

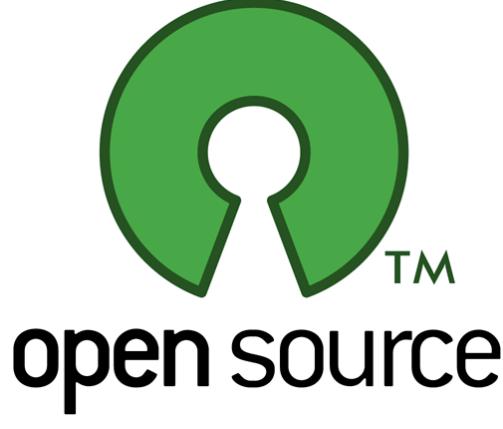
The HUBzero Platform for Scientific Collaboration

Michael McLennan

Director, HUBzero® Platform for Scientific Collaboration

Purdue University

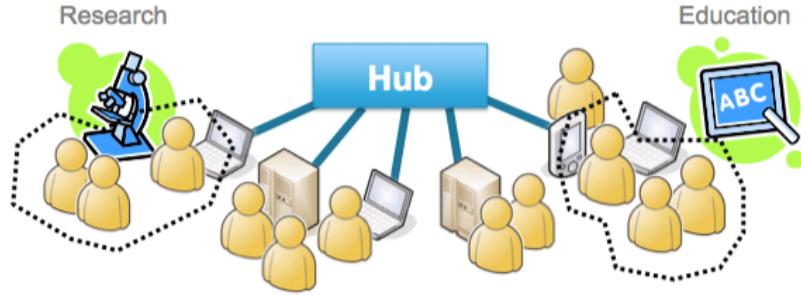
What is HUBzero?



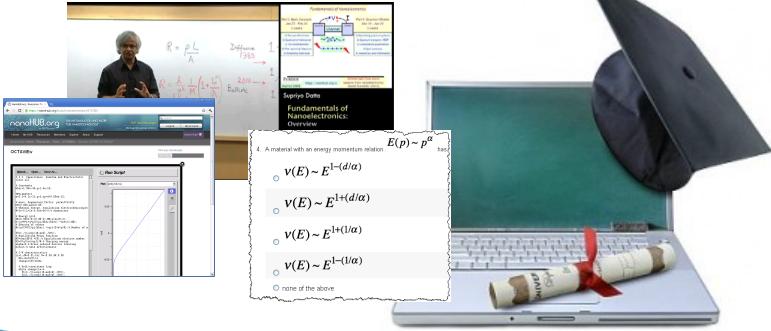
Open source software platform
used for building

“Science Gateways”
“Collaboratories”
“Hubs”

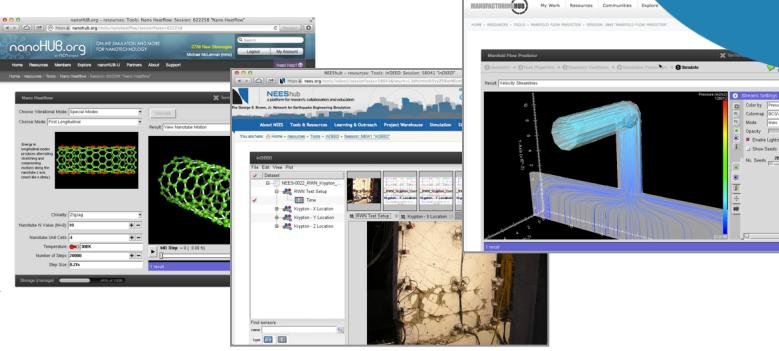
Platform for Scientific Collaboration



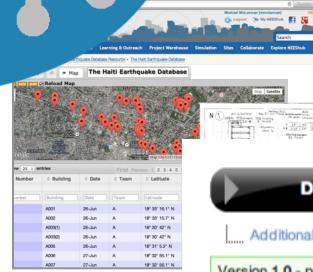
Group/Project Collaboration



Learning Management



Computational Tools

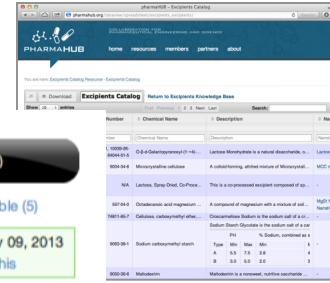


Download (JPG)

Additional materials available (5)

Version 1.0 - published on May 09, 2013
doi:10.4231/D3J268452 - cite this

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Databases / Publications

Started with nanoHUB.org



The screenshot shows the nanoHUB.org homepage. At the top, there's a search bar and a login/register button. Below the header, there's a banner with the text "What is nano?" and a 3D visualization of a nanotube. To the right of the banner is a map of the world with red dots indicating user activity. The main content area includes sections for "RESOURCES" (with tags like nanoelectronics, nanotransistors, research seminar, nanobio, quantum transport, etc.), "FEATURED" (with items like Resonant Tunneling Diode Simulation with NEGF, VolQD: Graphics Hardware Accelerated Interactive Visual Analytics, AGOME: Advancing Quantum Mechanics for Engineers, and Lecture 8: Mechanics of Defect Generation and Gate Dielectric Breakdown), "NOTABLE ONES" (with items like nanoHUB is anyone's gateway to nanotechnology, Peter Oosting: Engineering Lives in Nanobiotech, and Thermalactinolysis of Biomimetic Membranes), and "NEW IN RESOURCES" (with items like Anti-Reflective Coatings in Teaching Materials, Thermalactinolysis of Biomimetic Membranes, and NEGF 2D Toolkit).

Network for
Computational
Nanotechnology



Awards
EEC-0228390
EEC-0634750
OCI-0438246
OCI-0721680

705,725 Visitors
330,939 Users
349 Simulation Tools
4,568 Resources
1,110 Citations
22,649 Students at 185 Institutions





nanoHUB.org:

Your Workday on Steroids



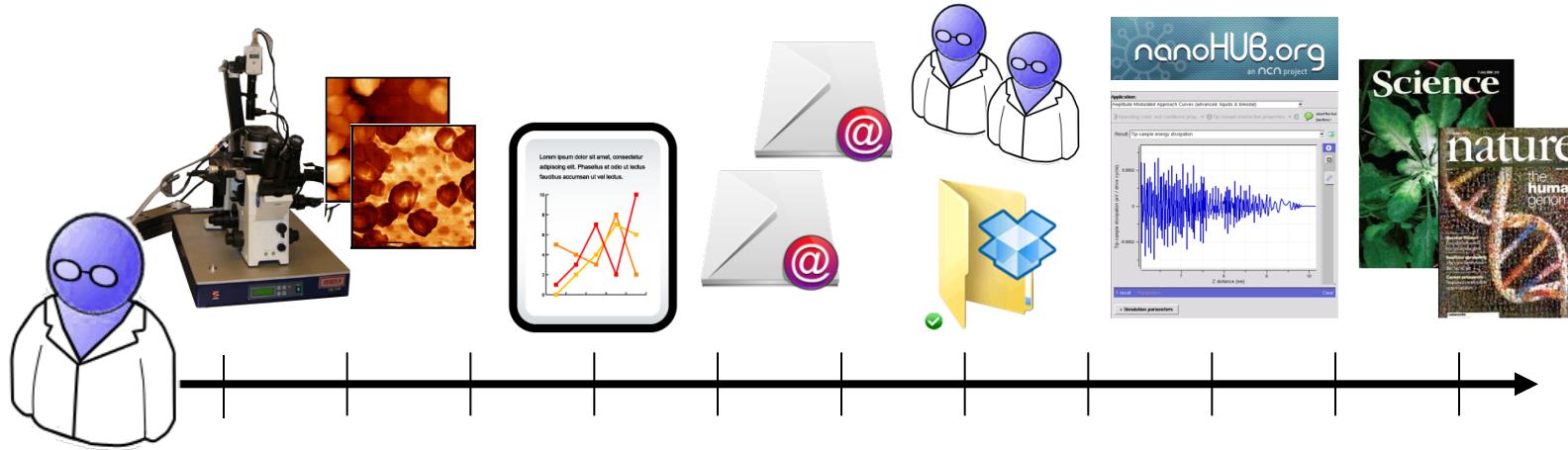
8 : 37 a.m



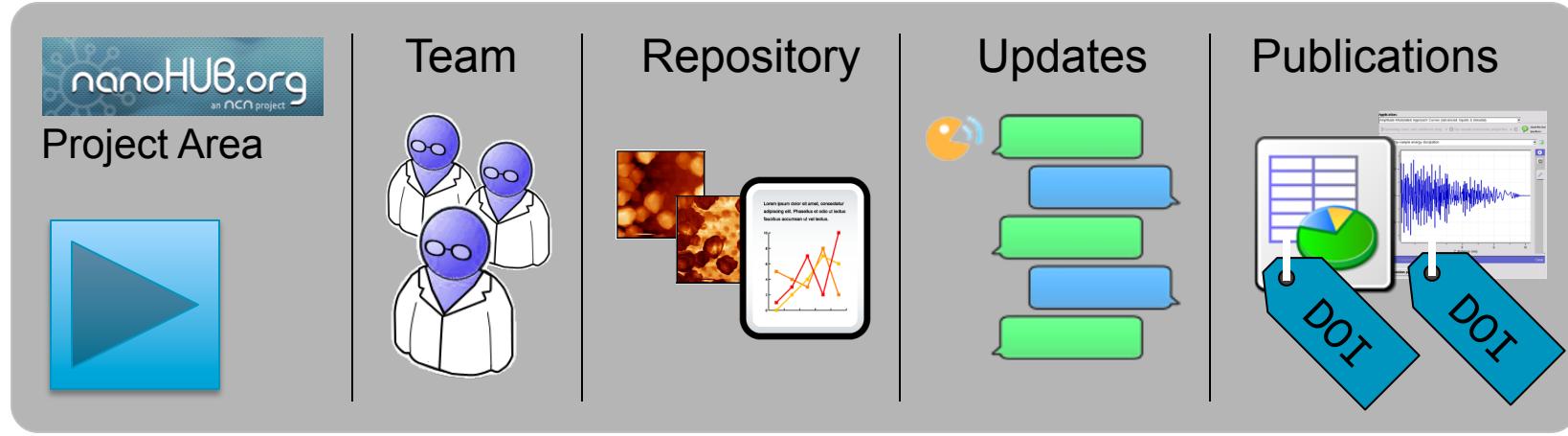
Email from Ale Strachan:

We should get started on our paper. Can you share the preliminary data from your experiments?

Collaborative Projects

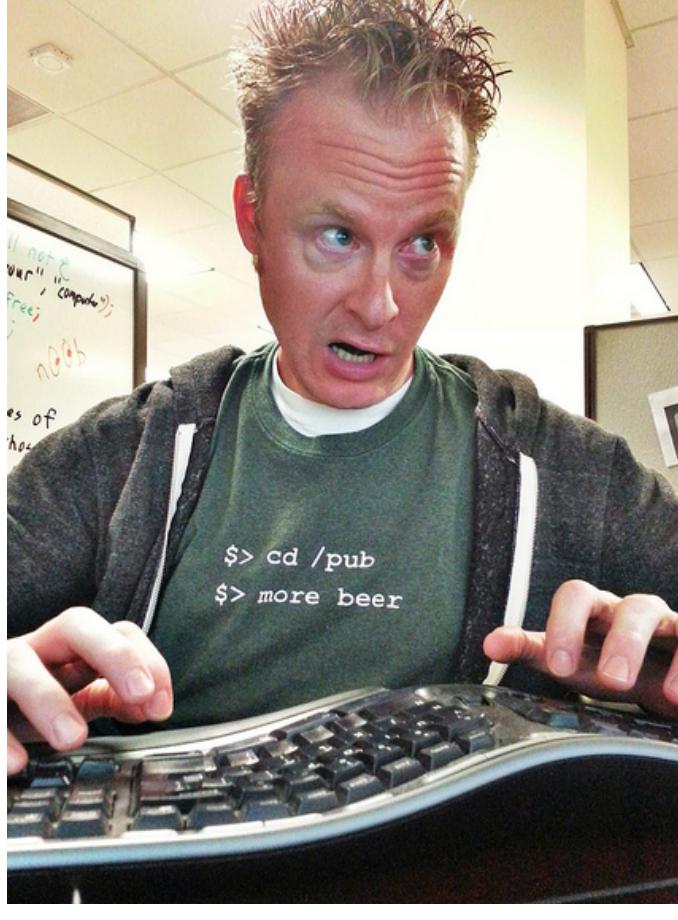


Researcher



Make Science/Engineering Reproducible

7



9:45am

Find some notes
for teaching your
quantum mechanics
class tomorrow.

Repository for Community Resources

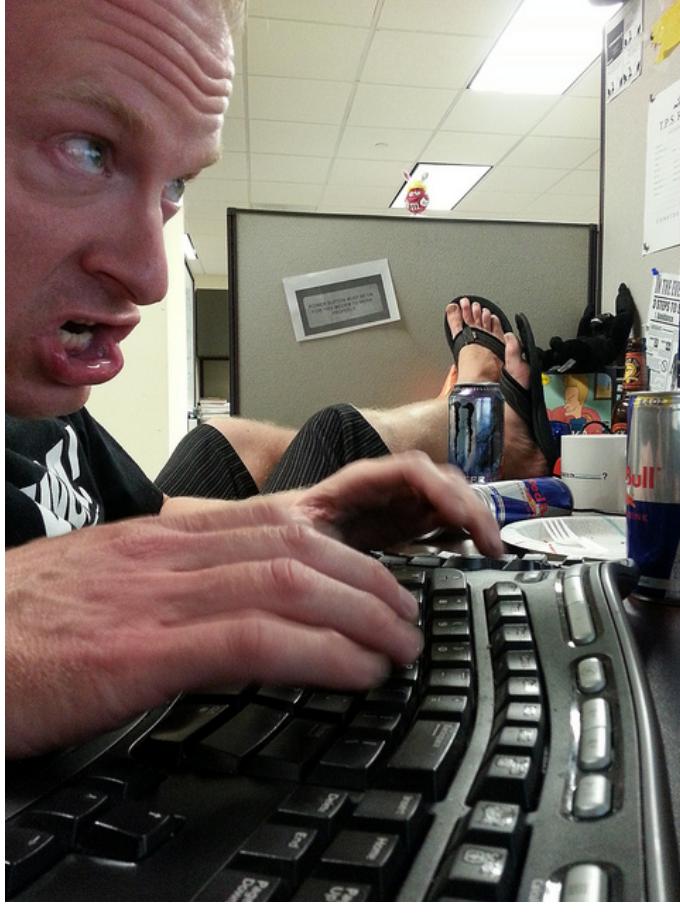


The screenshot shows the nanoHUB.org search interface. At the top, there's a search bar with the URL <https://nanohub.org/search/?term=quantum%20mechanics>. Below the search bar, the nanoHUB.org logo is displayed. The main content area shows a search result for 'quantum mechanics' with 1508 results. A sidebar on the left provides navigation links: Home, Resources, Members, Explore, nanoHUB, and ASU Computational Nanosciences Group.

This screenshot displays a scientific simulation interface. It features a TEM Cross Section image of an epitaxial layer structure with various layers labeled: AlAs/InGaAs/InAs/InGaAs/AlAs (2/1/2/1/2 nm), 100 nm n+ InGaAs, 100 nm n+ InGaAs, 30 nm n+ InAlAs/InGaAs, 25 nm AlAs, 40 nm InGaAs Channel, InAlAs/InGaAs Superlattice Buffer (44 nm period), and 120 nm InAlAs Buffer. To the right, there's a 'Basic Model Configuration' panel with parameters like Temperature (300K), Si doping (1e+10cm⁻³), Ge doping (1e+10cm⁻³), Substrate composition SiGe(1-x)Ge_x, Mat 1 Material (Silicon), and Mat 2 Material (Germanium). Below this is a 3D plot titled 'Density of States' showing energy levels across a range of values.



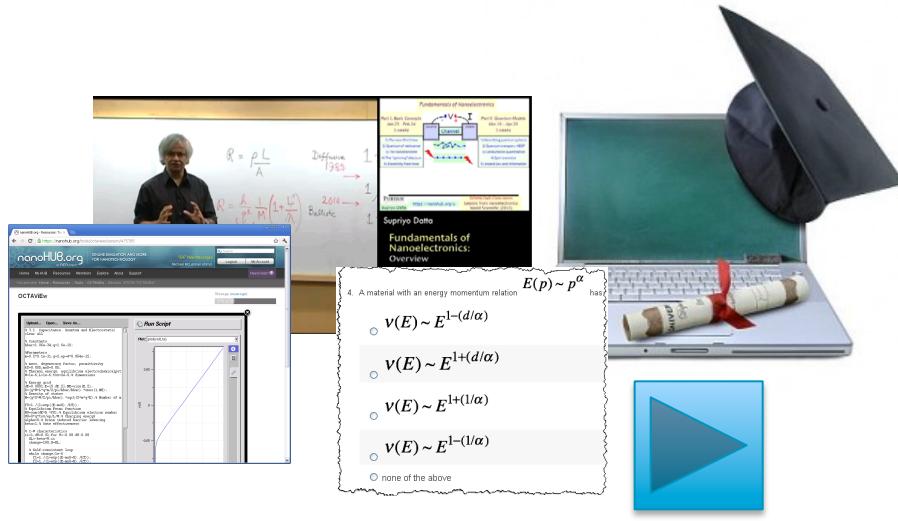
- ✓ Instant search
- ✓ Search inside documents
- ✓ Filter by types, tags, and other facets



10:13am

Put that course online
as part of the dissemination
plan for the grant.

Learning Management System



- ✓ Course builder
- ✓ Hands-on assignments
- ✓ Discussion forums
- ✓ Gradebook for instructors

Two Projects Using This Framework:



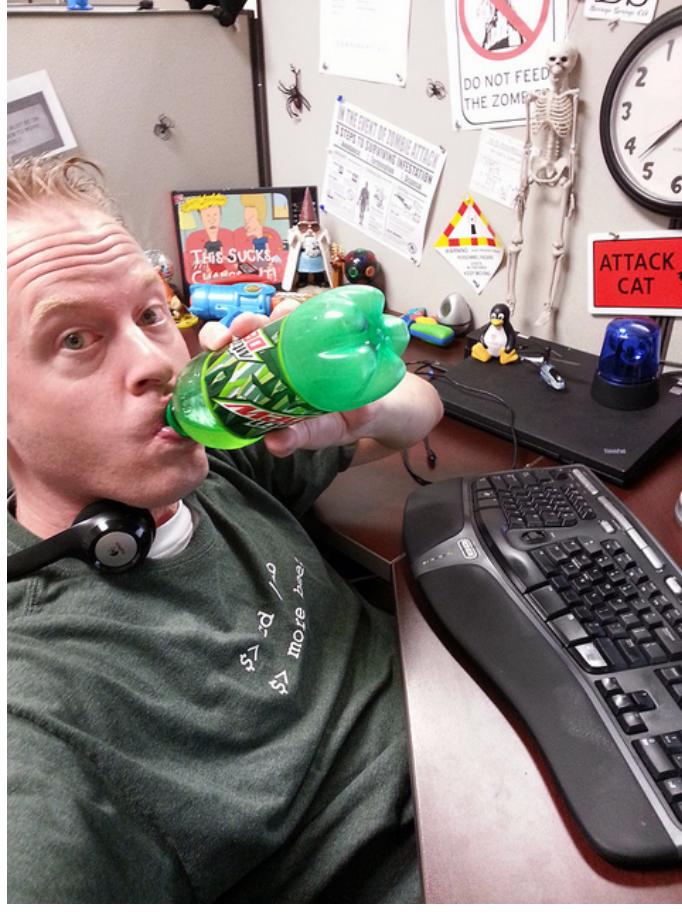
<http://nanohub.org/u>

11 nanotechnology courses

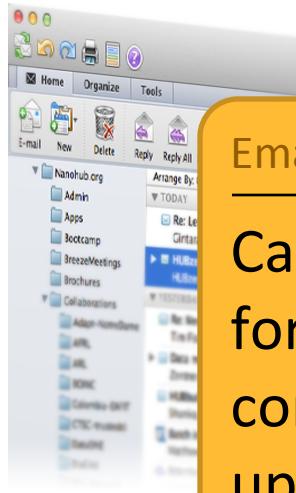


<http://purduenext.purdue.edu>

24 courses



11:14 am



Email from Tim Fisher:

Can you set up a web site
for the program
committee for our
upcoming workshop?

User Groups



The screenshot shows a web browser window for the nanoHUB.org website. The URL is https://nanohub.org/groups/ece606lundstrom. The page title is "ECE 606: Solid State Devices - Prof. Mark Lundstrom". The header includes the nanoHUB.org logo, navigation links (Home, Resources, Members, Explore, nanoHUB-U, Partners, About, Support), a search bar, and a login area showing "3175 New Messages" and "Michael McLennan (mmc)". Below the header is a breadcrumb trail: Home > Groups > ECE 606: Solid State Devices - Prof. Mark Lundstrom.

Course Information:

- Spring 2013: EE 115, TTH 4:30-5:45PM
- Instructor: M. S. Lundstrom (lundstro@purdue.edu)
- Office Hours: MWF 9:30-10:30AM, EE-334C
(or make an appointment for a different time by e-mail)

Course Description:

This course is about basic semiconductor physics and the physics of three important devices: 1) the PN junction, 2) the bipolar junction transistor (BJT), and 3) the metal-oxide-semiconductor field-effect transistor (MOSFET). The course is divided into three parts. The first part is an introduction to quantum mechanics and solid-state physics (energy bands, electrons and holes, the Fermi function), doping and carrier densities, carrier transport and generation-recombination, and the so-called semiconductor equations, which provide a complete, semi-classical, mathematical description of electrons and holes in semiconductors, subject to some important simplifying assumptions. The second part of the course applies these concepts to PN junctions and bipolar junction transistors (BJTs), and the third part treats the dominant electronic device today, the metal-oxide-semiconductor field-effect transistor (MOSFET).

The course covers a lot of ground, but it provides a basic understanding of semiconductors and devices, circuits and applications, and a starting point for further studies, for those who intend to focus on electronic devices.

Resources:

- Course Information (97.71 Kb)
- How to take this course (49.07 Kb)

Navigation:

- Request Group Membership
- Overview (highlighted)
- Members
- Announcements
- Calendar
- Collections
- Projects
- Usage

- ✓ Announcements
- ✓ Blog
- ✓ Calendar
- ✓ Collections
- ✓ Discussions
- ✓ Projects
- ✓ Wiki notes
- ✓ Wish lists

"Mini Site" with public and private parts



12:23pm

Look around for cool new
stuff while squeezing in
some lunch.

Collections



- ✓ Simple way to post links/documents
- ✓ Build your own collections
- ✓ Follow other users/groups and their collections

The collage displays four posts from a social media feed:

- Post 1:** A team of chemists and engineers at Penn State University have placed tiny synthetic motors inside live human cells, propelled them with ultrasonic waves and steered them magnetically. <http://t.co/QUQgwRGPqf> link. nanoHUB staff onto Nano News 10:38 am 06 Apr 2014.
- Post 2:** IEEE: First Single-Molecule LED. By coaxing light out of a single polymer molecule, researchers have made the world's tiniest light-emitting diode. <http://bit.ly/1d2FkPl> link. nanoHUB staff onto Nano News 10:33 am 06 Apr 2014.
- Post 3:** IEEE: Graphene Circuit Competes Head-to-Head With Silicon Technology. IBM has built on their previous graphene research and developed what is being reported as the best graphene circuit. <http://bit.ly/1evbfZB> link. nanoHUB staff onto Nano News 10:18 am 06 Apr 2014.
- Post 4:** Large thermoelectric power from a combination of magnets and superconductors. According to the newly published research, a very large thermoelectric effect can be created in a structure combining a ferromagnet (F) to a thin superconductor film (S) via an insulator (I) and where the superconductor is in the presence of a spin-splitting field due to the presence of a ferromagnetic insulator (FI) or a magnetic field (B). <http://t.co/yp18GRgZo> link. nanoHUB staff onto Nano News 10:26 am 06 Apr 2014.

Find and save your favorite stuff

15



1:42pm

Turn that MATLAB script
into something that other
people can use.

Deploying Live Tools for Others To Use



Magnetic Tape: \$10

```
----- XXXX XXXXX XXXX XX XX XXXX XX -----  
-- XX --  
--- XXXX XXXX XX XX XX XXXX XX XXXX XX ---  
-- XX XX XX X XX XX XX XX XX XX --  
-- XXXX XXXX XXX X XXXXX XX XX XXXXXXXX --  
-----  
SEQUEL: input deck  
  
title sequel the hard way  
# input file has units in angstroms  
scale cn=1.0e8  
input file=rtd.dat format=zevdmk  
device temp=300.0 area=1.0 bias=0.0  
solve itmax=0 prec=3 inject=r-to-l states=prop  
print tcoeff=r-to-l format1=* format2=* verbose=true  
output file=rtd data=t  
  
Executing a total of 1 calculation(s).  
1SEQUEL 2.1 page 2  
calculation 1 of 1 Summary of Input Information  
  
-----  
30E+20 /cm**3 !  
32E-01 m0 !  
3.03  
300.0000 K  
1.0000000 cm**2  
0.0000000 V  
1.0000000 Kb T  
1.1790000E+07 /cm**3  
propagating  
  
Fortran F77  

```

Live Tool: Priceless

Device: 2-barrier device

Ambient temperature: 300K

Applied bias: 0V

Result: Transmission Coefficient

Thickness B1: 5nm

Thickness W: 5nm

Thickness B2: 5nm

Contact B1 W B2 Contact

Doping (cm⁻³)

1E19

1E18

1E17

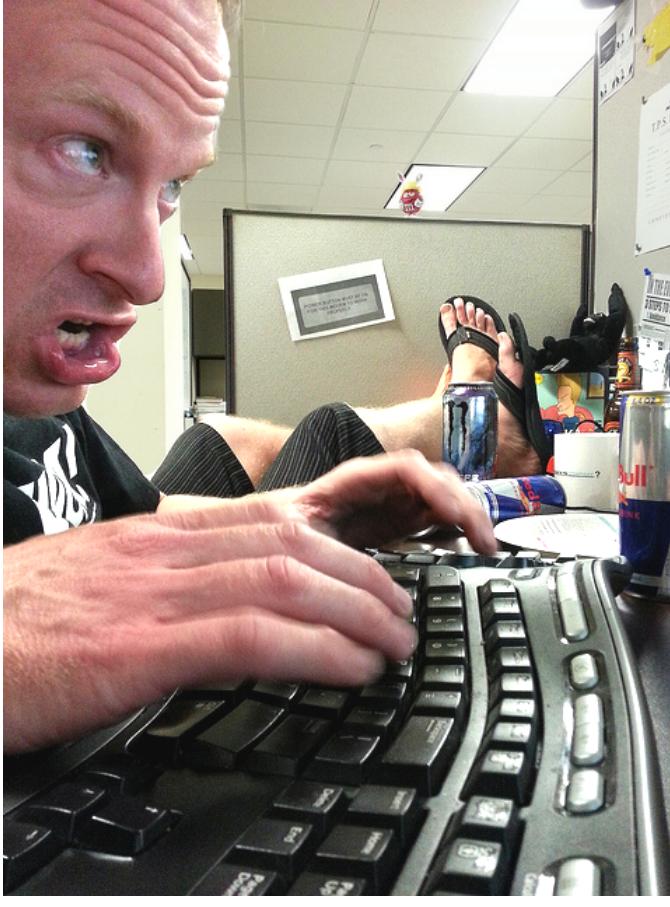
Doping

10.0 RANKING

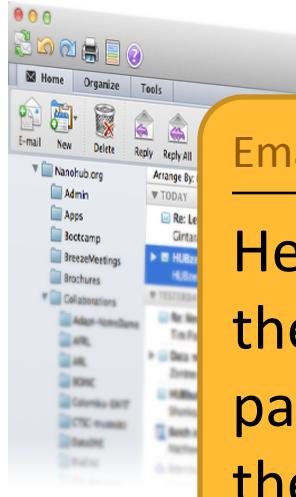
Intermediate-Advanced

- 1753 users, detailed usage
- 318 users in 38 classes
- 4 Citation(s)
- 2 questions (Ask a question)
- 2 review(s) (Review this)
- 0 wish(es) (Add a new wish)

Share: ...



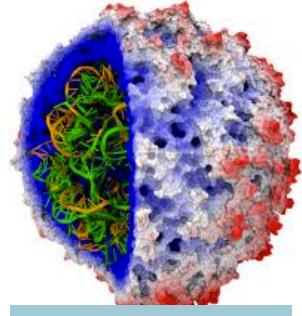
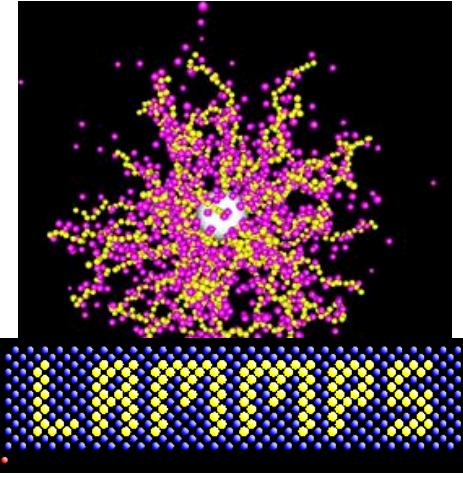
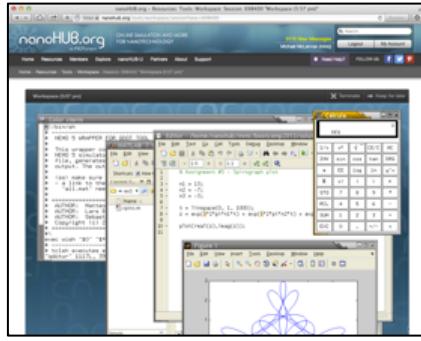
3:20pm



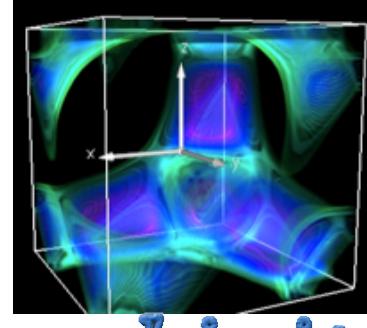
Email from Ale Strachan:

Here's a spreadsheet with the Smolyak sparse grid parameters. Can you run the simulations for us?

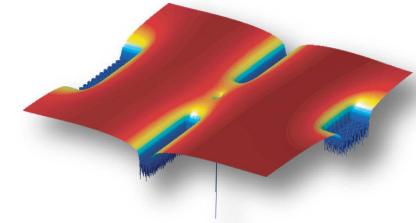
Research Computing



NAMD



ab init



NEHO

Access research codes and remote supercomputers

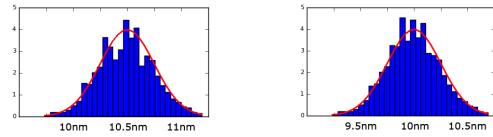
19

Powerful Computational Support



Uncertainty Quantification

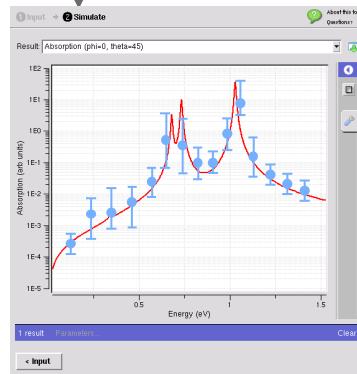
Parameter Probability Distributions



Simulation Model



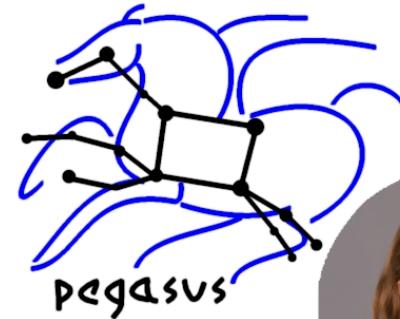
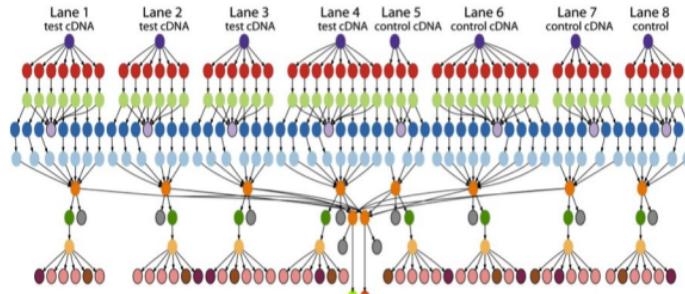
Alejandro
Strachan



Uncertainty in Outputs

Automated Workflow

Pegasus "DAX" Workflow



Ewa
Deelman
20



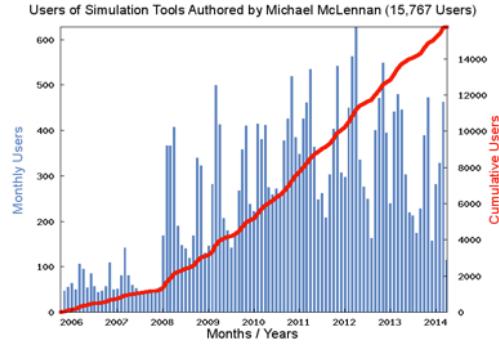
5:42pm

Post a copy of that
technical report so that
others can access it.

Dissemination and Digital Publication



- ✓ Tools
- ✓ Seminars
- ✓ Teaching Materials
- ✓ Tech Reports

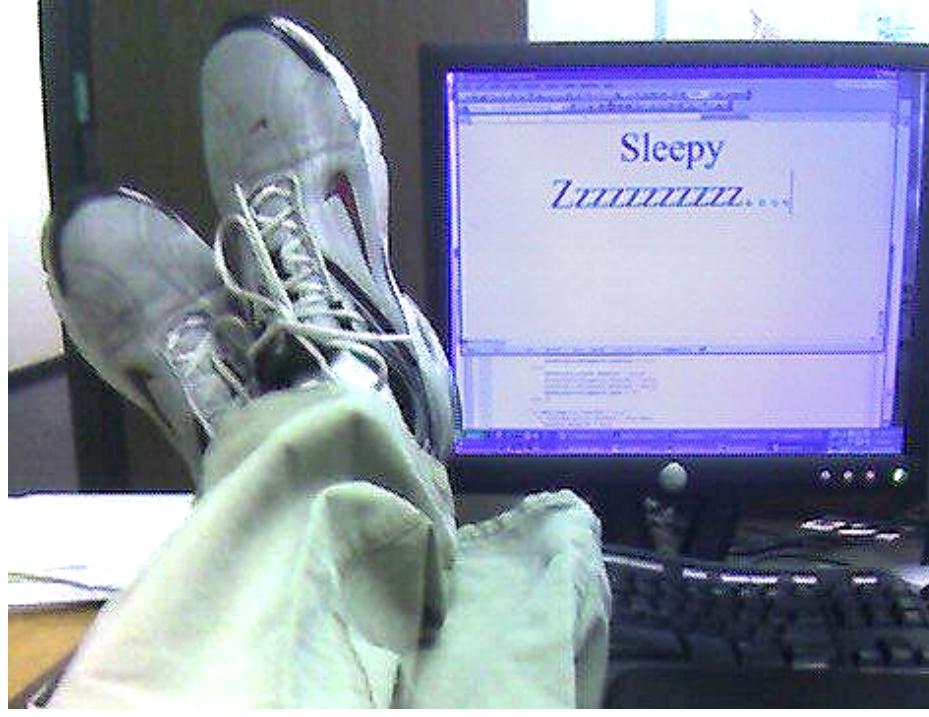


Disseminate your work to a worldwide audience

22

7:12pm

Done for the day



60+ Hubs for many disciplines



~1,800,000
visitors total

visitors	users	
705,725	330,939	nanoHUB.org an NCF project
364,304	118,016	NEEShub George E. Brown, Jr. Network for Earthquake Engineering Simulation
63,487	32,236	pharmaHUB.org
62,495	5,492	habri central Resources for the Study of the Human-Animal Bond
53,507	13,487	vhub.org
49,559	23,168	GLOBALHUB
47,972	6,976	ciHUB.org BETA
47,085	12,788	cceHUB
46,083	5,166	PURR
45,833	5,473	iemHUB a CIEM project
45,176	9,069	molecularHUB.org
41,048	8,078	StemEdHub.org

Sept 29-30, 2014

HUBbub 2014, Indianapolis

24



Global community



- Non-profit organization
- Independent owner of HUBzero code
- Promotes dissemination and outreach
- Coordinates software contributions

Only \$5,000 to join – 20 hours of tech support

<https://hubzero.org/about/foundation>

25



More information



Michael McLennan
Director, HUBzero® Project
mmclennan@purdue.edu
<http://hubzero.org/pressroom>

- Simulation/modeling tools
- Data management
- Collaboration and social networking
- Analytics to measure impact