

Using the HUBzero™ Platform for Scientific Computing

Michael McLennan
Senior Research Scientist and Hub Software Architect
Rosen Center for Advanced Computing
Purdue University

Why Cyberinfrastructure?



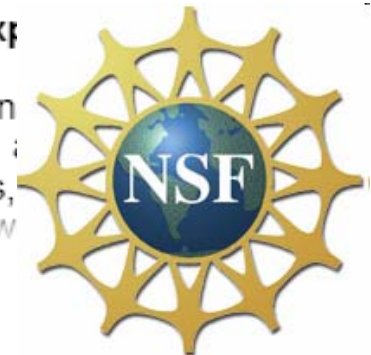
Title: Center for Genomic Studies on Mental Disorders (U24)

Request for Applications (RFA) Number: RFA-MH-08-100

Center will function as a single, national resource. A new critical feature of the Center will be the development of a genomic **cyberinfrastructure** that represents the coordinated aggregate of software, hardware, and communication technologies, as well as human expertise, required to support current and future discoveries in the study of mental disorders. This cyberinfrastructure will integrate relevant and often disparate genetic and genomic resources to provide a useful, usable, and enabling framework for human genetic research and

2. Educational Opportunities Using **Cyberinfrastructure** and Virtual or Mixed Reality (Exp)

Applications of networked computing and communication, sophisticated user input, and dynamic environments have only begun to realize the potential benefit of these new technologies to improve, enhance, and transform education. Many innovative projects in cyberlearning, virtual environments and laboratories, visualization, and tutoring systems have required the development of new technology. How



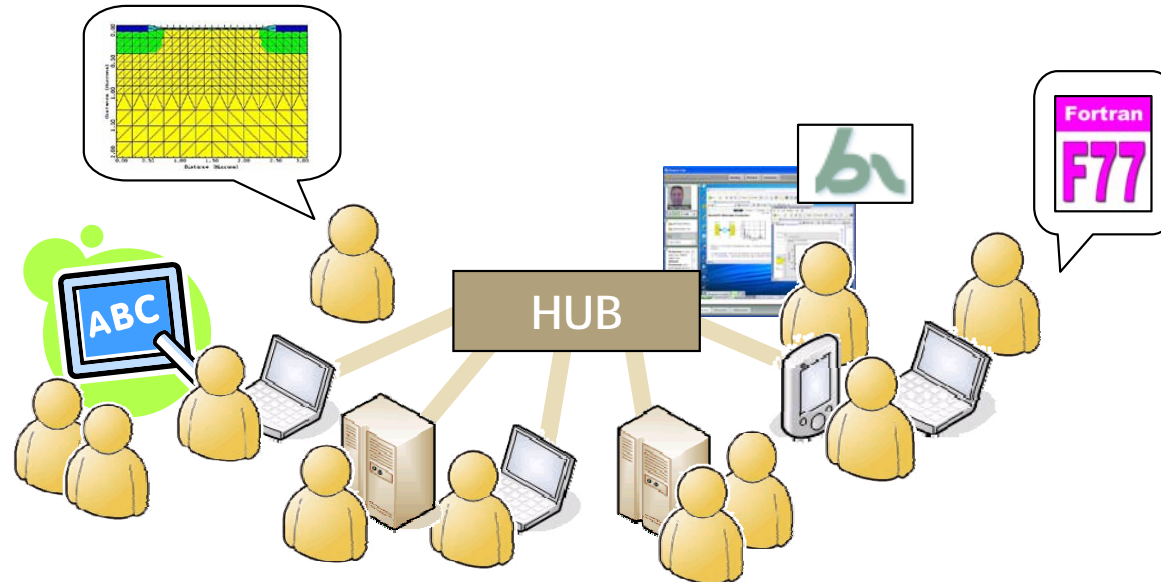
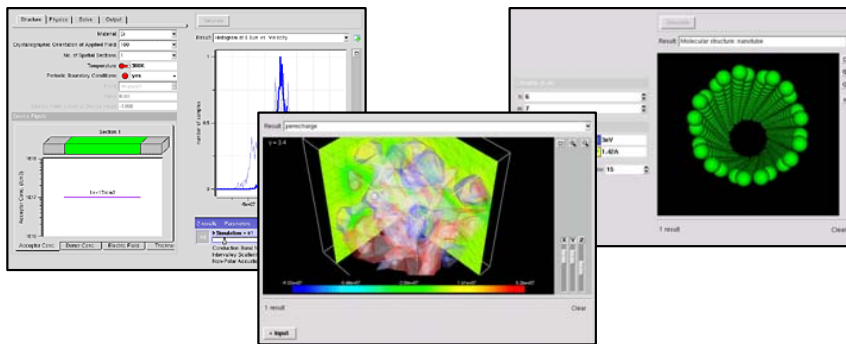
- Supporting the acquisition and development of instrumentation that contributes to, or takes advantage of, existing investments in **cyberinfrastructure**, while avoiding duplication of services already provisioned by NSF investments. Please consult the NSF document, "Cyberinfrastructure

across the United States. It should have known expertise in the targeted program areas of interdisciplinary graduate education and professional development. It is also expected that the lead institution will have known expertise in the IT field, developing and maintaining **cyber-communities** and communication modes, and in addressing the needs of the community the Resource Center is meant to support.

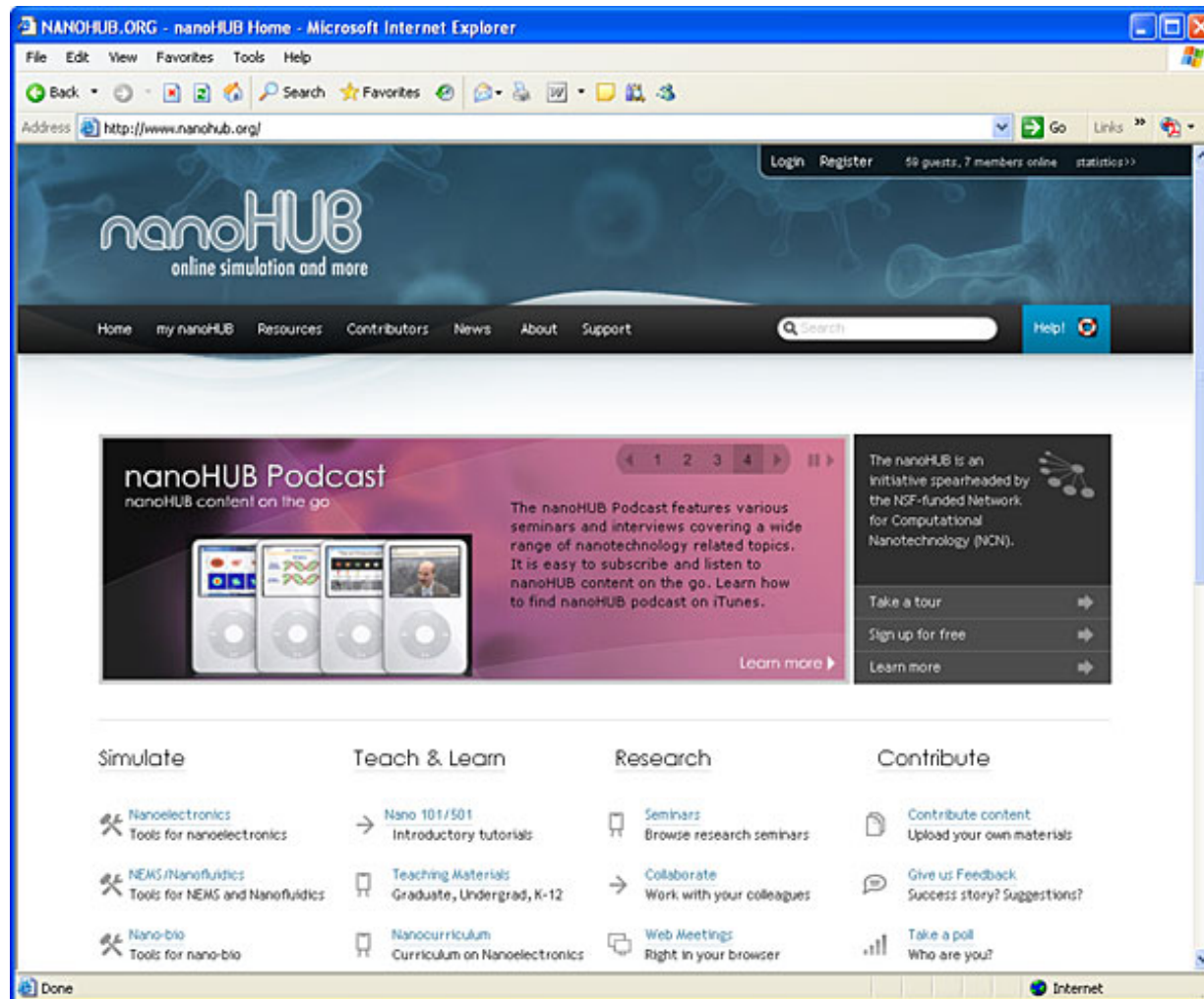
Cyberinfrastructure = HUB

Online simulation...

...and more!



Example: nanoHUB.org

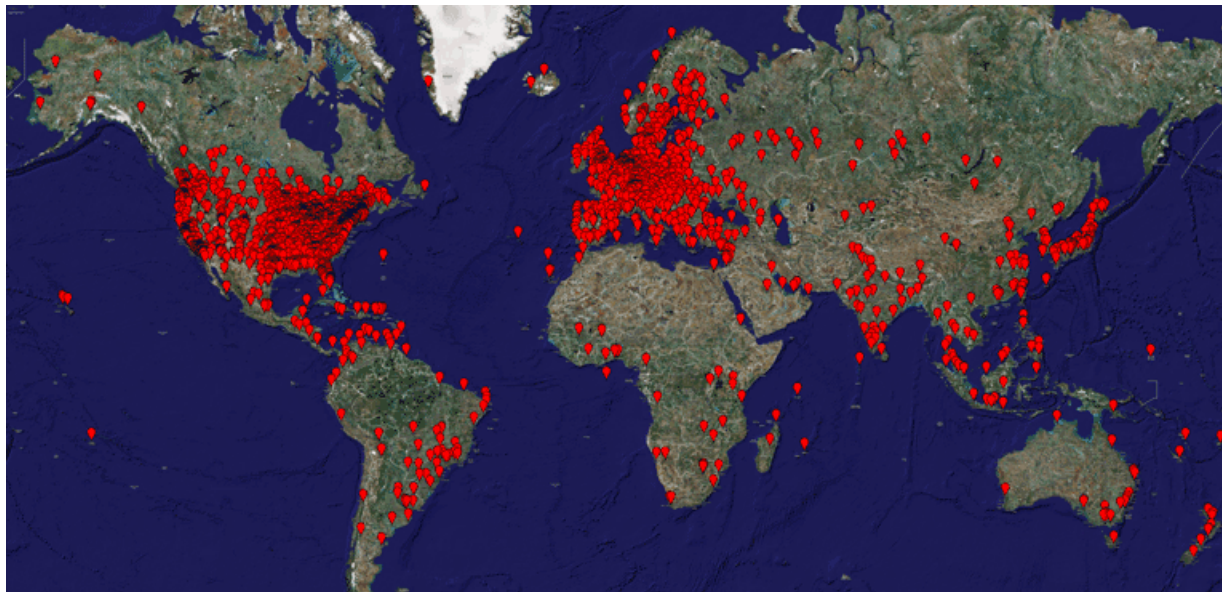
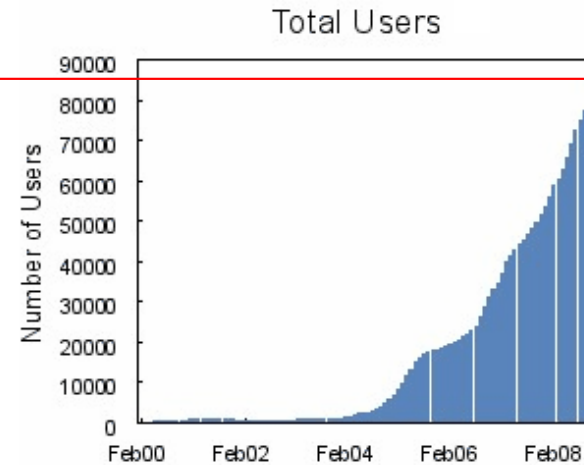


[demo >>](#)

nanoHUB Usage Statistics

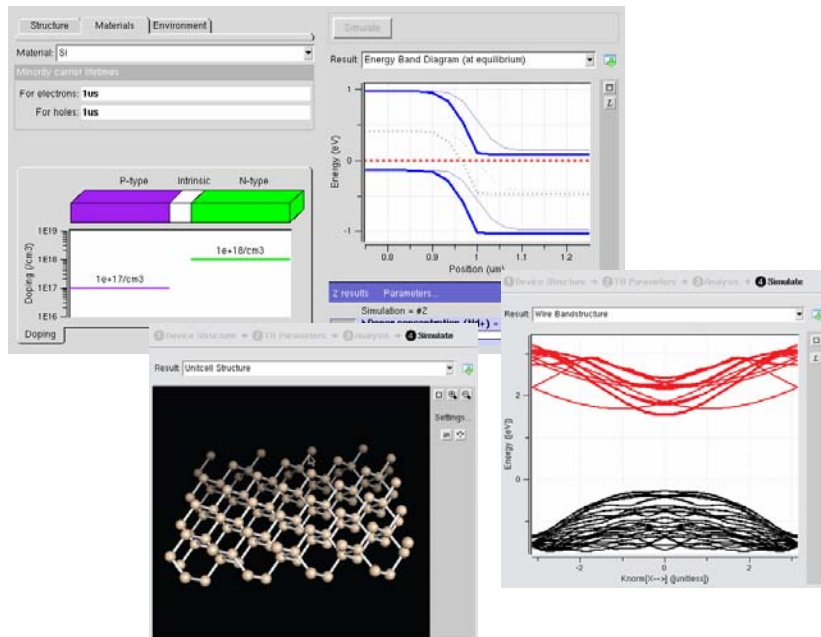
85,184 users worldwide

- >5,000,000 hits/month
- All Top 50 US Engr Schools
- 14% of all .edu domains
- 333 International Ed Institutions
- 233 US K-12 schools



Supporting Education

ECE 612 Nanoscale Transistors (Fall 2006)

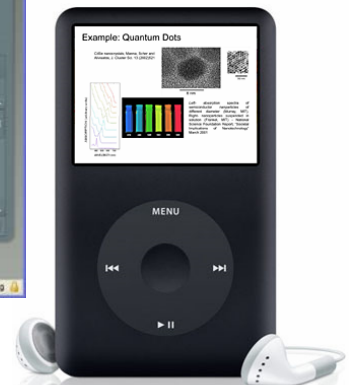
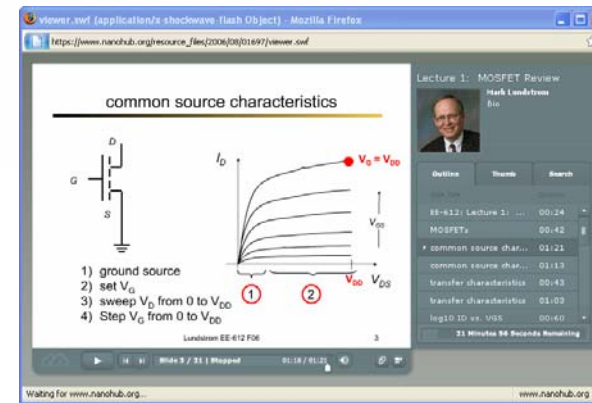


Simulation tools:

- Demonstrations in class
- Homework assignments
- Class projects

Contributor(s) [Mark Lundstrom](#)
Purdue University, West Lafayette

Abstract **Please Note:** An updated version of this course is in production for the physics of advanced transistors



Teaching Materials:

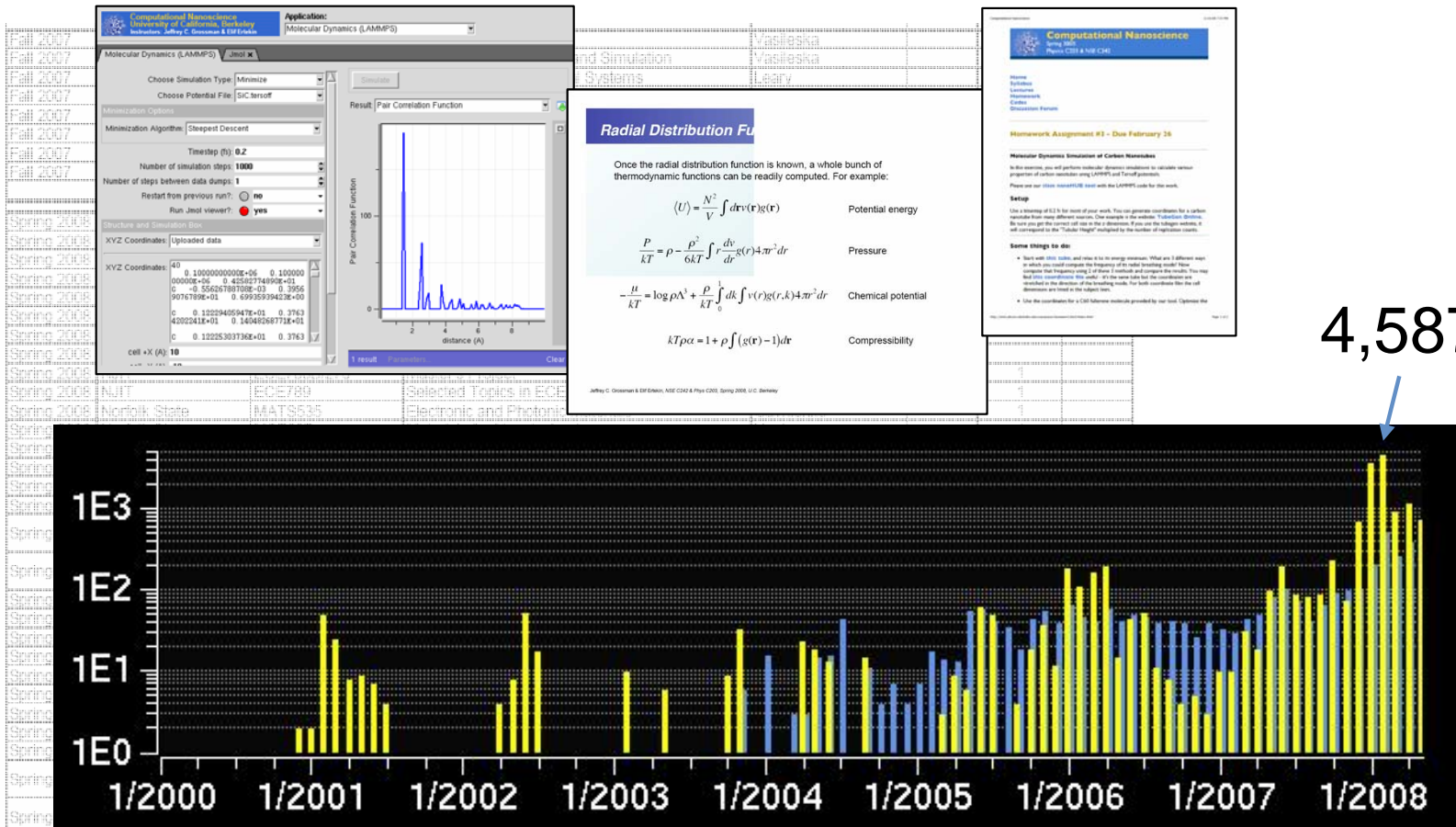
- Complete courses
- Tutorials and Podcasts
- Homework assignments

44 classes at 18 institutions

Fall 2007	Arizona St.	EEE434/591	Quantum Mechanics	Vasileska		1	
Fall 2007	Arizona St.	EEE533	Semiconductor Devices and Simulation	Vasileska		1	
Fall 2007	Purdue	BME695N	Engineering Nanomedical Systems	Leary		1	
Fall 2007	Purdue	ME697S	Continuum Mechanics	Koslowski		1	
Fall 2007	Purdue	MSE550	Properties of Solids	Strachan		1	
Fall 2007	Northwestern	CHEM171	Accelerated Inorganic Chemistry	Schatz	1		
Fall 2007	Southern Illinois	ECE593	Nanoelectronic Devices	Ahmed		1	
Fall 2007	Stanford	EE212	VLSI Fabrication Techniques	Plummer	1		
		# of Institutions: 5	# of Courses: 8		# of Instructors: 7	2	6
							8
Spring 2008	Arizona St.	EEE/CSE 101	Introductory Engineering Design	Vasileska	1		
Spring 2008	Arizona St.	EEE352	Properties of Electronic Materials	Ferry	1		
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	UIUC	ECE398JC	Electronic and Photonic Devices	Choquette	1		
Spring 2008	UIUC	ECE498JL	Nanotechnology	Lyding	1		
Spring 2008	NIJIT	ECE417/270	Independent Study	Sosnowski	1		
Spring 2008	NIJIT	ECE700B/270	Master's Project	Sosnowski		1	
Spring 2008	NIJIT	ECE789	Selected Topics in ECEII	Hanafi		1	
Spring 2008	Norfolk State	MAT535	Electronic and Photonic Materials	Gavrilenko	1		
Spring 2008	Norfolk State	MSE607	Materials for Nanotechnology	Noginova	1		
Spring 2008	Norfolk State	PHY580	Quantum Mechanics	Noginov		1	
Spring 2008	Northwestern	CHEM101	General Chemistry	Schatz/Ratner/Hatch	1		
Spring 2008	Northwestern	CHEM102	General Chemistry	Spears/Mirkin/Hatch	1		
Spring 2008	Northwestern	CHEM172	Accelerated General Chemistry	Spears/Hatch	1		
Spring 2008	Northwestern	CHEM342-2 [Section 20]	Quantum Chemistry	Weitz	1		
Spring 2008	Northwestern	CHEM342-2 [Section 21]	Quantum Chemistry	Schatz	1		
Spring 2008	Northwestern	CHEM488	Computational Chemistry	Seideman	1		
Spring 2008	Portland State	ECE416	IC Technologies	Natter	1		
Spring 2008	Portland State	ECE510	Leakage in CMOS Nanometer Technologies	Chiang		1	
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	U. Mass / Amherst	PHY490N	Introduction to Nanotechnology and Nanomanufacturing	Tuominen	1		
Spring 2008	U. Nevada, LV	ECG756	Advanced Topics in Semiconductor Devices II	Das		1	
Spring 2008	U. of Texas, Austin	EE396V	Semiconductor Nanostructures	Tutuc		1	
Spring 2008	Utah	ECE6264	Advanced Silicon Devices	Miller		1	
Spring 2008	Washington/Seattle	EE331	Devices/Circuits I	Amirparviz	1		
Spring 2008	Wright State	PHY640-01	Nanoengineering and Nanoscience	Lok		1	
Spring 2008	Wright State	PHY681	Nanotechnology	Lok		1	
		# of Institutions: 17	# of Courses: 36		# of Instructors: 32	19	17
							36

Table 1.4, NCN Annual Report, 2008

44 classes at 18 institutions

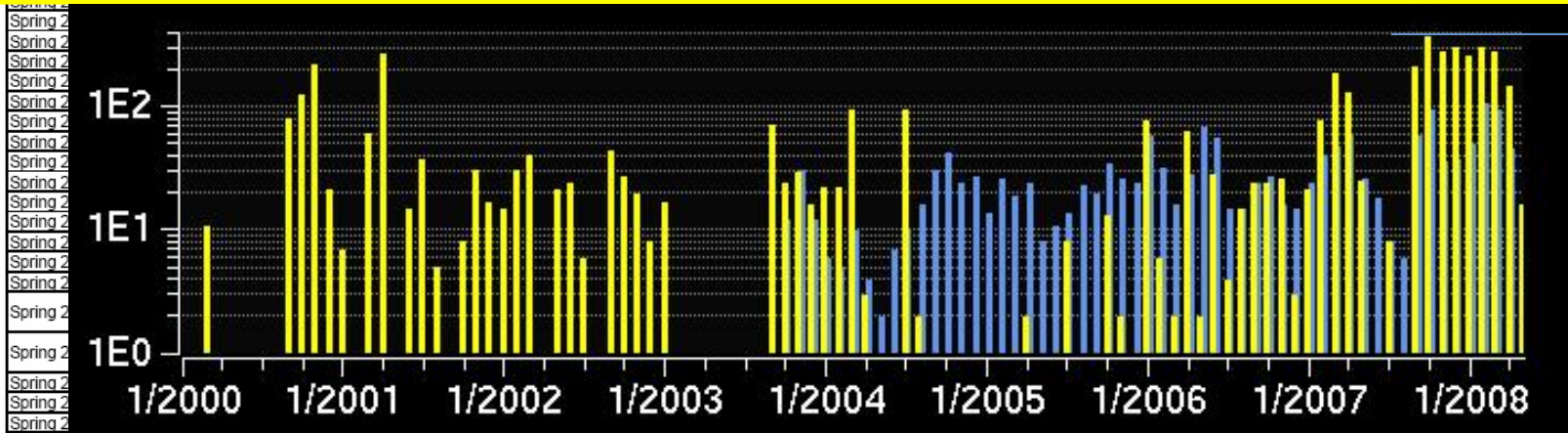


4,587 runs!

Spring 2008	UC Berkeley	PHYC203/NSEC242	Computational Nanoscience	Grossman/Ertekin
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44 classes at 18 institutions

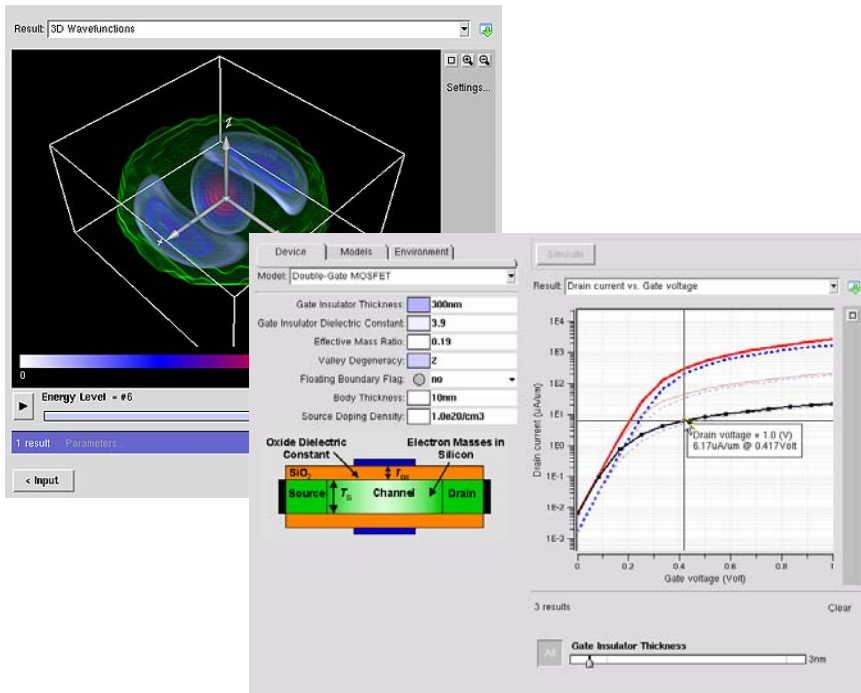
Spring 2008	Arizona St.	EEE/CSE 101	Introductory Engineering Design	Vasileska
Spring 2008	Arizona St.	EEE352	Properties of Electronic Materials	Ferry
Spring 2008	Arizona St.	EE533	Semiconductor Transport	Vasileska



369 runs

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		
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Supporting Research



The video player shows a presentation slide titled "Piezoelectric Transducers: Strain Sensing and Energy Harvesting (and Frequency Tuning)". The slide includes a diagram of a piezoelectric microphone structure with labels: EN1, UF-IMG(B2), Piezoelectric (PZT), Diaphragm (Si), Electrode (Pt or TlPt), and Package (Acrylic). The video player interface shows a search bar and a list of related videos.

- [2] The justification for this value of switching energy in practical present-day circuits can be found e.g. in Mukhopadhyay S, Switching energy in CMOS logic: how far are we from physical limit? Available from <<http://www.nanohub.org/resources/1250//>>.
- [3] Zhirnov VV, Cavin RK, Hutchby JA, Bourjanoff GI. Limits to

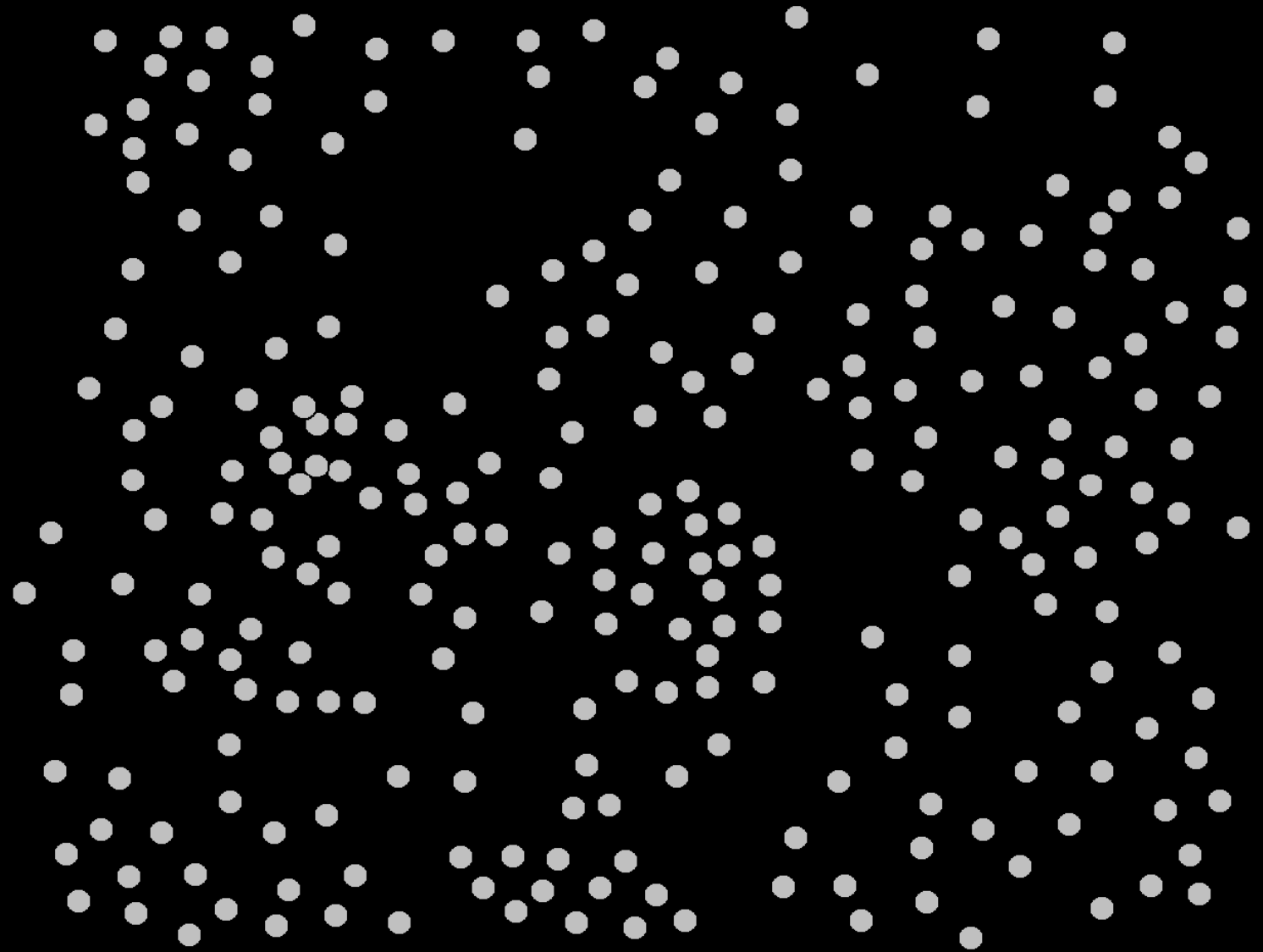
Simulation tools:

- Used by theorists
- Used by experimentalists

Tutorials and Seminars:

- Cutting edge research
- Cited in journal articles
- Preprints and tech pubs

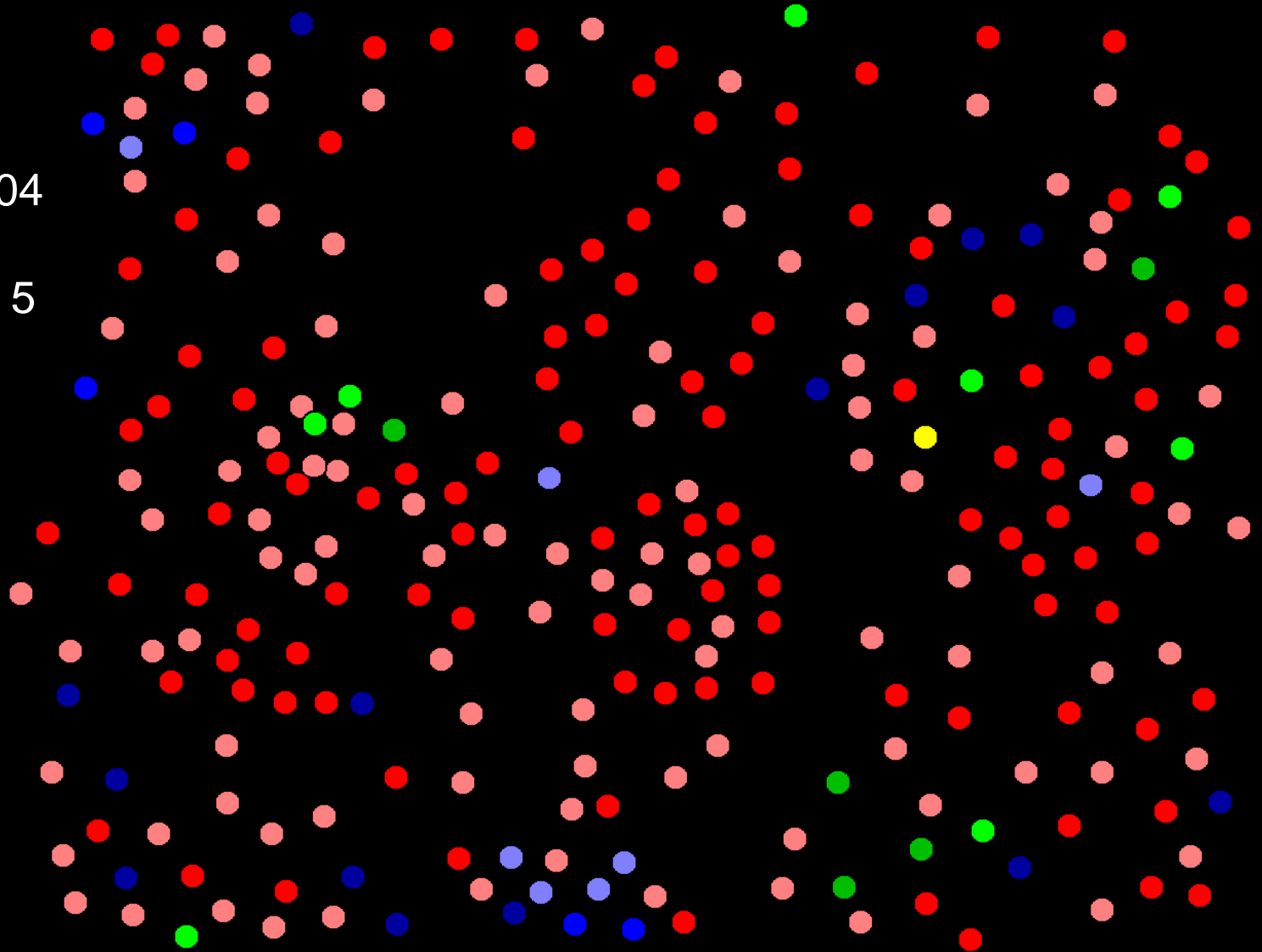
265 Citations



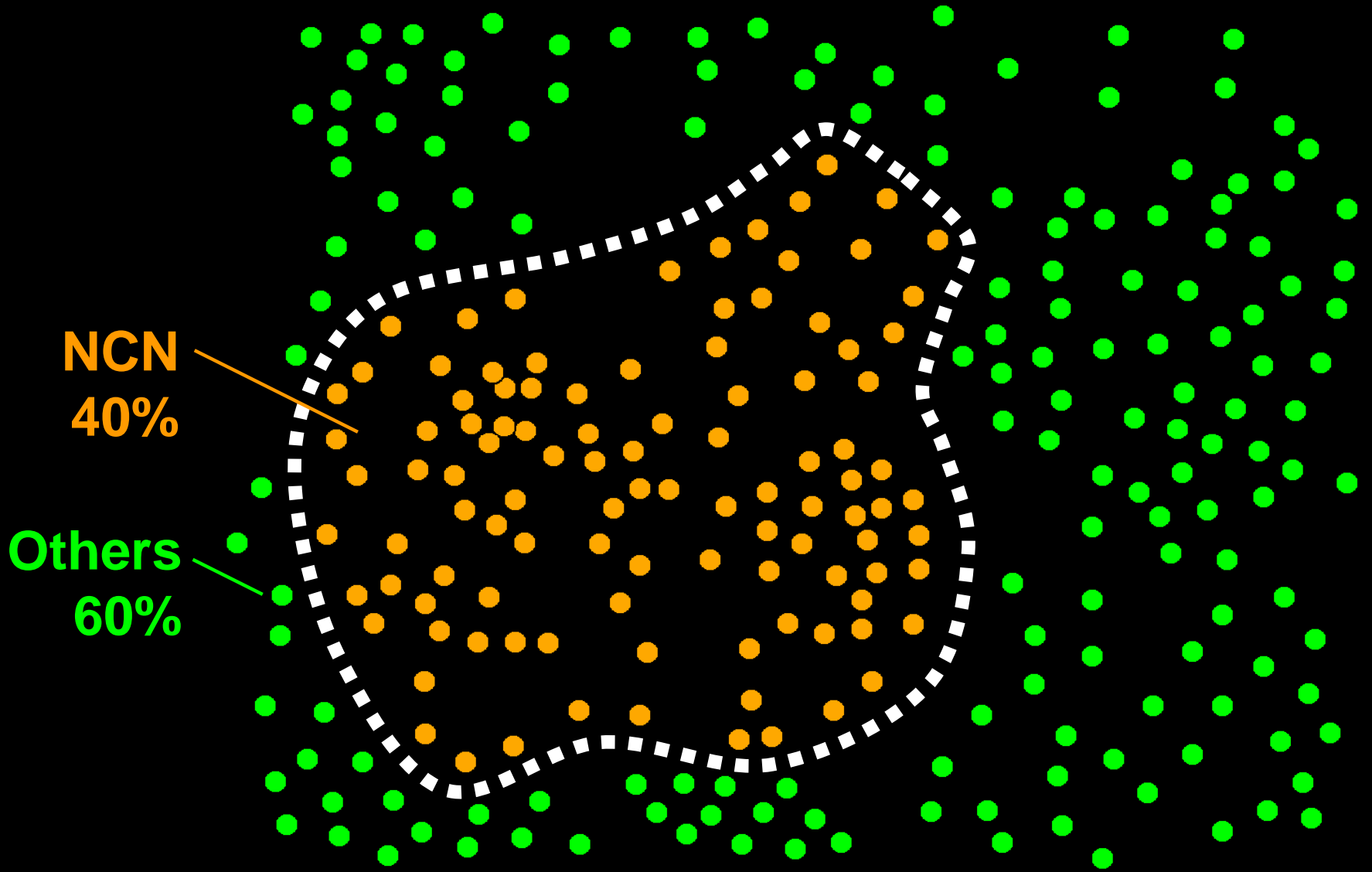
265 Citations... Published where?

● Journals 119
● Proceedings 104
● Ph.D. thesis 8
● Masters thesis 5
● Books 1
89%

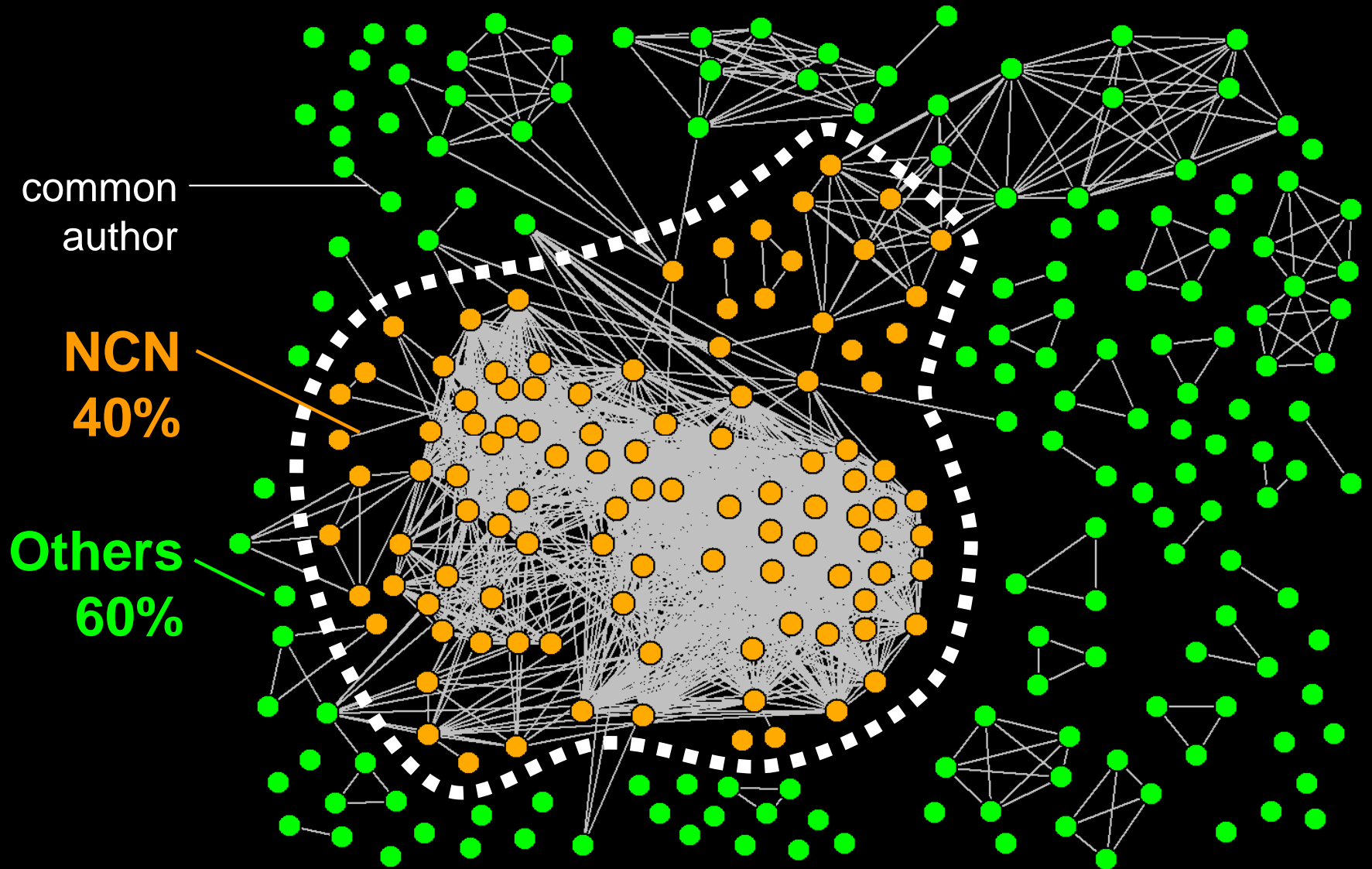
● Conferences 8
● Magazines 5
● TechReps 15
11%



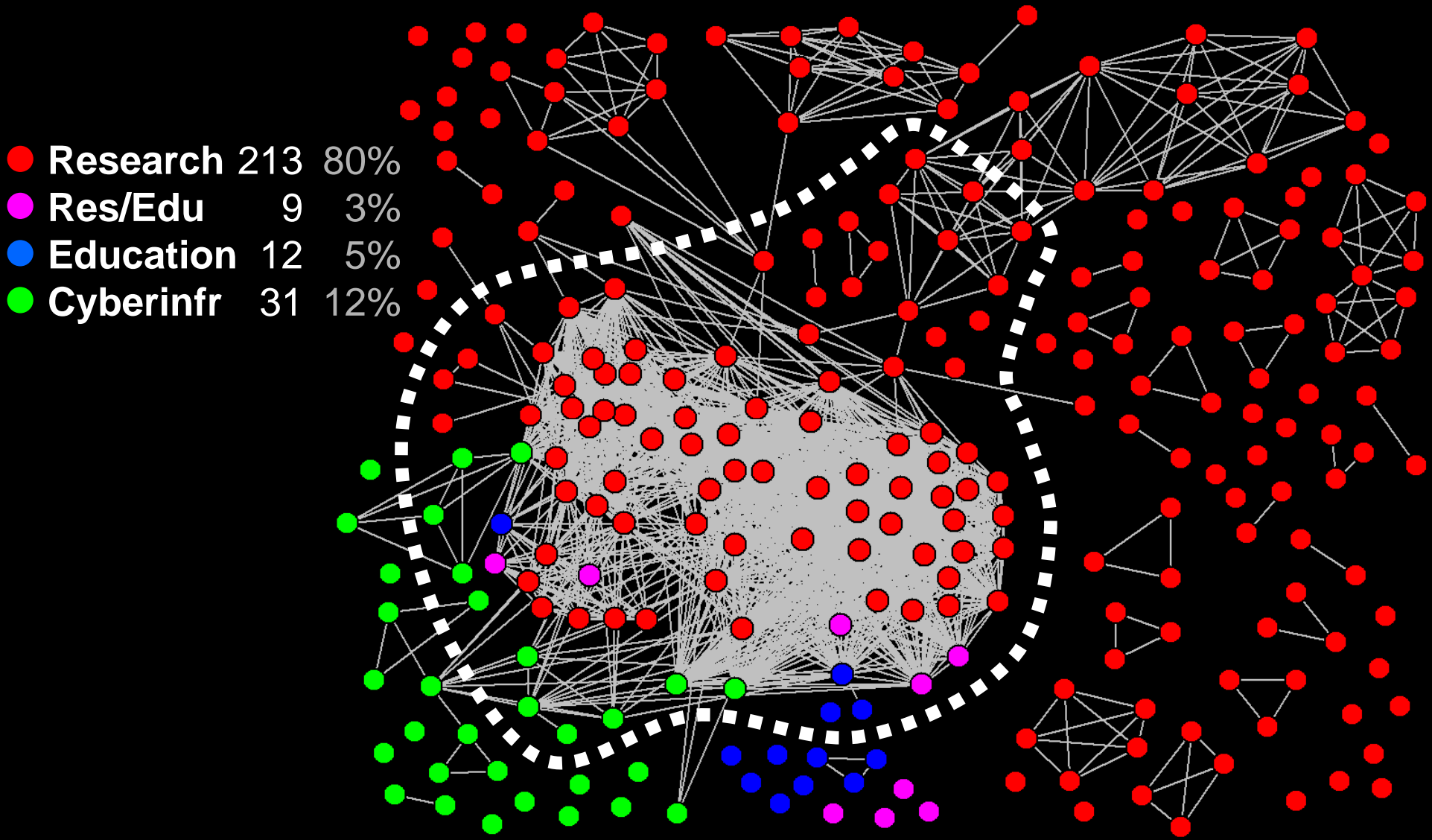
265 Citations... Who?



265 Citations... Who? With whom?



265 Citations... Cited for what?



265 Citations... Examples

Device Physicist
Enrico Sangiorgi
University of Bologna, Italy

Scaling the High-Performance Double-Gate SOI MOSFET down to 32 nm Technology Node with SiO₂-based Gate Stacks

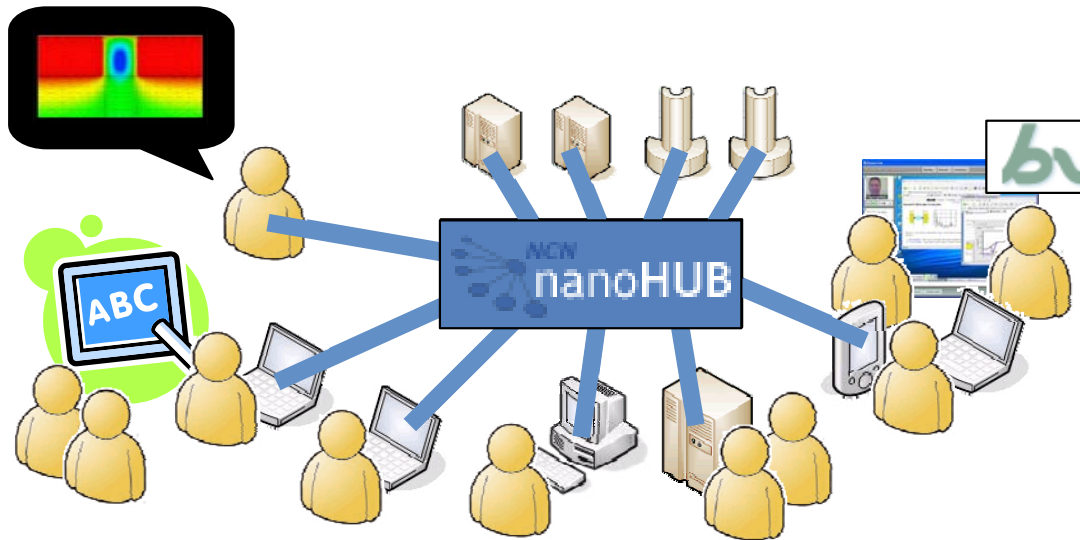
Analysis of Scaling Strategies for Sub-30 nm Double-Gate SOI N-MOSFETs

Electrical characteristics related to silicon film thickness in advanced FD SOI-MOSFETs

Experimentalist
Akiko Ohata
IMEP Minatec, France

Ultra-thin fully-depleted SOI MOSFETs: Special charge properties and coupling effects

General Framework

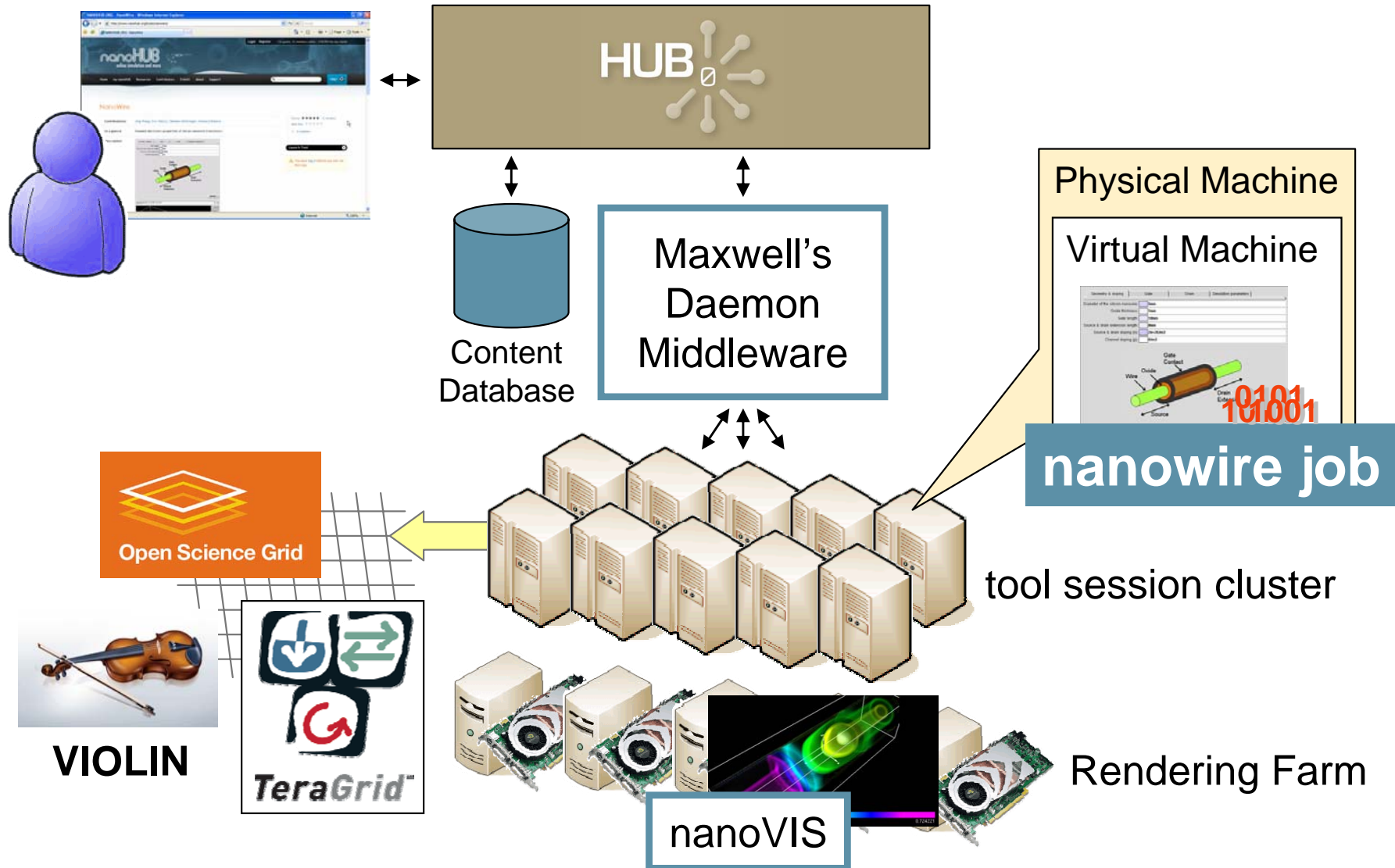


<http://hubzero.org>

What exactly is HUBzero?

- Unique middleware for simulation and modeling
- Content management system for scientists
- Collaboration and social networking

Cyberinfrastructure for Running Tools

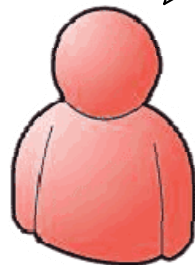


Rappture: Rapid Application Infrastructure

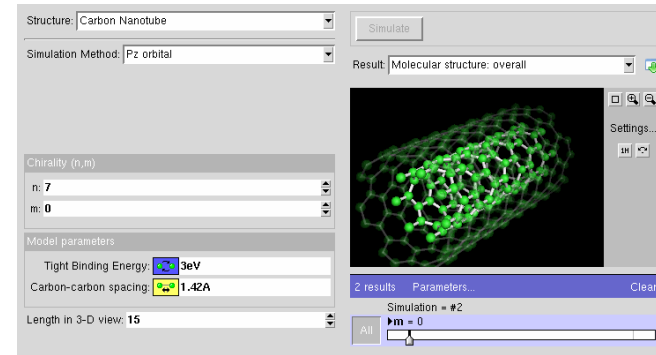
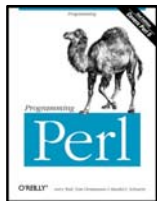
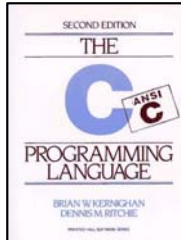
Rappture



Simulation Code



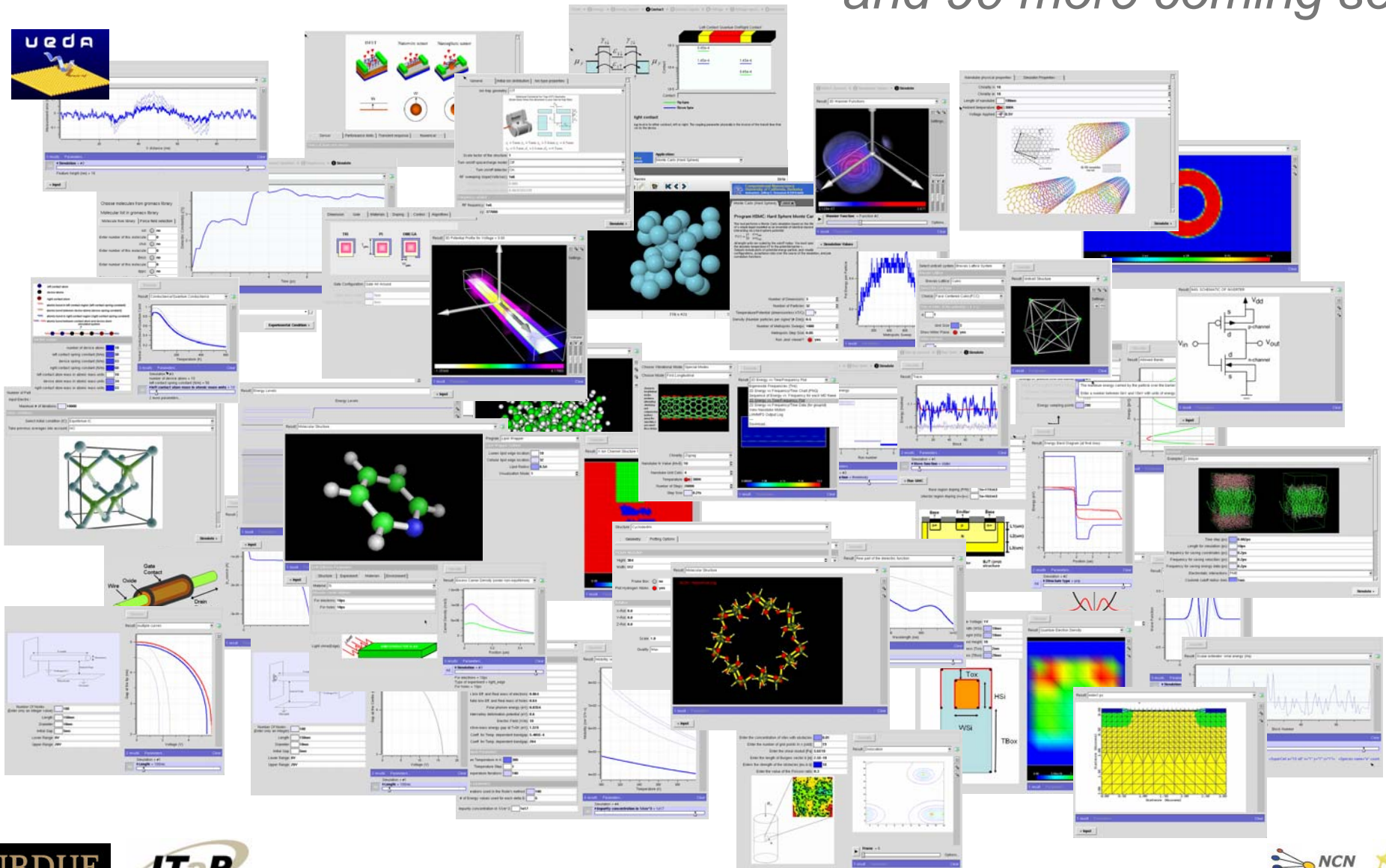
Scientist



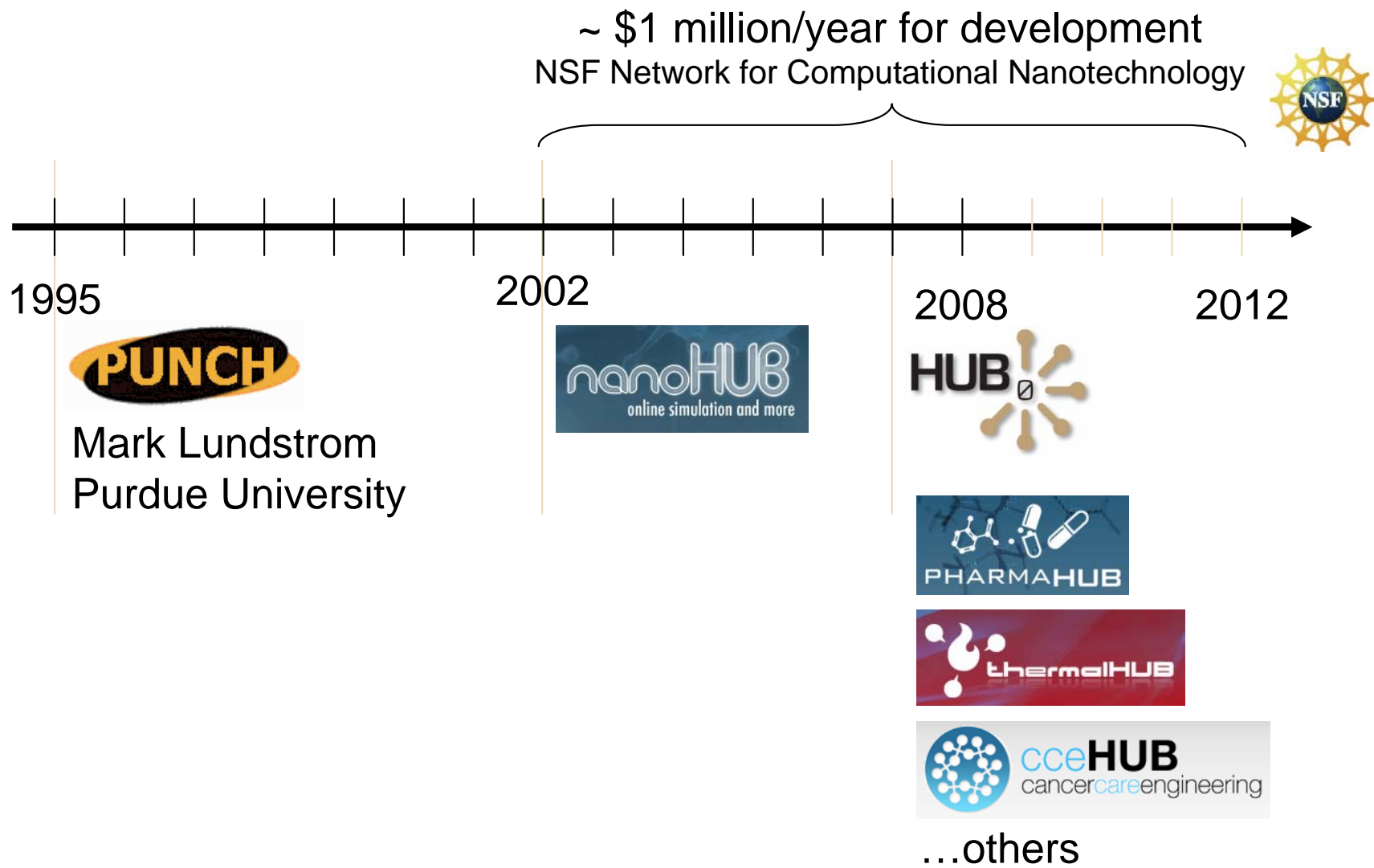
- Created by NCN in Nov 2004
- Works with your favorite programming language
- Open Source
- Online at <http://rappture.org>
- Used by 180 projects and 200 developers

Over 125 tools online!

and 90 more coming soon



Leveraging the Platform



New Hubs Online

IndianaCTSI.org – Anantha Shekhar, IUPUI
clinical and translational research in healthcare
online since 10/1/2007 with 1,434 visitors

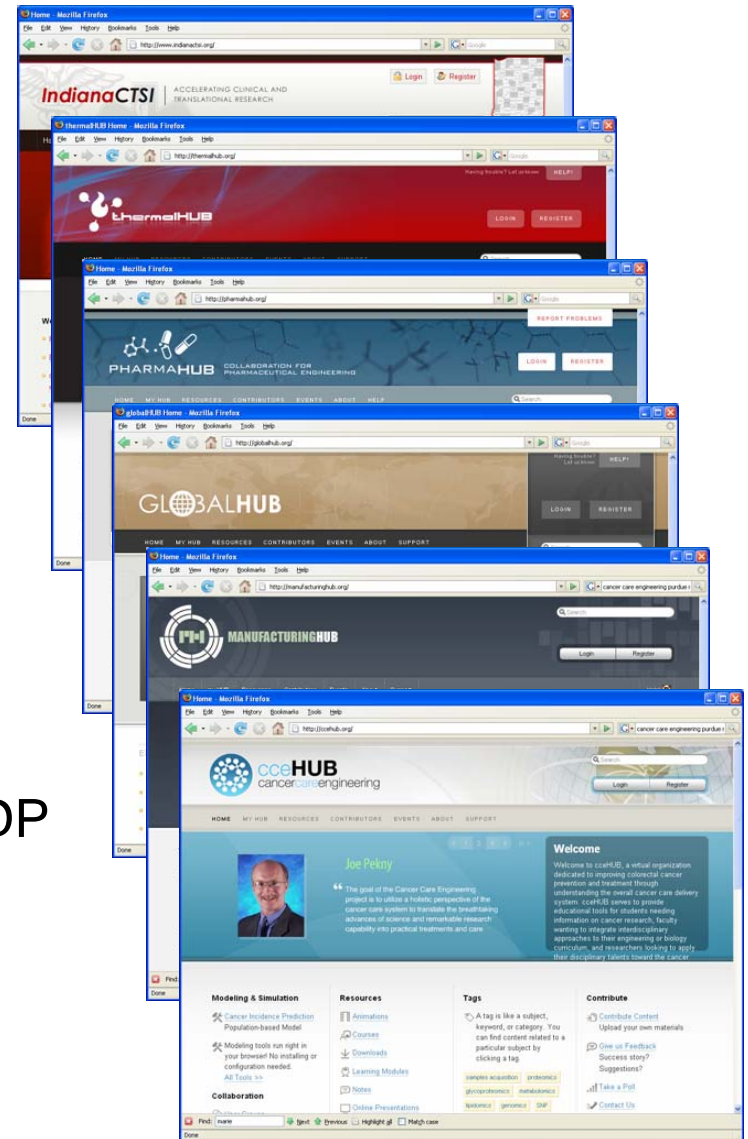
thermalHUB.org – Tim Fisher, ME Purdue
heat transfer
online since 12/6/2007 with 4,029 visitors

pharmaHUB.org – Rex Reklaitis, ChE Purdue
pharmaceutical product development and manufacturing
online since 12/11/2007 with 1,411 visitors

GlobalHUB.org – Dan Hirleman, ME Purdue
global engineering education
online since 12/17/2007 with 686 visitors

manufacturingHUB.org – John Sullivan, Purdue DP
advanced manufacturing techniques
online since 5/30/2008

cceHUB.org – Marietta Harrison, Purdue DP
cancer care engineering
online since 6/11/2008



How do I set up my own Hub?

Service offered by the
Hub Technology Group in the
Rosen Center for Advanced Computing



Dell 1950 server
750GB storage
16GB RAM

Hardware	\$6,000
Data backups	\$7,500
6 weeks setup	\$12k
6 weeks maintenance/year	\$12k
First year	\$25,653
Each additional year	\$12,911

+ indirect costs ~\$58,800 for 1 year
~\$78,500 for 2 years
~\$98,200 for 3 years

“Starter” Hub:
200 simultaneous tool sessions
Thousands of active browsers
500 users with 1GB storage

details at
hubzero.org

HUBzero is changing the way science is done

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



<http://hubzero.org>

