

The HUBzero Platform for Scientific Collaboration

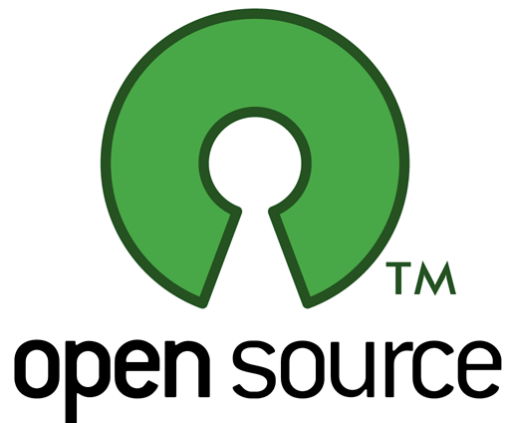
Michael McLennan

Director, HUBzero® Platform for Scientific Collaboration

Purdue University



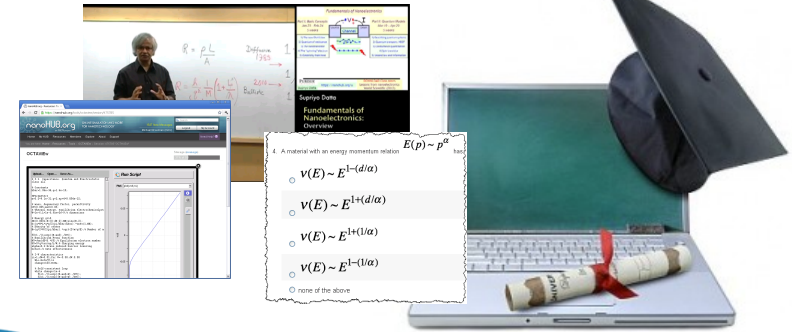
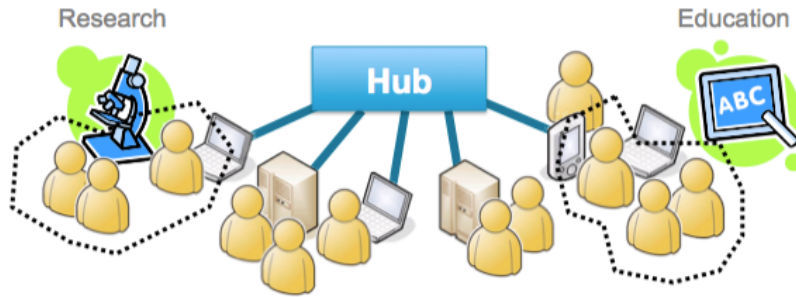
What is HUBzero?



Open source software platform
used for building

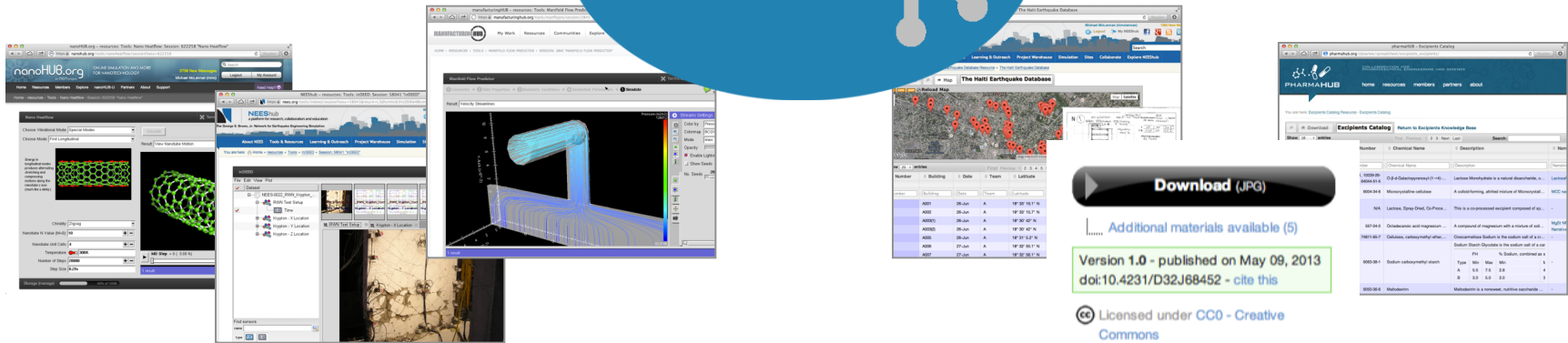
“Science Gateways”
“Collaboratories”
“Hubs”

Platform for Scientific Collaboration



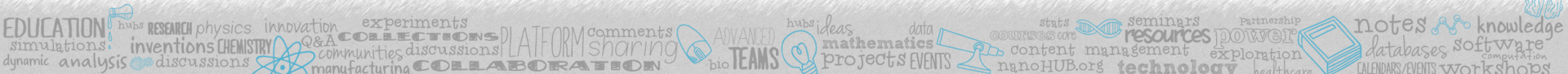
Group/Project Collaboration

Learning Management

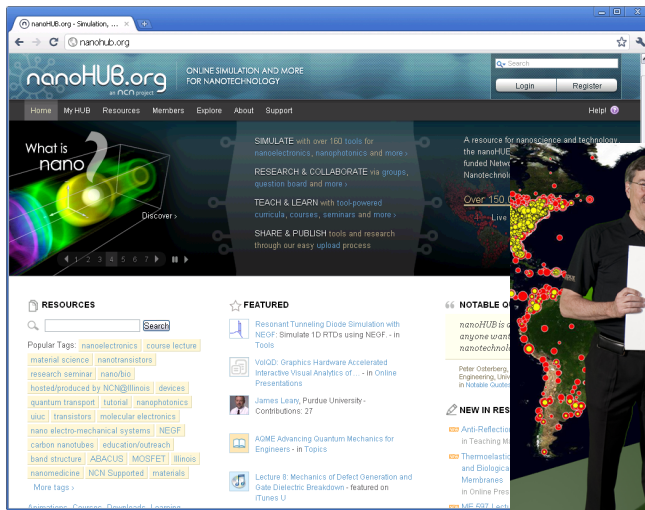


Computational Tools

Databases / Publications



Started with nanoHUB.org



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

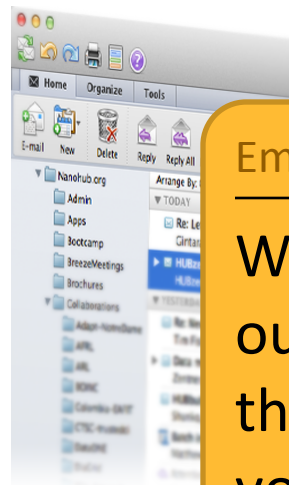




nanoHUB.org: Your Workday on Steroids



8:37 am



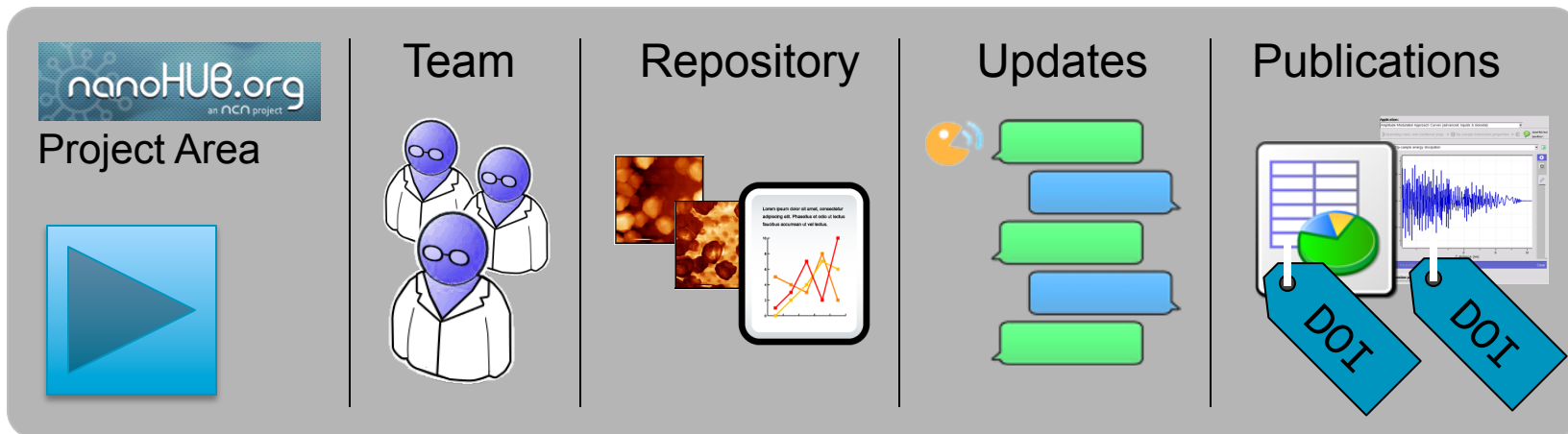
Email from Ale Strachan:

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

Collaborative Projects

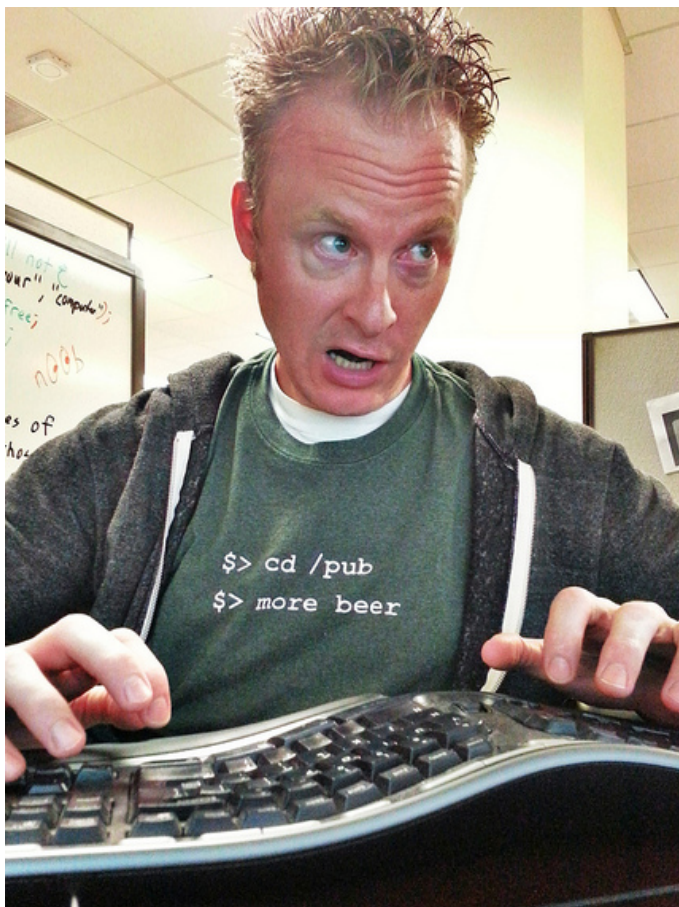


Researcher



Make Science/Engineering Reproducible





9:45am

Find some notes for teaching your quantum mechanics class tomorrow.

Repository for Community Resources



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

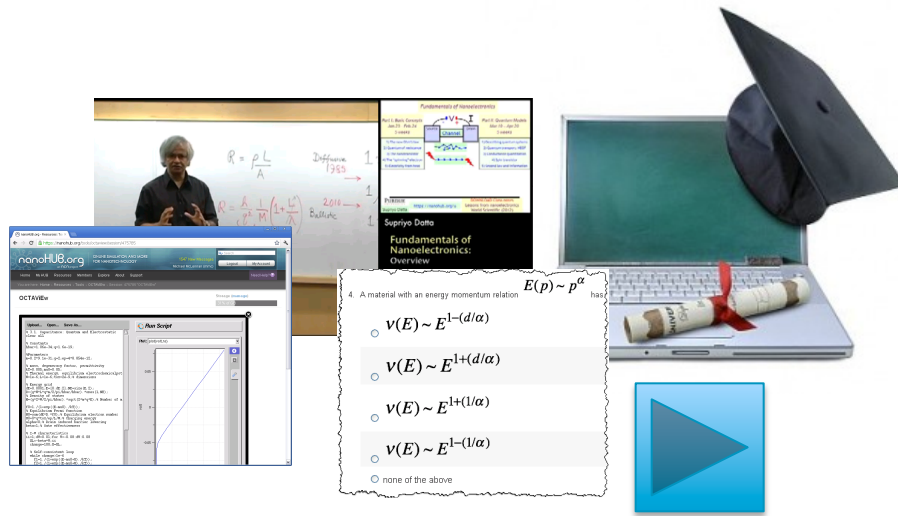




10:13am

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>

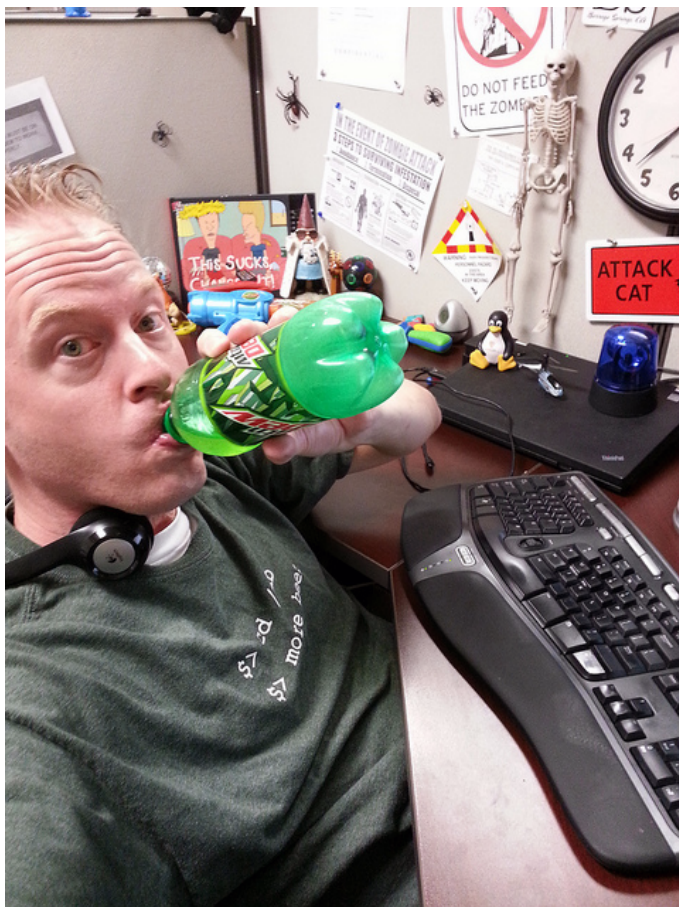
11 nanotechnology courses



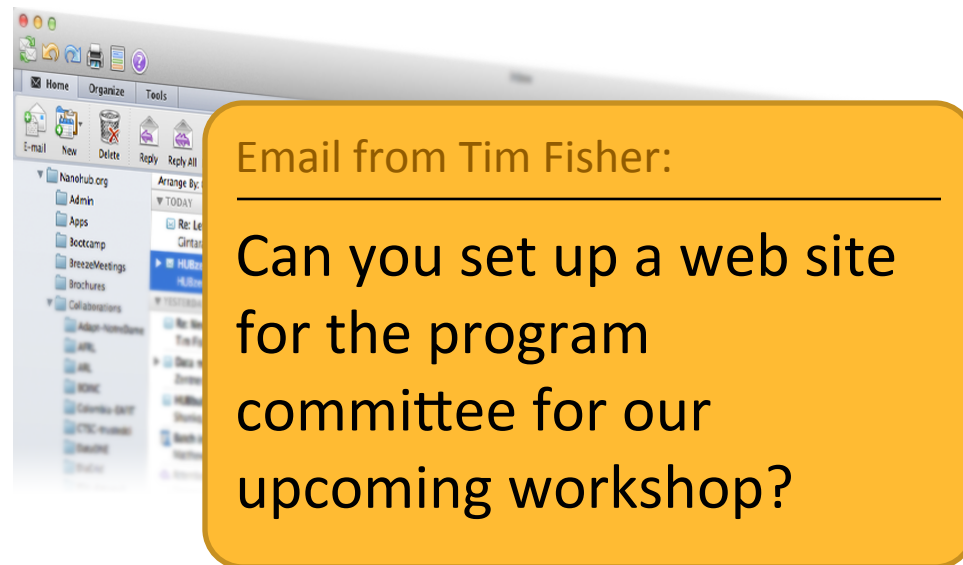
<http://purduenext.purdue.edu>

24 courses

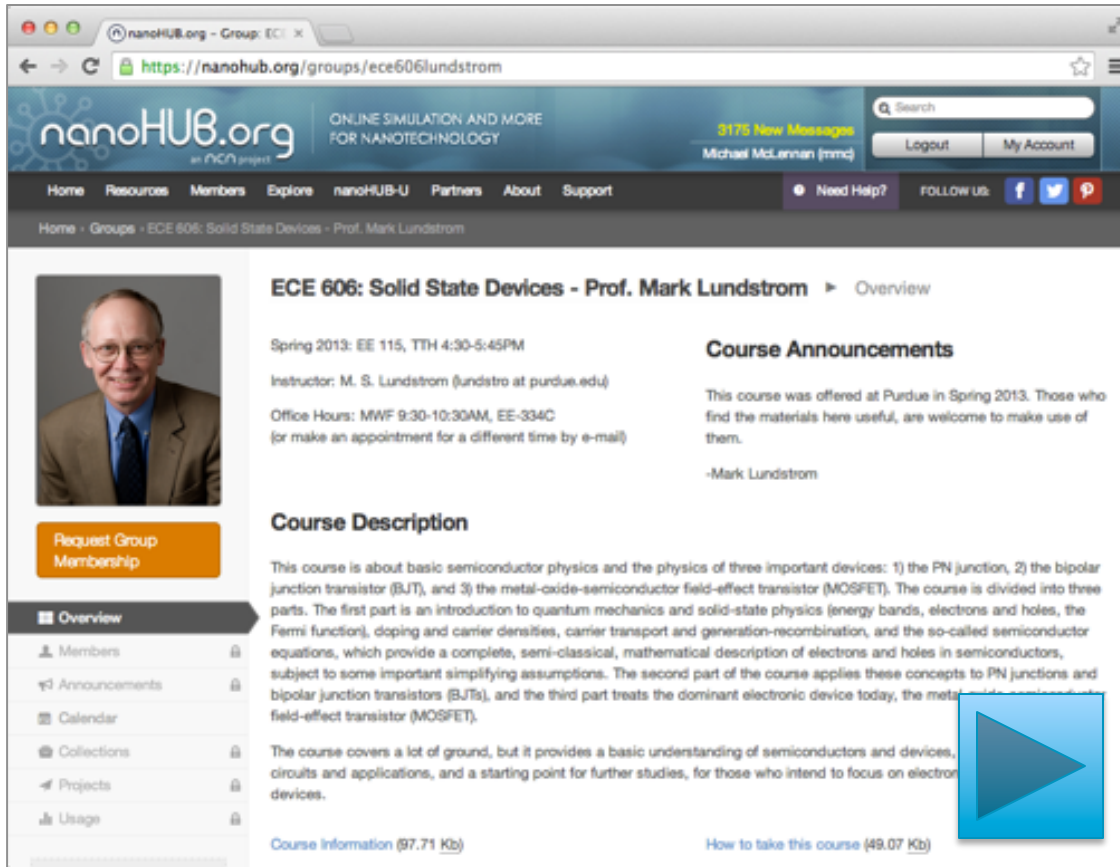




11:14 am



User Groups



The screenshot shows a web browser window displaying the nanoHUB.org website. The page is for a user group titled "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), and a search bar. The main content area features a profile picture of Prof. Mark Lundstrom, a "Request Group Membership" button, and a sidebar with navigation options: Overview, Members, Announcements, Calendar, Collections, Projects, and Usage. The main text provides course details for Spring 2013, including the instructor's name, office hours, and a "Course Description" section. A large blue play button icon is overlaid on the bottom right of the course description.

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

“Mini Site” with public and private parts



12:23pm

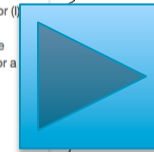
Look around for cool new stuff while squeezing in some lunch.

Collections



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

The screenshot displays a grid of content on the nanoHUB platform. On the left, there are two posts from 'nanoHUB staff onto Nano News' dated April 6, 2014. The top post is titled 'A team of chemists and engineers at Penn State University have placed tiny synthetic motors inside live human cells...' and includes a 'nanobio applications' tag. The bottom post is titled 'IEEE: Graphene Circuit Competes Head-to-Head With Silicon Technology' and features an image of a circuit board. In the center, there is a post titled 'IEEE: First Single-Molecule LED' with a 3D molecular model and a 'light emitting diodes' tag. On the right, there is a post titled 'Large thermoelectric power from a combination of magnets and superconductors' with a diagram of a layered structure (F/S/I/F) and a 'thermoelectric power generation' tag. At the bottom right, there is a promotional banner for an 'ONLINE COURSE INTRODUCTION TO BIOELECTRICITY' from Purdue University, featuring an instructor named Pedro Brazool.



Find and save your favorite stuff



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  XX  XX XX XX XX XX XX XX XX  SEQUAL 2.1
----- XXXX XXXXX XX XX XX XXXXXX XX -----  Purdue University
      XX  XX  XX X  XX XX XX XX XX XX  August 1988
-- XXXX XXXXXX XXX X XXXXX XX XX XXXXXX

SEQUAL: input deck

title sequal the hard way
# input file has units in angstroms
scale  cn=1.0e8
input  file=rt.d dat format=zevdmk
device temp=300.0 area=1.0 bias=0.0
solve  itmax=0 prec=3 inject=-to-1 states=prop
print  tcoeff=-to-1 format1=* format2=* verbose=true
output file=rt.d dat=t

Executing a total of 1 calculation(s).
1SEQUAL 2.1 page 2
calculation 1 of 1 Summary of Input Information
    
```



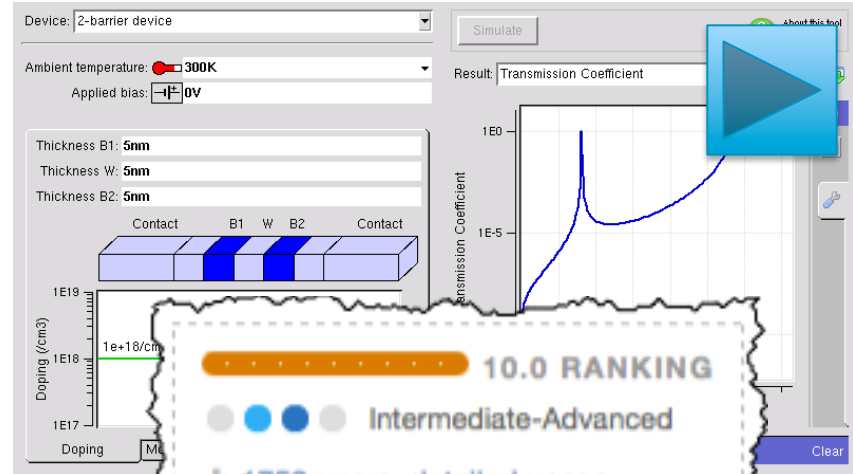
```

300.0000 K
1.0000000 cn**2
3.0000000 U
1.0000000 Kb T
1.17900000E+07 /cn**3
ppagating
    
```

Fortran
F77



Live Tool: Priceless

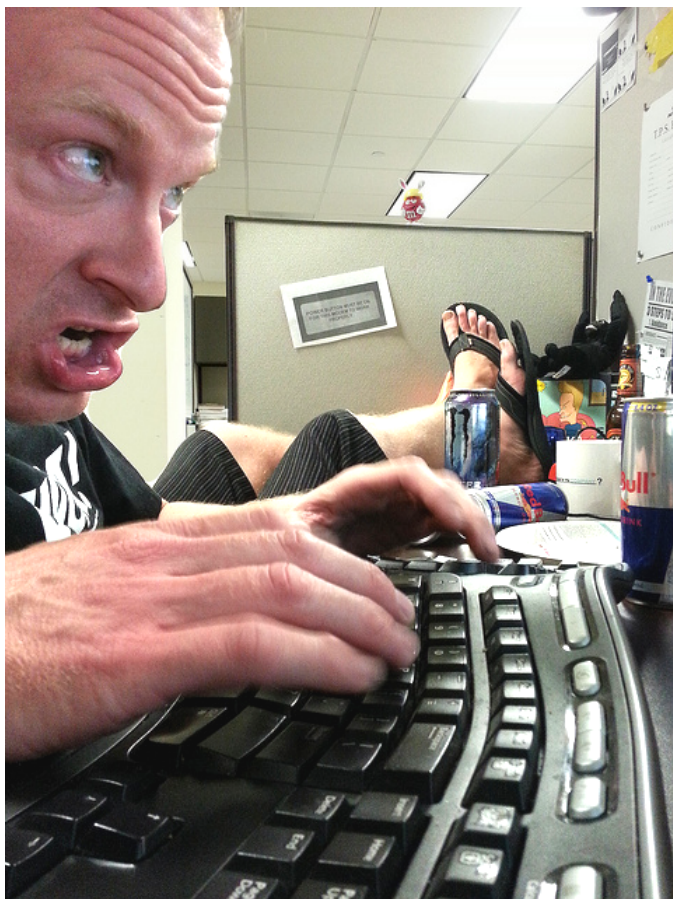


10.0 RANKING

● ● ● 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: ...



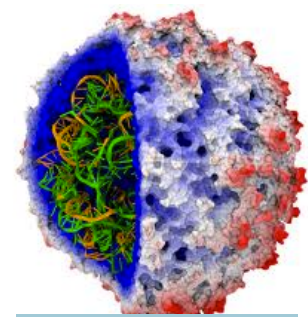
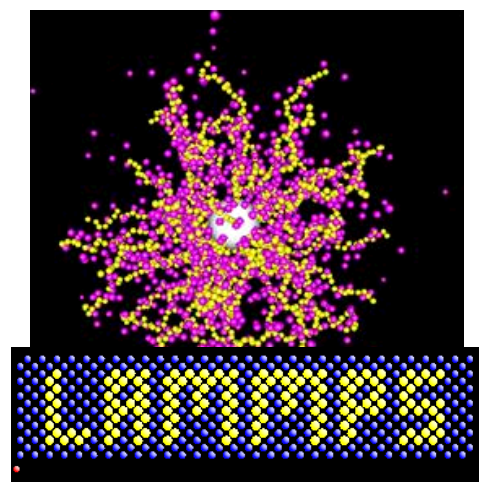
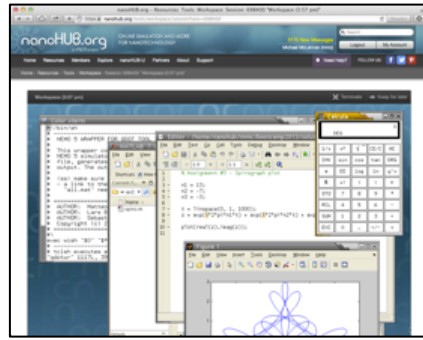
3:20pm



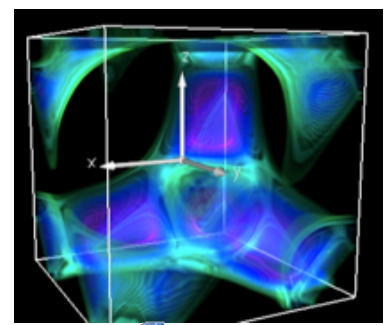
Email from Ale Strachan:

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

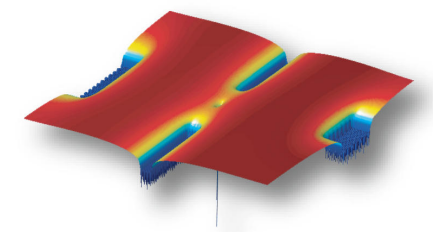
Research Computing



NAMD



abinit



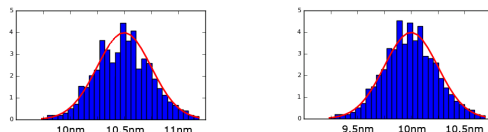
NEMO

Access research codes and remote supercomputers

Powerful Computational Support

Uncertainty Quantification

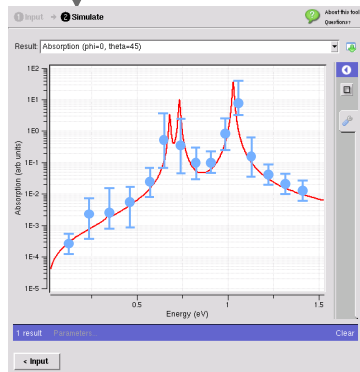
Parameter Probability Distributions



Simulation Model



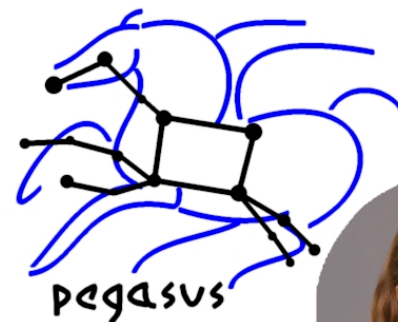
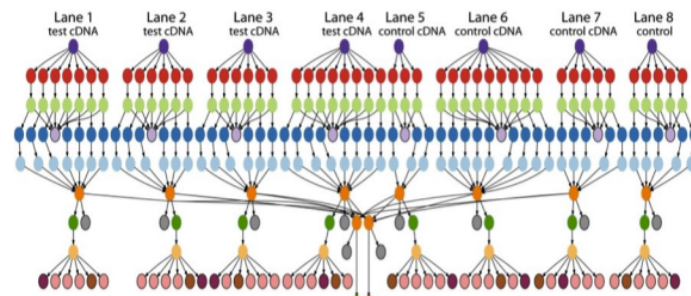
Alejandro Strachan



Uncertainty in Outputs

Automated Workflow

Pegasus "DAX" Workflow



Ewa Deelman



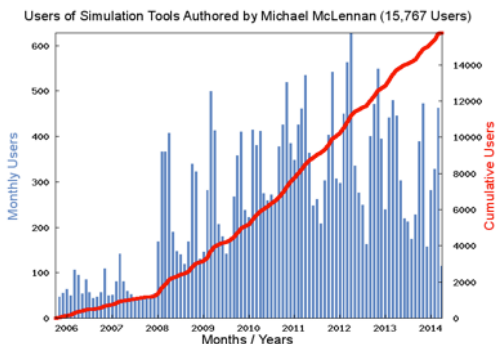
5:42pm

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

Dissemination and Digital Publication



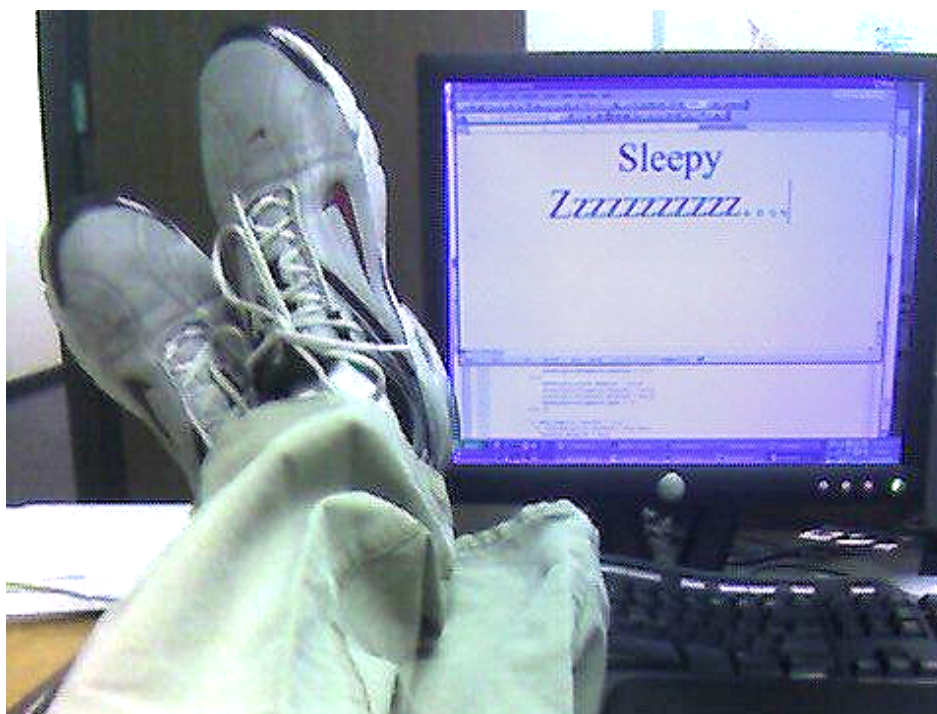
- ✓ Tools
- ✓ Seminars
- ✓ Teaching Materials
- ✓ Tech Reports



Disseminate your work to a worldwide audience

7:12pm

Done for the day



60+ Hubs for many disciplines



~1,800,000
visitors total

visitors	users
705,725	330,939
364,304	118,016
63,487	32,236
62,495	5,492
53,507	13,487
49,559	23,168
47,972	6,976
47,085	12,788
46,083	5,166
45,833	5,473
45,176	9,069
41,048	8,078



nanoHUB.org



nees.org



pharmaHUB.org



HABRIcentral.org



vhub.org



GlobalHUB.org



ciHUB.org



cceHUB.org



PURR



iemhub.org



molecularHUB.org



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>



More information



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<http://hubzero.org/pressroom>

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

