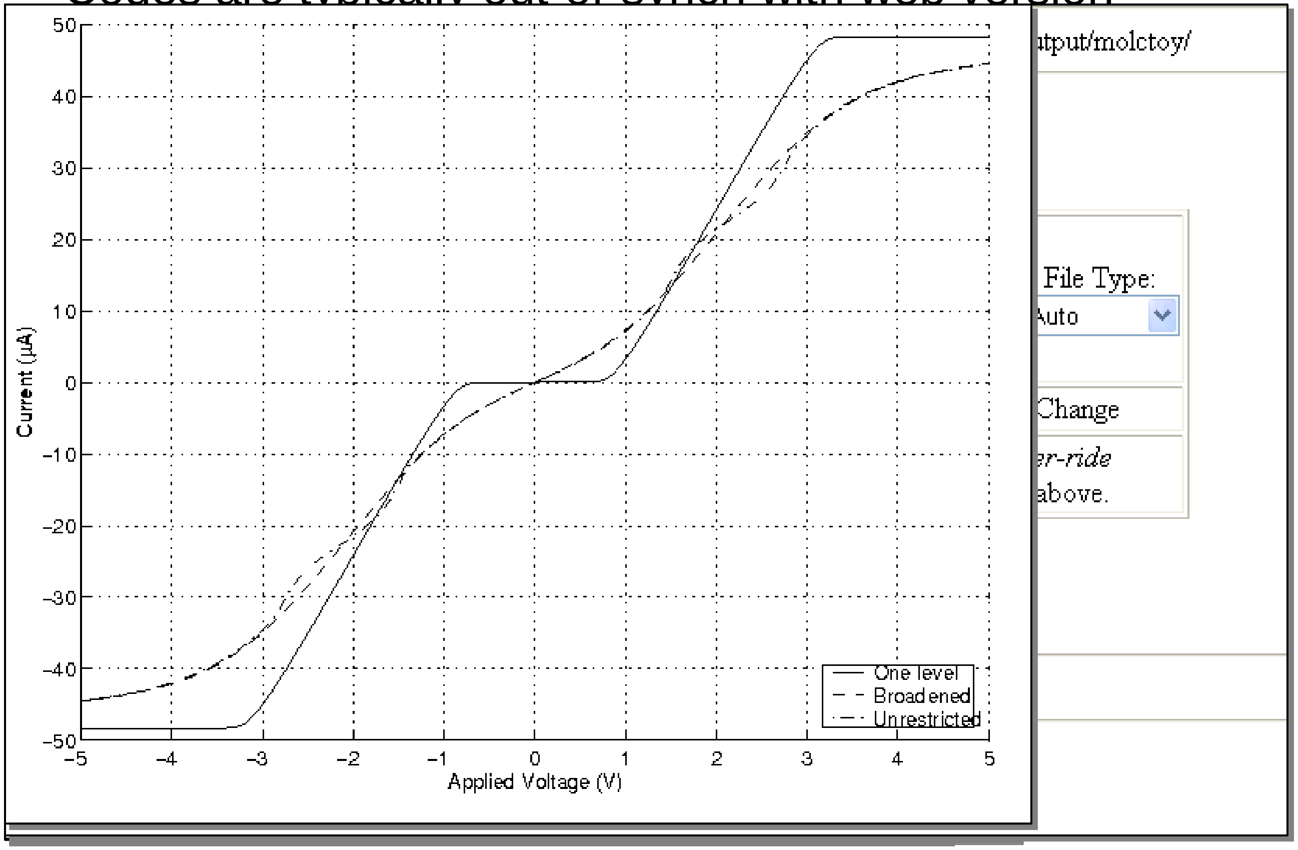
What is it?

- *Live Demo>>*
- *PPT Demo>>*
- *Short Video>>*

Impact ?
Scalability ?
Future ?

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

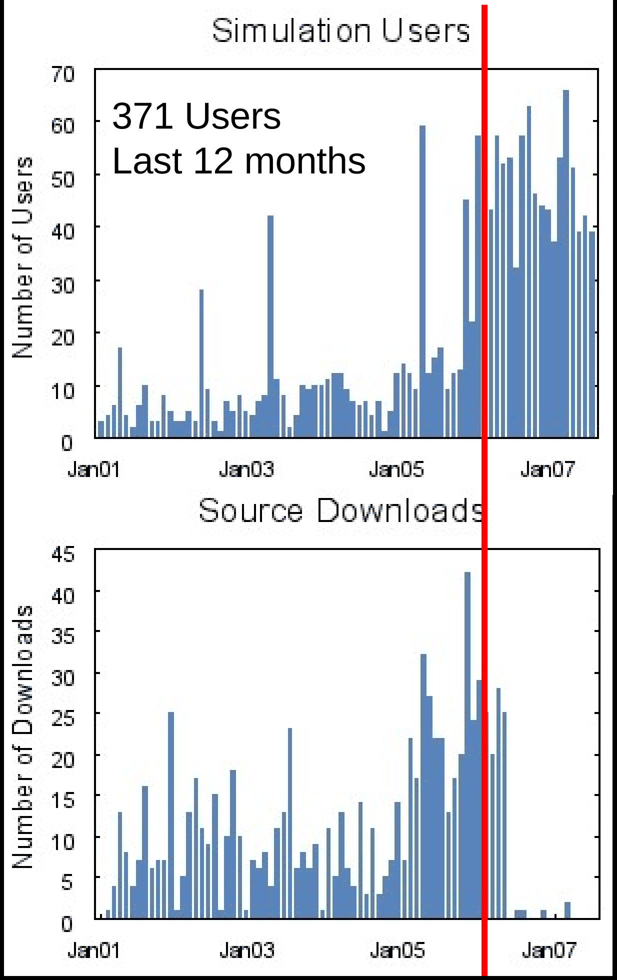
Typical Questions:

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

Symptoms of:

- No VISUAL feedback.
- Not interactive.

Case in point



Rappture version Feb 06

371 Users
Last 12 months

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

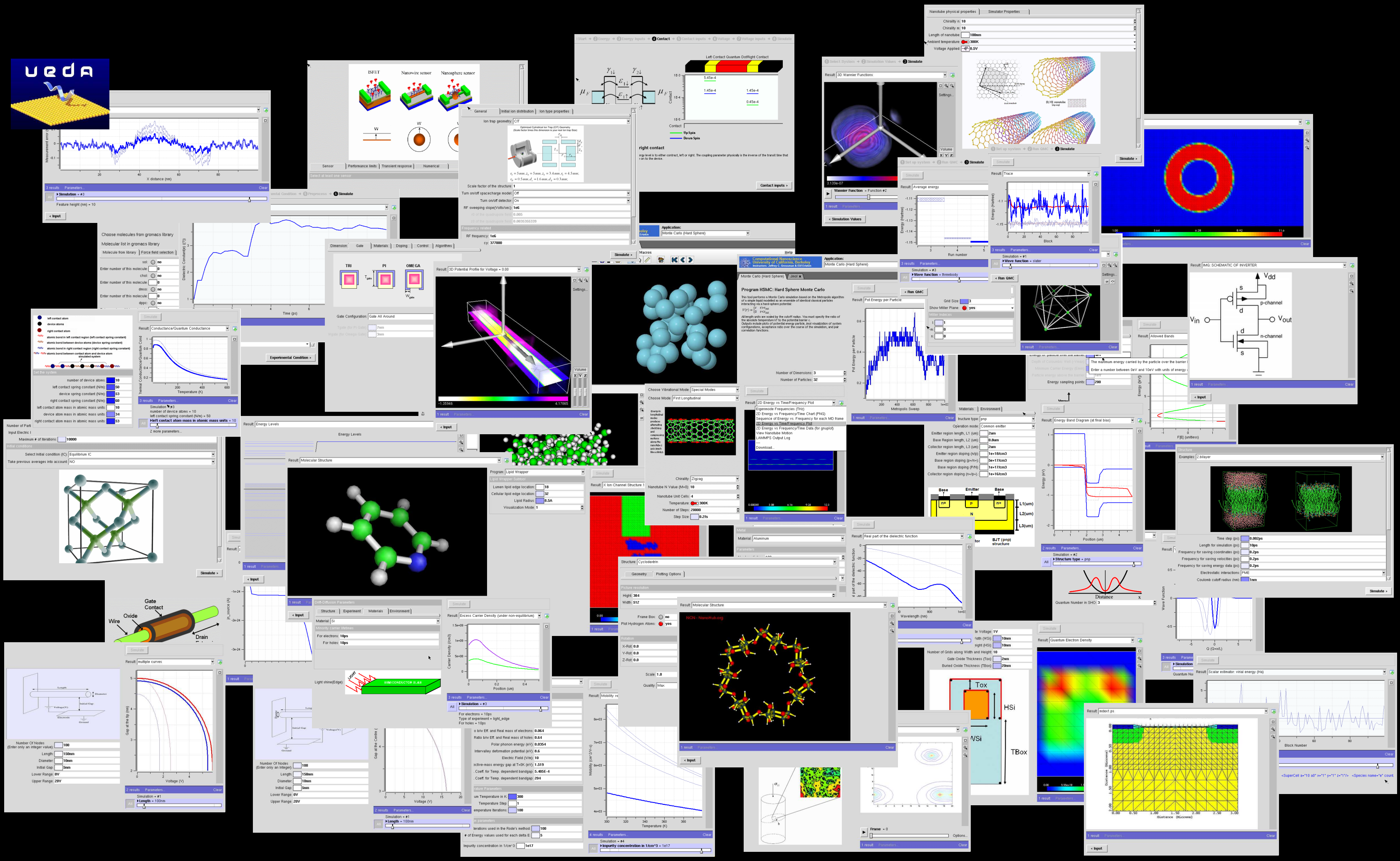
Effect of channel positioning on the 1⁄f noise in silicon-on-insulator metal-oxide-semiconductor

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

Over 120 tools online!

and 57 more coming soon



Rappture Toolkit

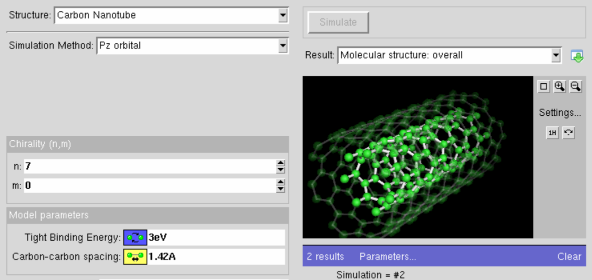
Rappture

+

Simulation Code

Scientist

=



Structure: Carbon Nanotube

Simulation Method: Pz orbital

Chirality (n,m)

n: 7

m: 0

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length in 3-D view: 15

Result: Molecular structure: overall

2 results Parameters... Clear

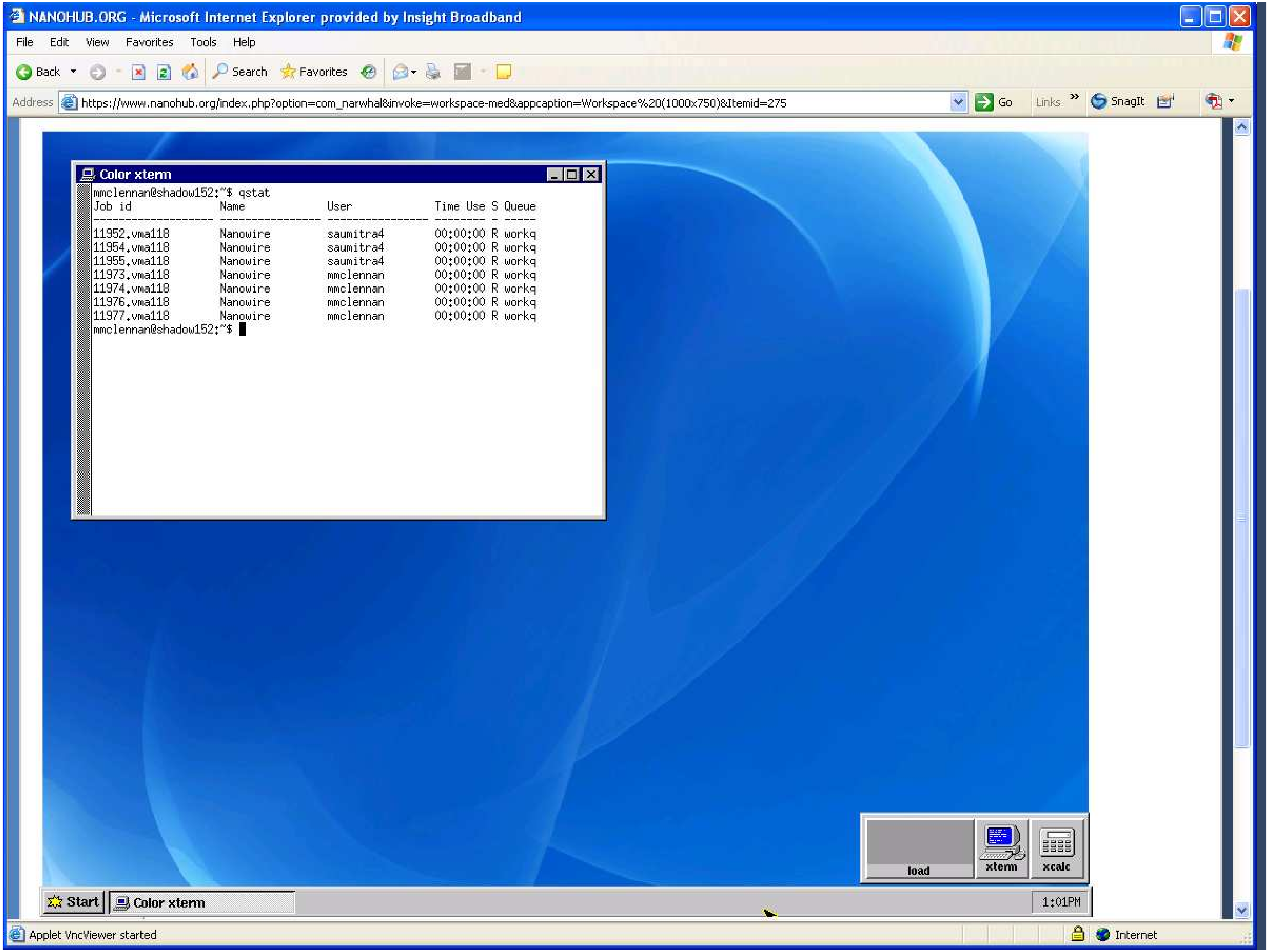
Simulation = #2

m = 0

- Created by NCN in Nov 2004
- Works with your favorite programming language
- Open Source
- Online at http://rappture.org
- Used by 180 projects and 200 developers

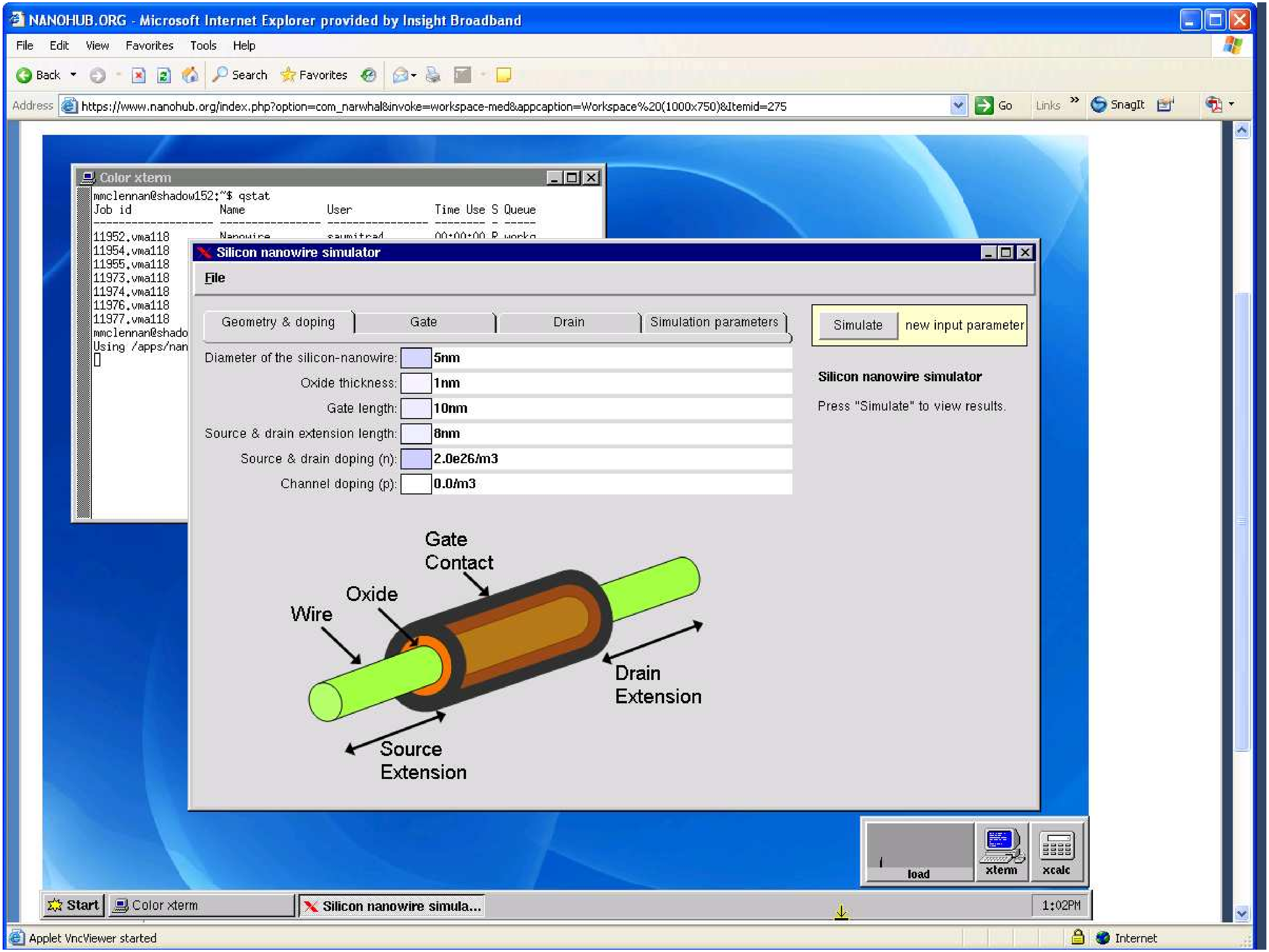
nanoHUB Workspaces

A full-fledged Linux desktop,
as close as your Web browser



Address: https://www.nanohub.org/index.php?option=com_narwhal&invoke=workspace-med&appcaption=Workspace%20(1000x750)&Itemid=275

```
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
11973.vma118        Nanowire         mmclennan        00:00:00 R workq
11974.vma118        Nanowire         mmclennan        00:00:00 R workq
11976.vma118        Nanowire         mmclennan        00:00:00 R workq
11977.vma118        Nanowire         mmclennan        00:00:00 R workq
mmclennan@shadow152:~$ 
```



https://www.nanohub.org/index.php?option=com_narwhal&invoke=workspace-med&appcaption=Workspace%20(1000x750)&Itemid=275

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

Diameter of the silicon-nanowire: 5nm

Oxide thickness: 1nm

Gate length: 10nm

Source & drain extension length: 8nm

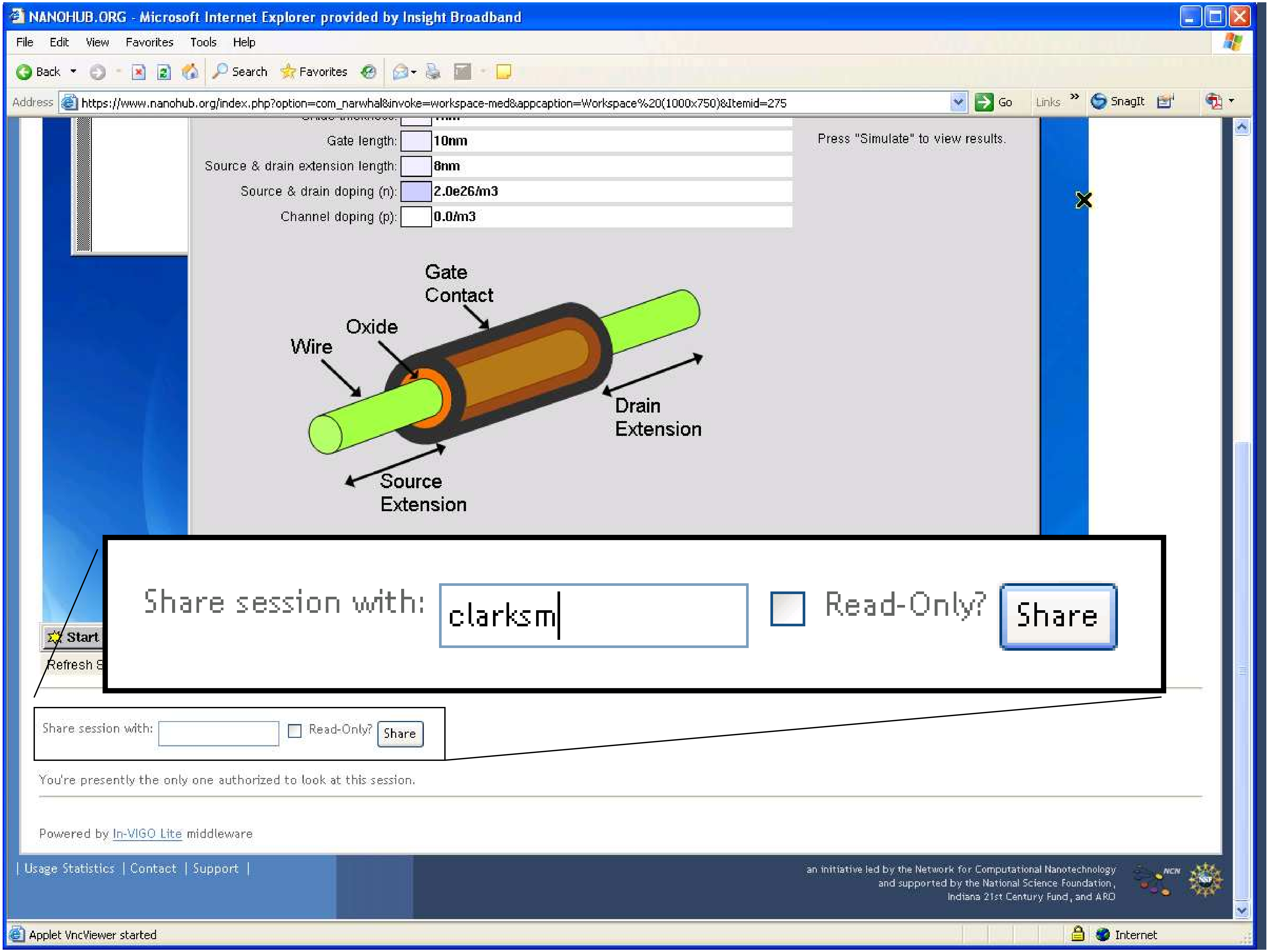
Source & drain doping (n): 2.0e26/m3

Channel doping (p): 0.0/m3

Silicon nanowire simulator

Press "Simulate" to view results.

Applet VncViewer started



NANOHUB.ORG - Microsoft Internet Explorer provided by Insight Broadband

Address: https://www.nanohub.org/index.php?option=com_narwhal&invoke=workspace-med&appcaption=Workspace%20(1000x750)&Itemid=275

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.

Share session with: clarksm ☐ Read-Only?

Share session with: ☐ Read-Only?

You're presently the only one authorized to look at this session.

Powered by In-VIGO Lite middleware

an initiative led by the Network for Computational Nanotechnology and supported by the National Science Foundation, Indiana 21st Century Fund, and ARO

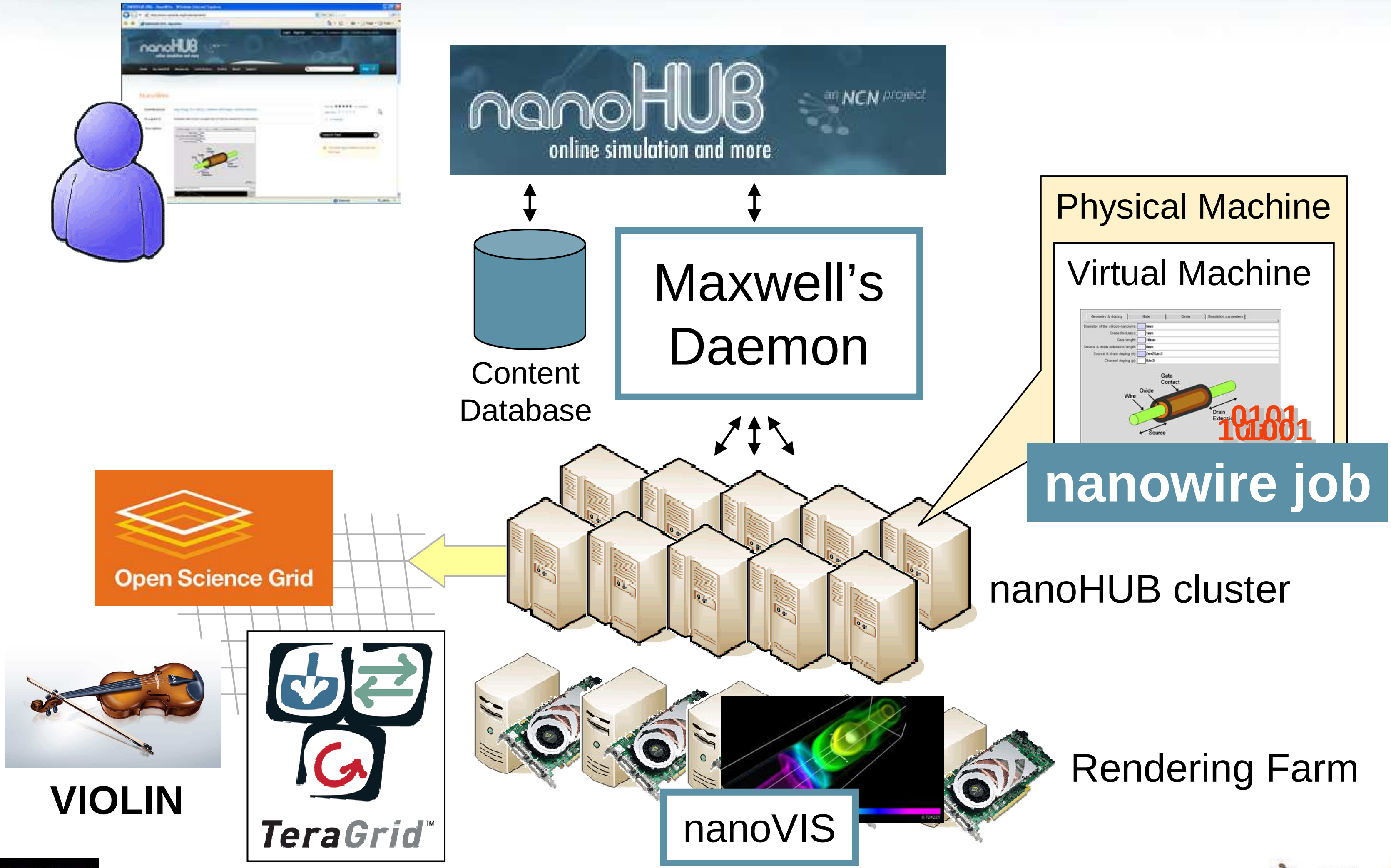
Applet VncViewer started

>1,250

Resources

Upload Your Own Content *anytime*

Cyberinfrastructure for Running Tools



Content Database

Maxwell's Daemon

Physical Machine

Virtual Machine

nanowire job

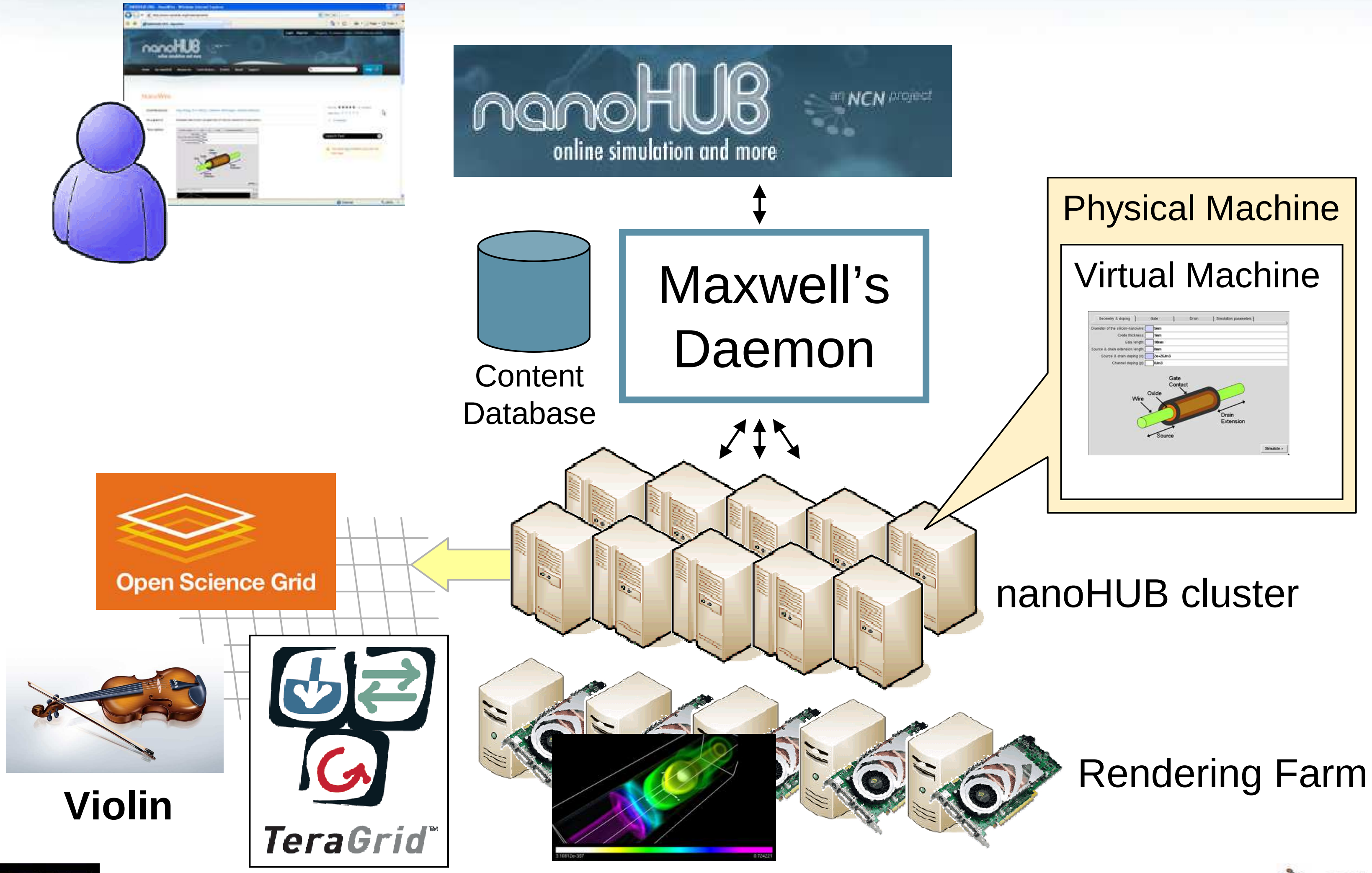
nanoHUB cluster

Rendering Farm

nanoVIS

VIOLIN

Cyberinfrastructure for Running Tools



nanoHUB online simulation and more
an NCN project

Content Database

Maxwell's Daemon

Physical Machine

Virtual Machine

nanoHUB cluster

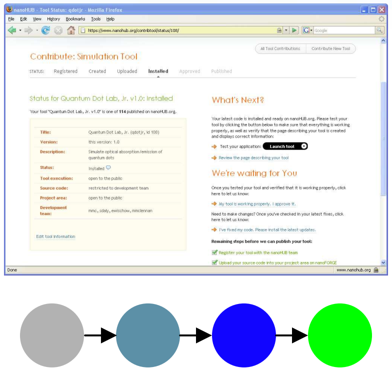
Rendering Farm

Open Science Grid

Violin

TeraGrid™

Other Cyberinfrastructure

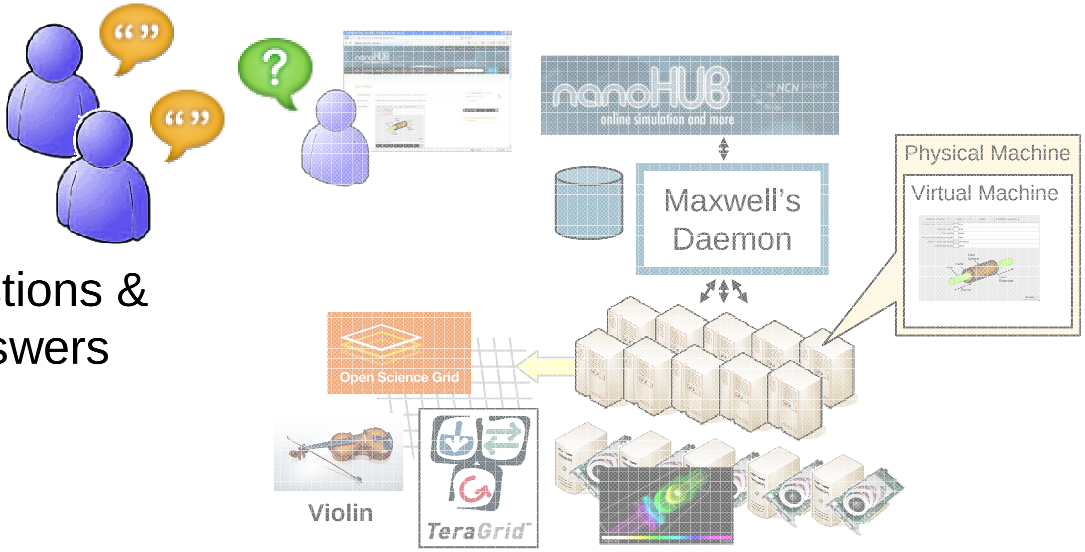


Tool Development

Recommendations

+

Incentive System

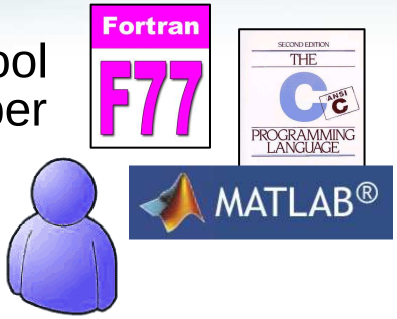


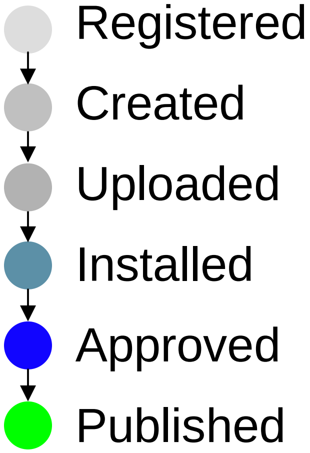
Questions & Answers

Citations & Digital Object Identifiers

Tool Development Framework

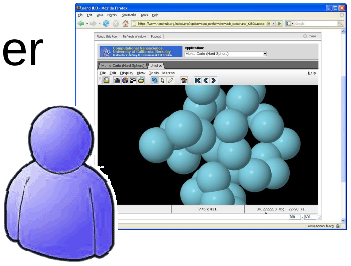
Tool Developer

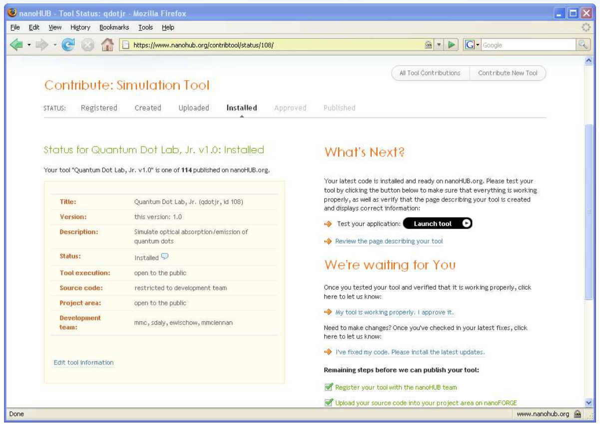




- Registered
- Created
- Uploaded
- Installed
- Approved
- Published

End User





Contribute: Simulation Tool

STATUS: Registered Created Uploaded **Installed** Approved Published

Status for Quantum Dot Lab, Jr. v1.0: Installed

Your tool "Quantum Dot Lab, Jr. v1.0" is one of **114** published on nanoHUB.org.

Title:	Quantum Dot Lab, Jr. (qdotjr, id 108)
Version:	this version: 1.0
Description:	Simulate optical absorption/emission of quantum dots
Status:	Installed
Tool execution:	open to the public
Source code:	restricted to development team
Project area:	open to the public
Development team:	mmc, sdaly, ewischow, mmclennan

Edit tool information

What's Next?

Your latest code is installed and ready on nanoHUB.org. Please test your tool by clicking the button below to make sure that everything is working properly, as well as verify that the page describing your tool is created and displays correct information:

- Test your application: Launch tool
- Review the page describing your tool

We're waiting for You

Once you tested your tool and verified that it is working properly, click here to let us know:

- My tool is working properly. I approve it.

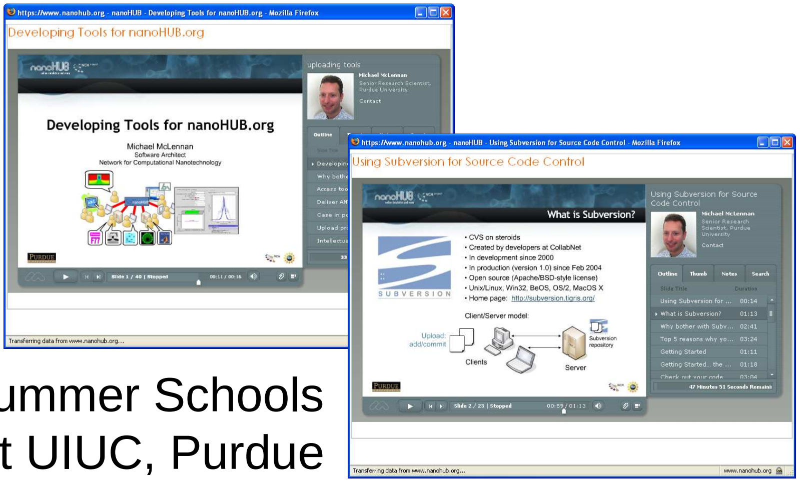
Need to make changes? Once you've checked in your latest fixes, click here to let us know:

- I've fixed my code. Please install the latest updates.

Remaining steps before we can publish your tool:

- ☑ Register your tool with the nanoHUB team
- ☑ Upload your source code into your project area on nanoFORGE

Web-based Publishing System

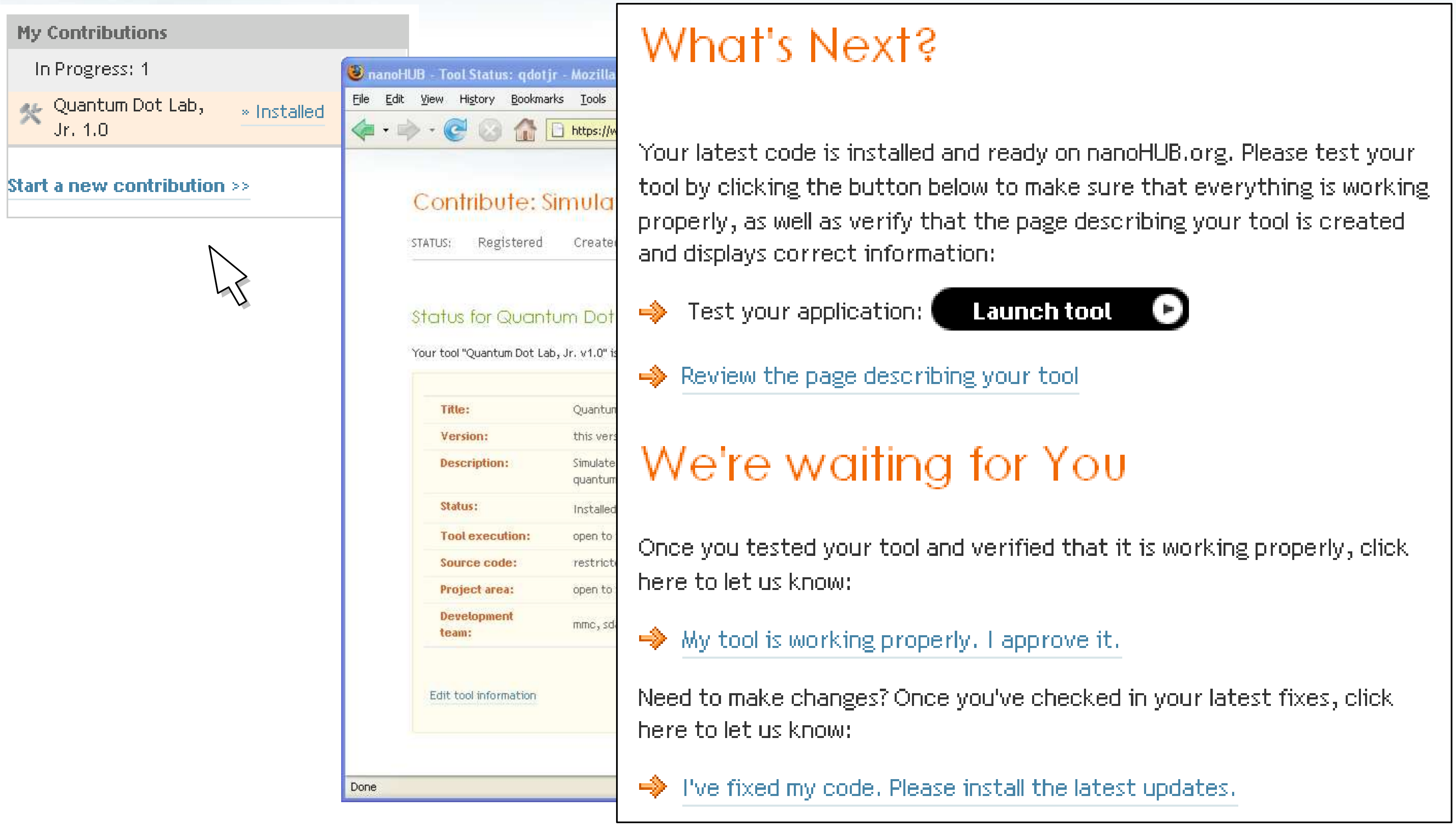


- CVS on steroids
- Created by developers at CollabNet
- In development since 2000
- In production (version 1.0) since Feb 2004
- Open source (Apache/BSD-style license)
- Unix/Linux, Win32, BeOS, OS/2, MacOS X
- Home page: http://subversion.tigris.org/

Slide Title	Duration
Using Subversion for …	00:14
What is Subversion?	01:13
Why bother with Subv…	02:41
Top 5 reasons why yo…	03:24
Getting Started	01:11
Getting Started… the …	01:18
Check out your code	03:04

Summer Schools
at UIUC, Purdue
Online seminars

Web-based Publishing System



My Contributions

In Progress: 1

Quantum Dot Lab, Jr. 1.0 » Installed

Start a new contribution >>

Contribute: Simula

STATUS: Registered Create

Status for Quantum Dot

Your tool "Quantum Dot Lab, Jr. v1.0" i

Title: Quantum

Version: this vers

Description: Simulate quantum

Status: Installed

Tool execution: open to

Source code: restricte

Project area: open to

Development team: mmc, sd

Edit tool information

What's Next?

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➾ Review the page describing your tool

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Need to make changes? Once you've checked in your latest fixes, click here to let us know:

➾ I've fixed my code. Please install the latest updates.

Usage since April 2007

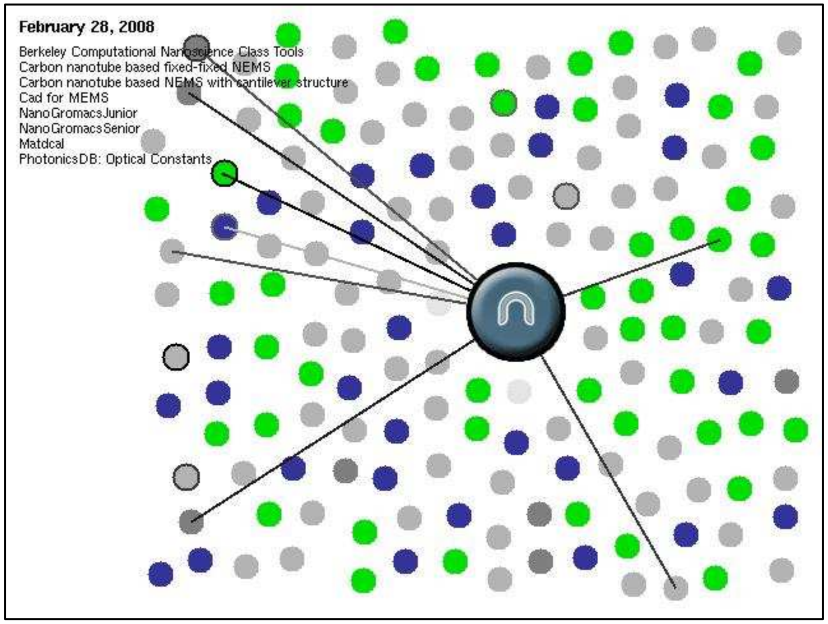
199 Projects

During the past year…
110 Active Projects

89 Active Developers

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

State changes they made:	459
State changes we helped with:	474
TOTAL:	933



[Time Development for One Tool >>]

[Time Development for All Tools >>]

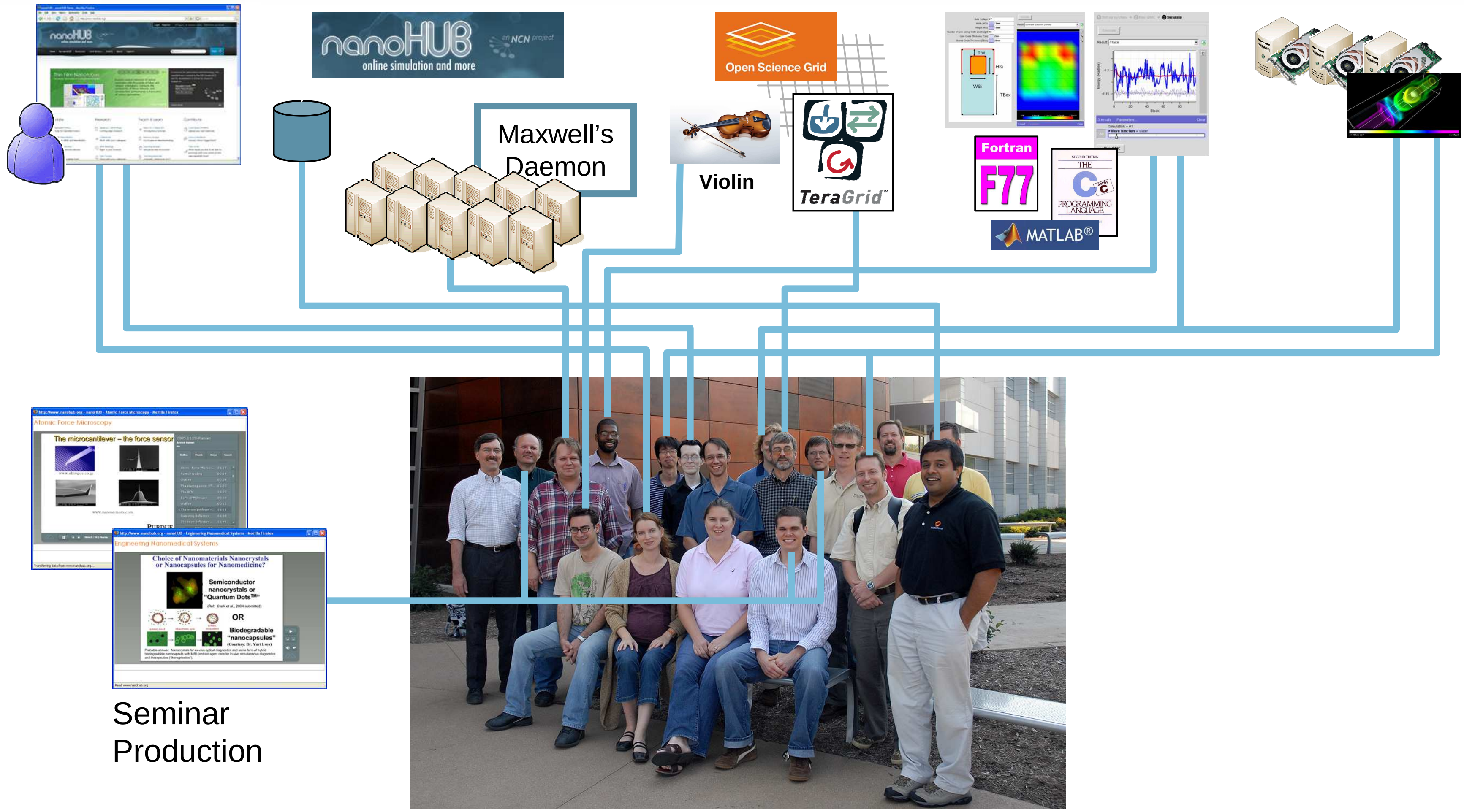
Automated Infrastructure is Easy to Manage

0.5 FTE
Managing Tool Contributions

nanoHUB Team

Wide Range of Expertise

Web Databases Hardware Middleware Grid Computing Scientific Applications Visualization

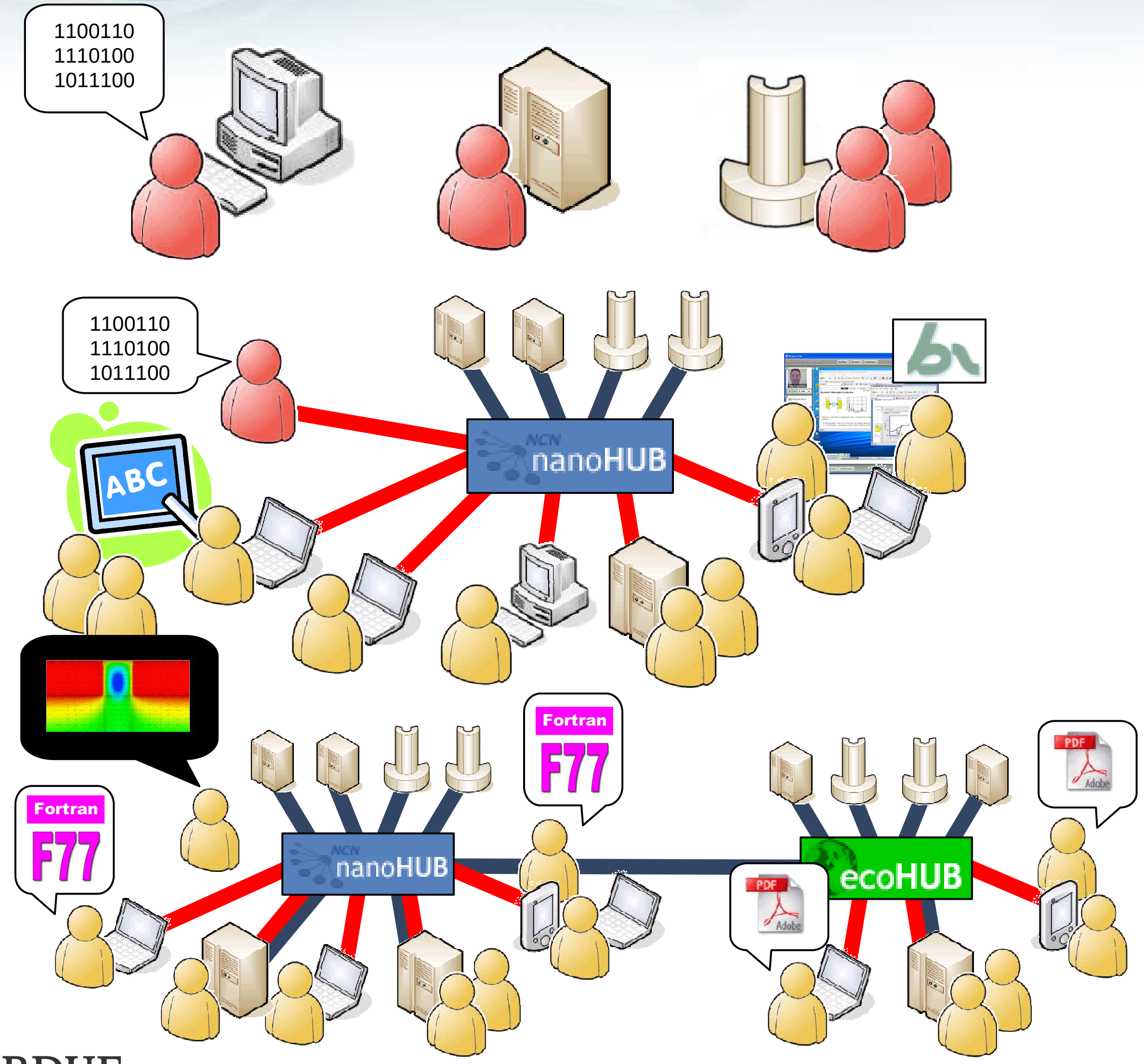


Maxwell's Daemon

Violin

Seminar Production

Evolution of Scientific Computing



Scientific & HPC Computing

few users with specialized knowledge

Science Gateways

cyberinfrastructure, more users

Cyber Communities

ecosystem, users support each other

New Hubs Online Now

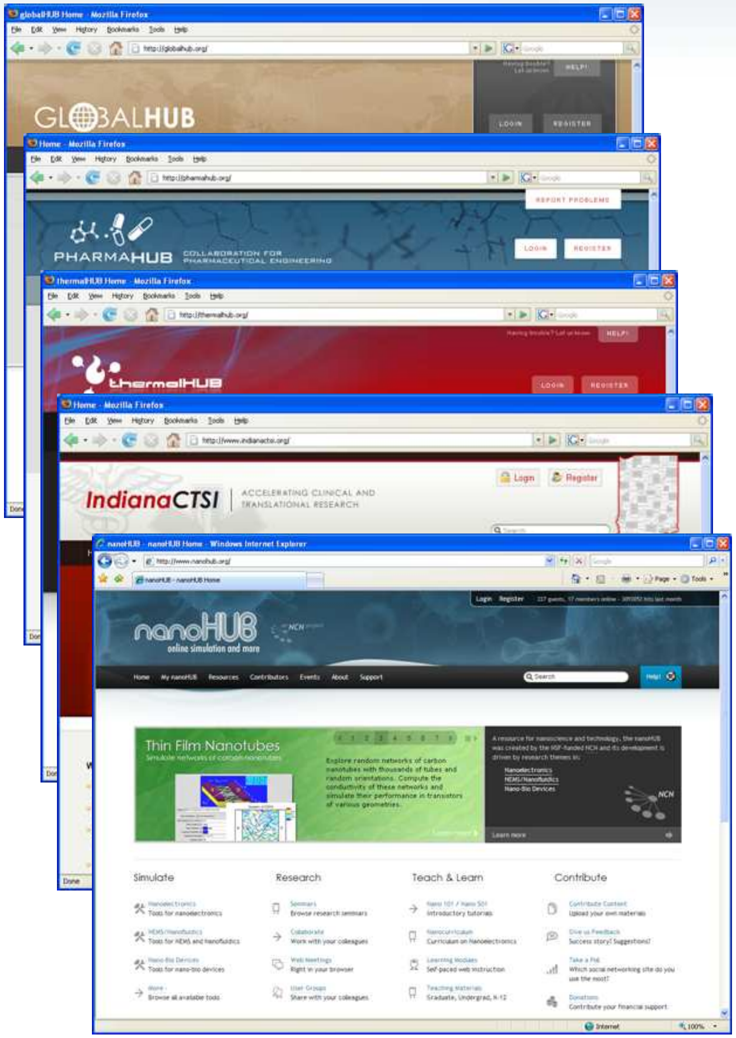
GlobalHUB.org – Dan Hirleman, ME at Purdue
global engineering education
online since 12/17/2007

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

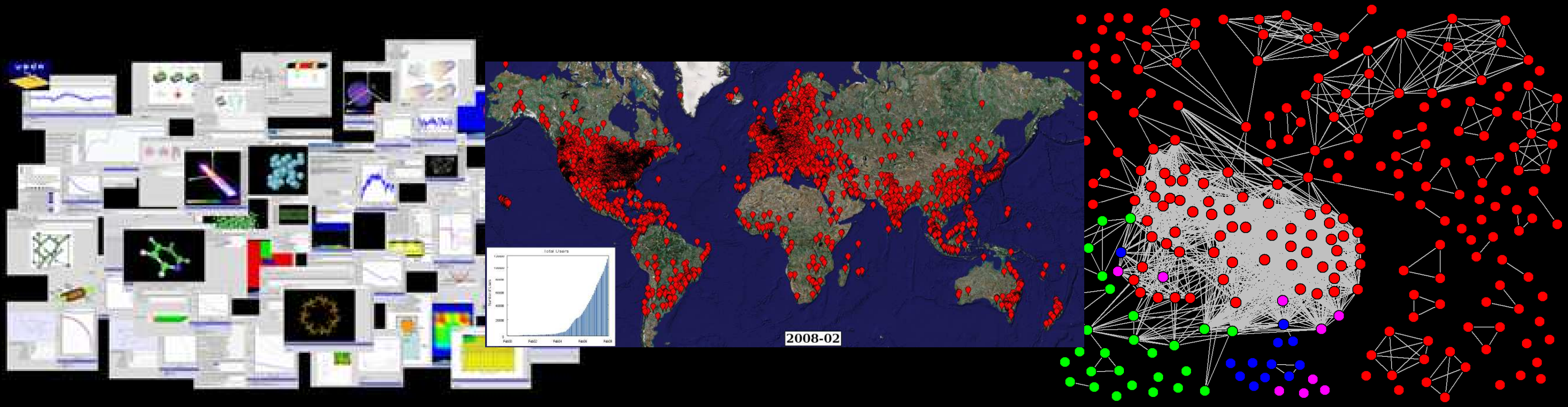
IndianaCTSI.org – Anantha Shekhar, IU School of Medicine, Connie Weaver at Purdue
accelerating clinical and translational research in healthcare
online since 10/1/2007

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



Changing...

- the sharing of information
- expectations of experimentalists/educators
- the pace of tool deployment
- the face of cyberinfrastructure



A global following