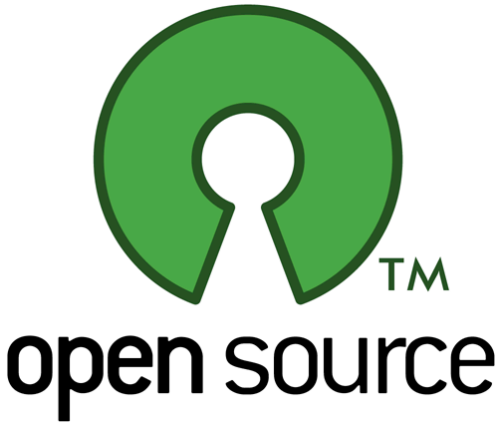
The HUBzero Platform for Scientific Collaboration

Michael McLennan
Director, HUBzero® Platform for Scientific Collaboration
Purdue University

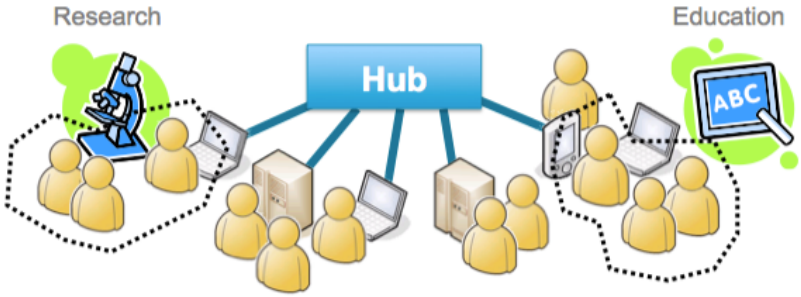
What is HUBzero?



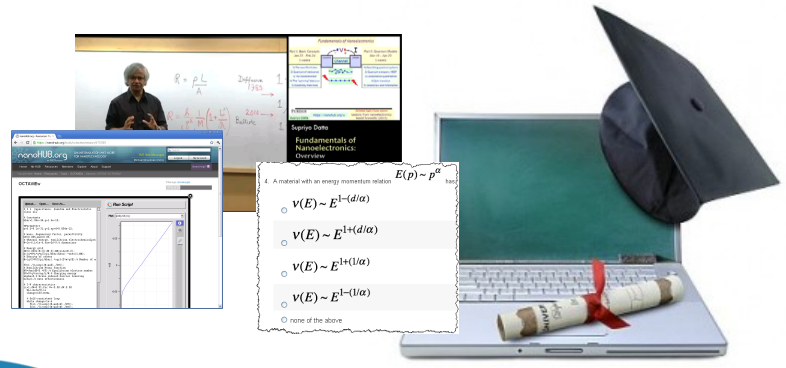
Open source software platform used for building

"Science Gateways"
"Collaboratories"
"Hubs"

Platform for Scientific Collaboration

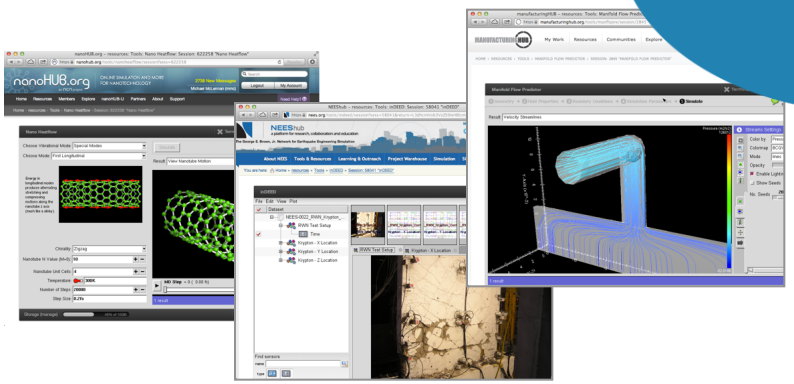


Group/Project Collaboration



Learning Management

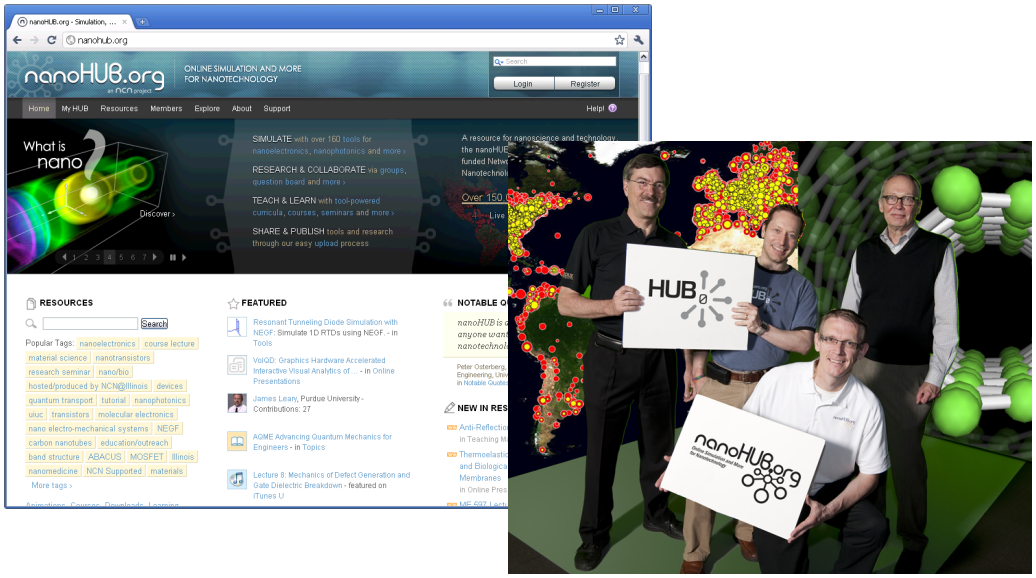
hubzero



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

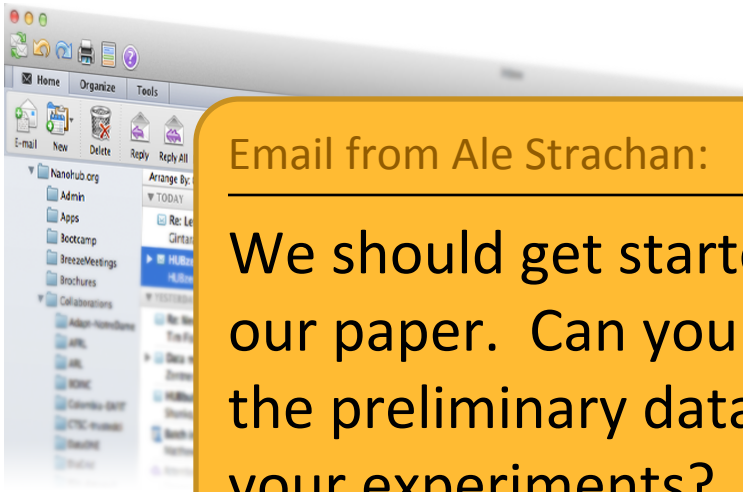
hubzero

nanoHUB.org
an NCN project

nanoHUB.org:

Your Workday on Steroids

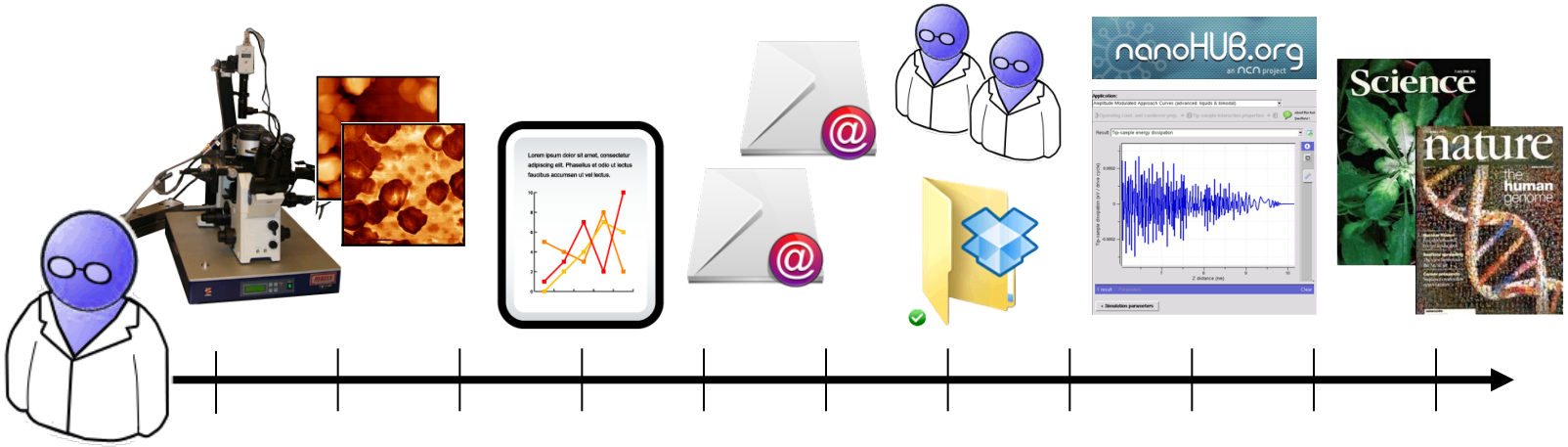
8:37am



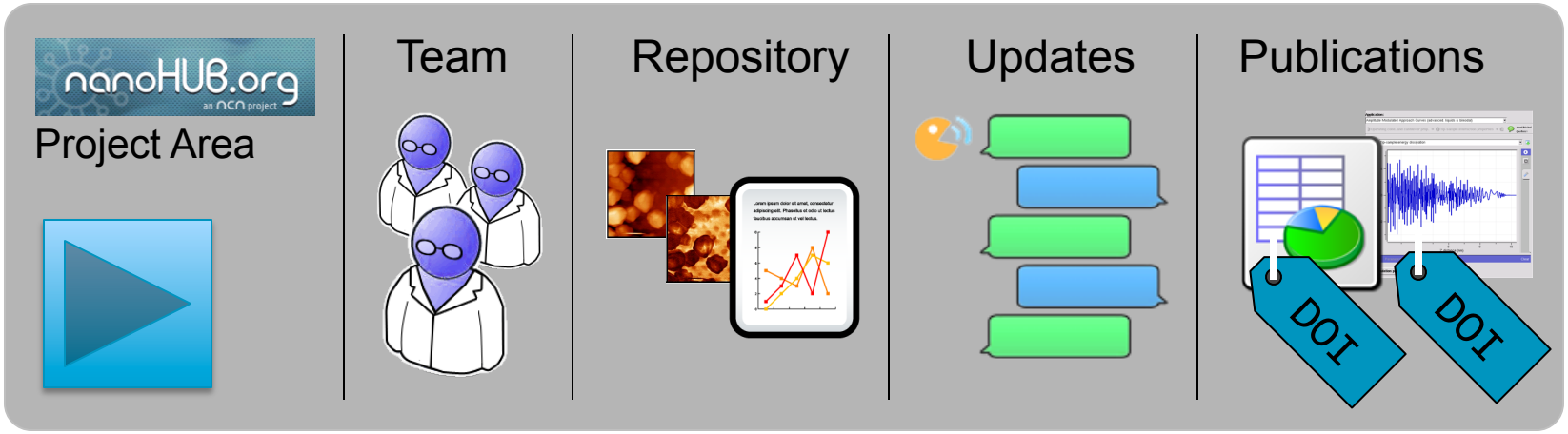
Email from Ale Strachan:

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

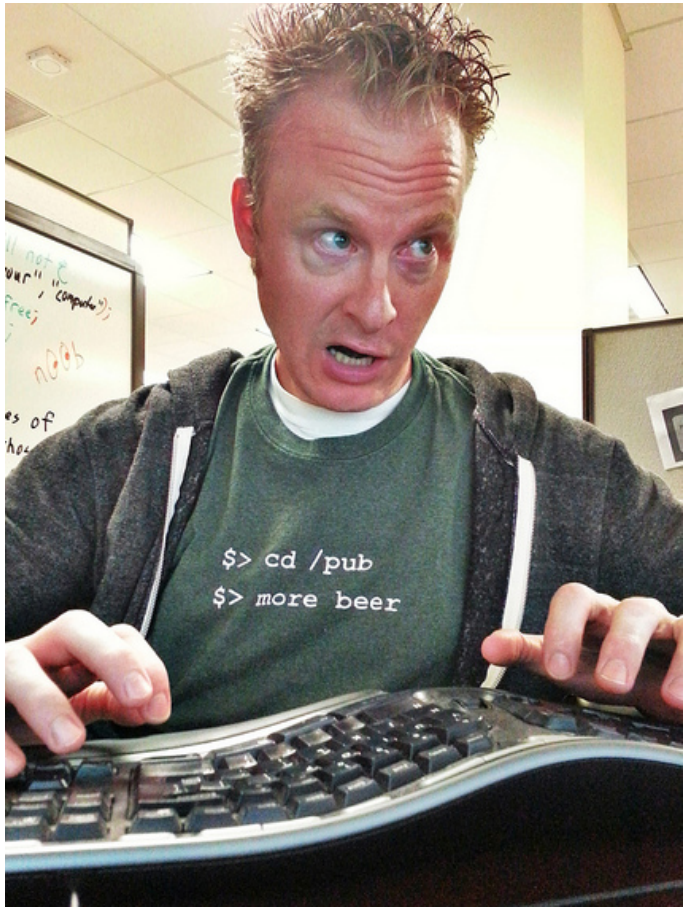
Collaborative Projects



Researcher



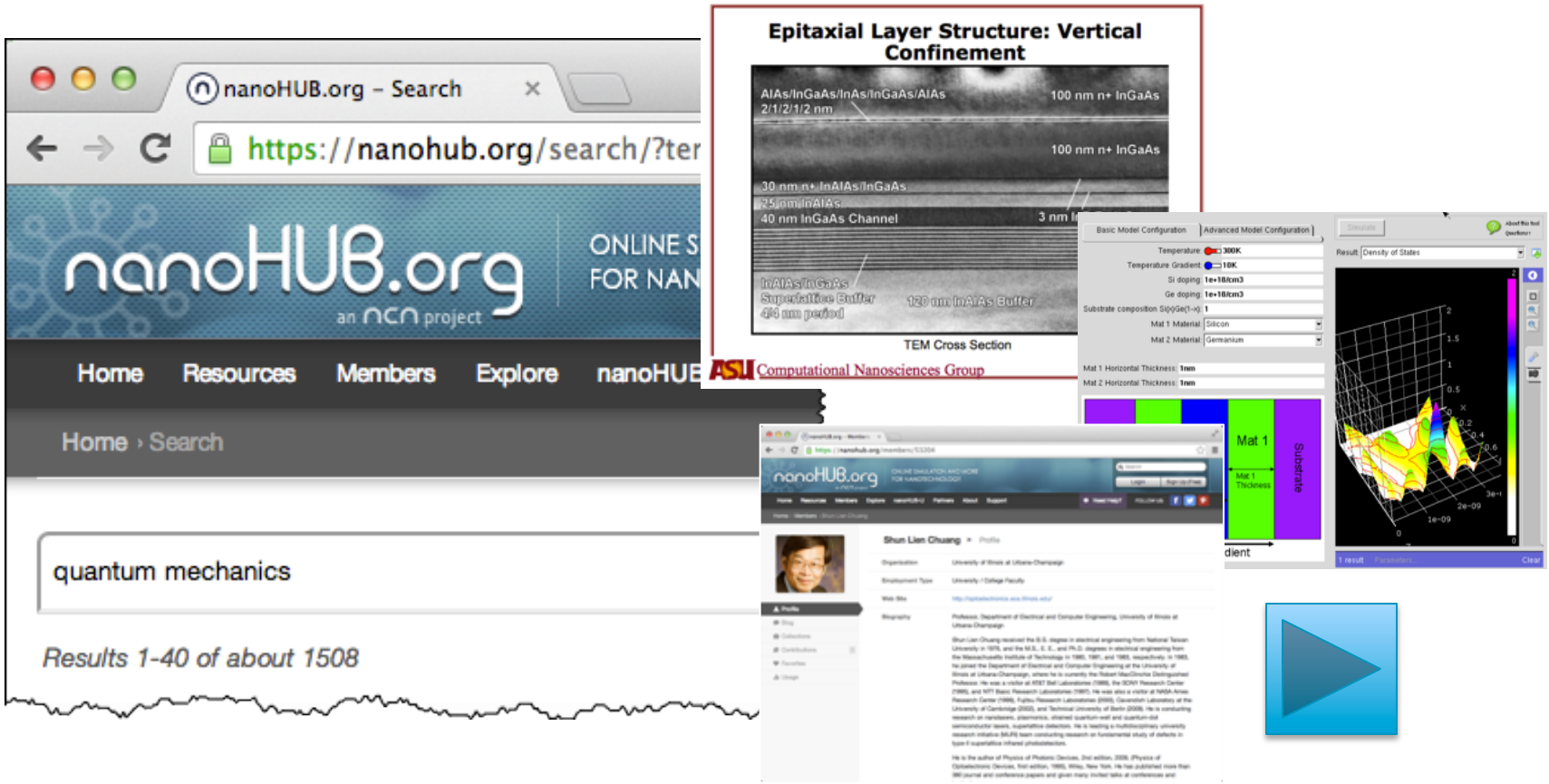
Make Science/Engineering Reproducible



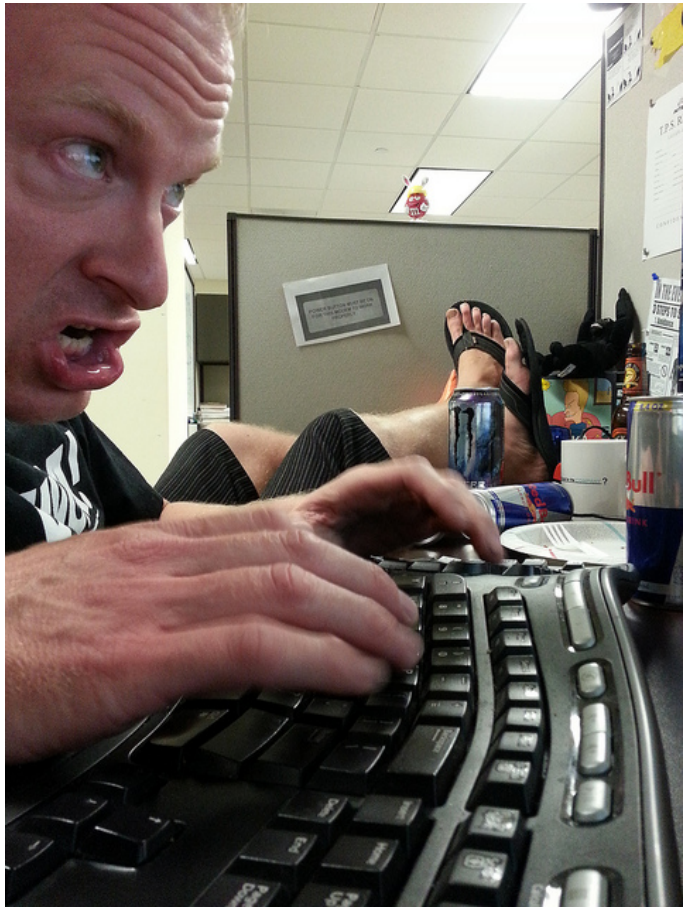
9:45am

Find some notes for teaching your quantum mechanics class tomorrow.

Repository for Community Resources



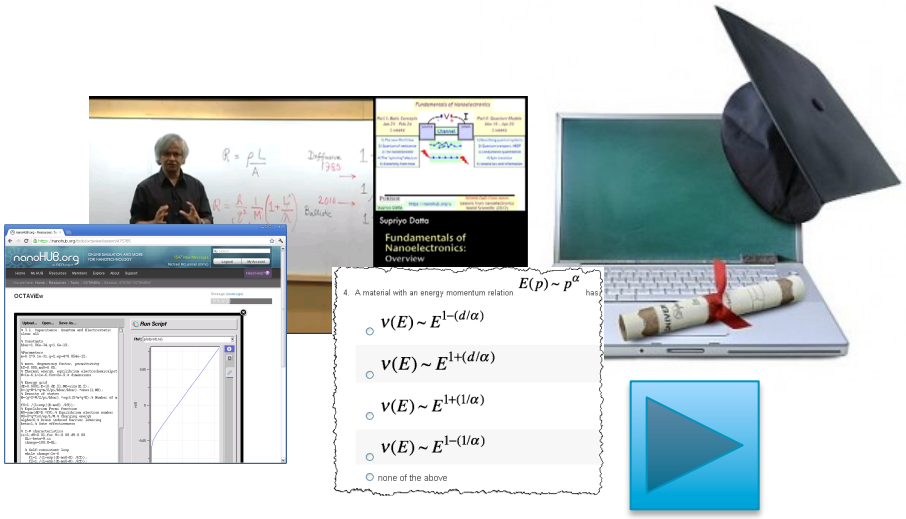
- ✓ Instant search
- ✓ Search inside documents
- ✓ Filter by types, tags, and other facets



10:13am

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

Learning Management System

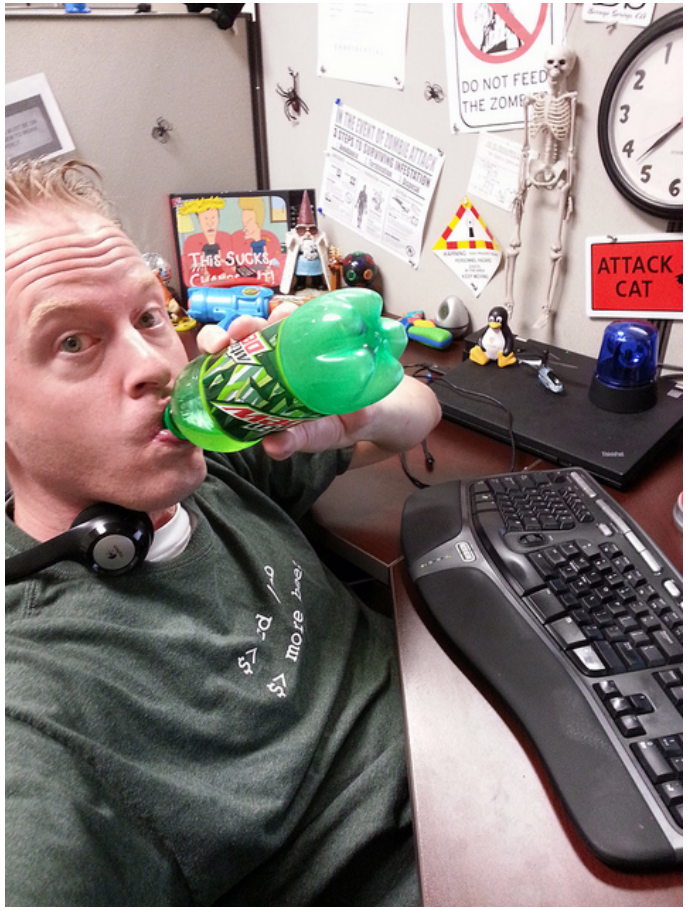


- ✓ Course builder
- ✓ Hands-on assignments
- ✓ Discussion forums
- ✓ Gradebook for instructors

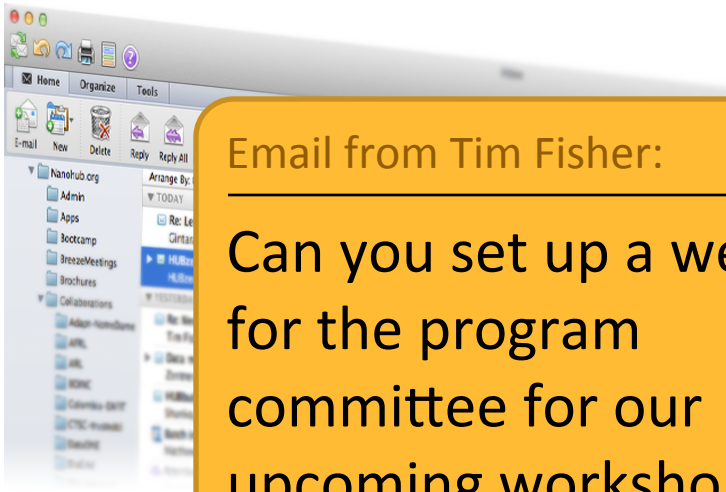
Two Projects Using This Framework:

http://nanohub.org/u
11 nanotechnology courses

http://purduenext.purdue.edu
24 courses



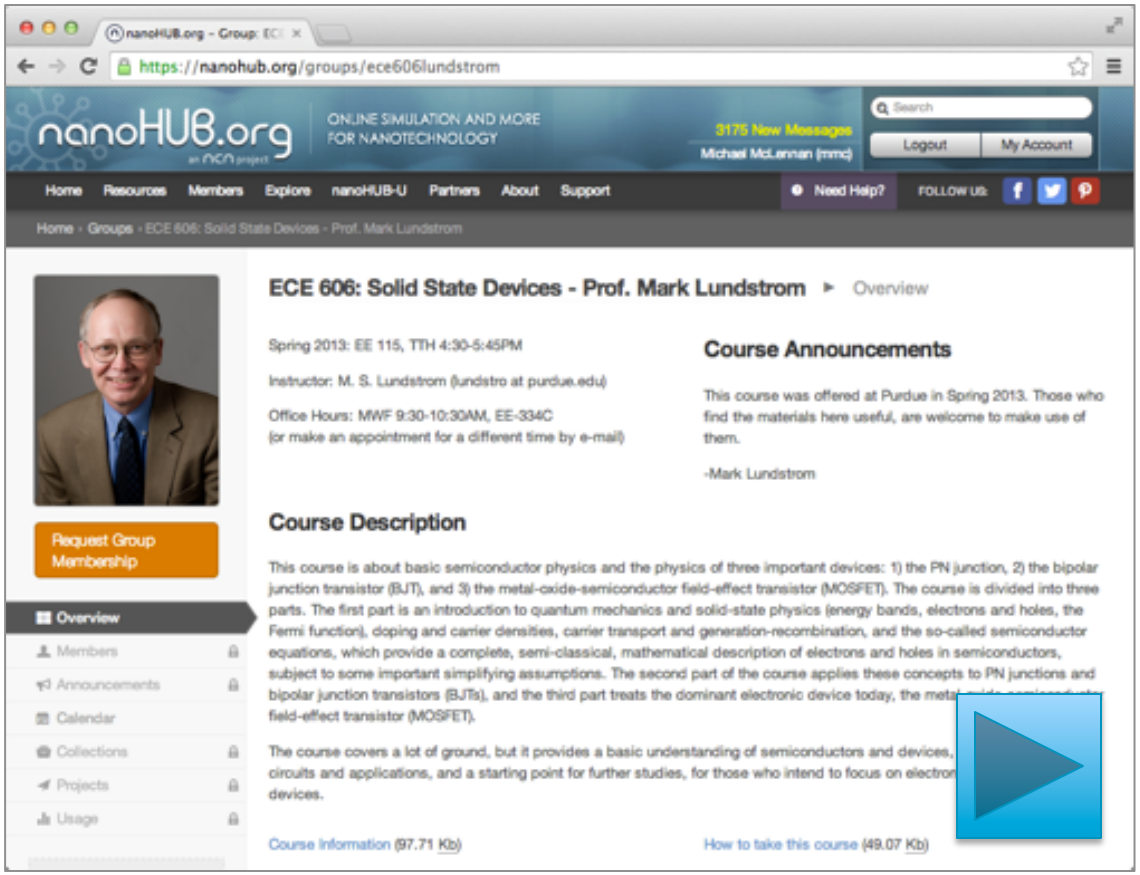
11:14am



Email from Tim Fisher:

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

User Groups



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

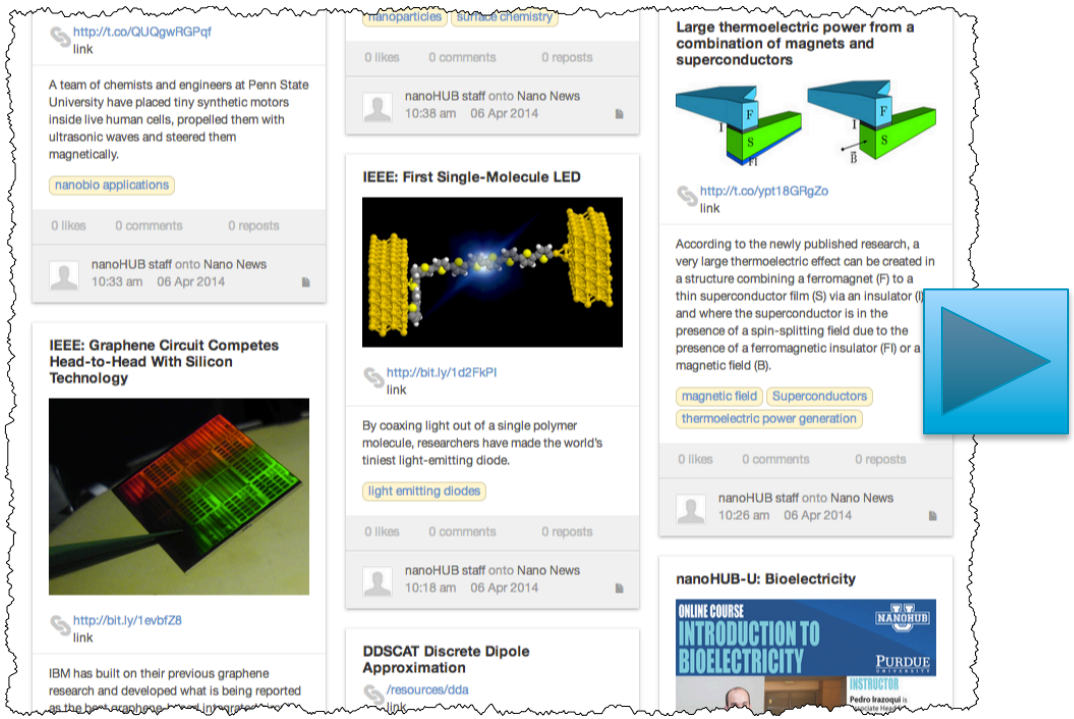
"Mini Site" with public and private parts

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



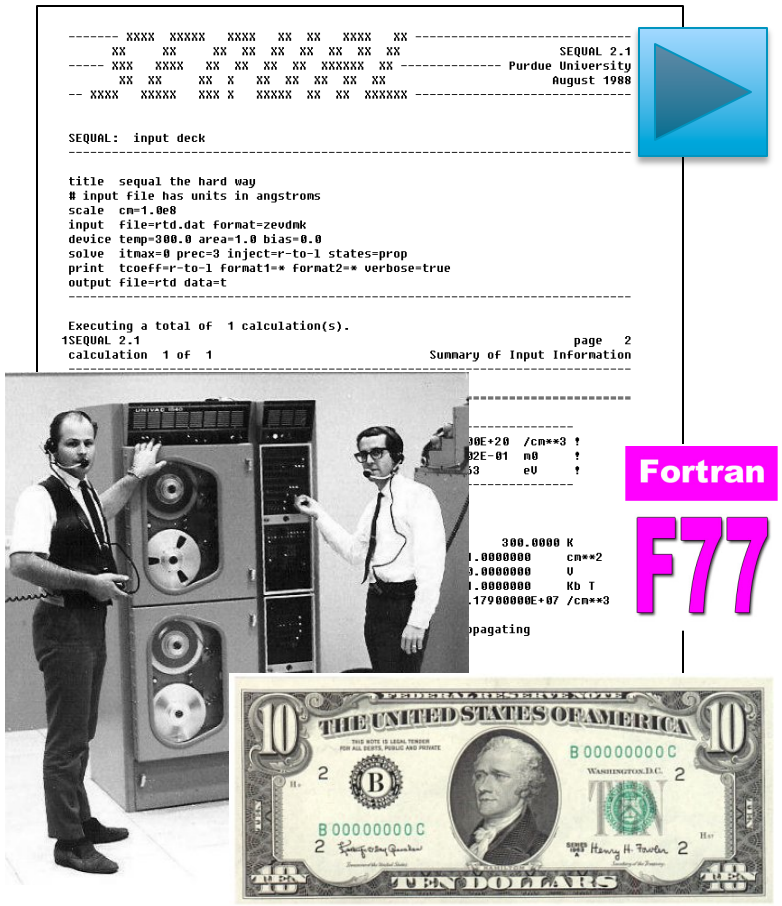
Find and save your favorite stuff

1:42pm

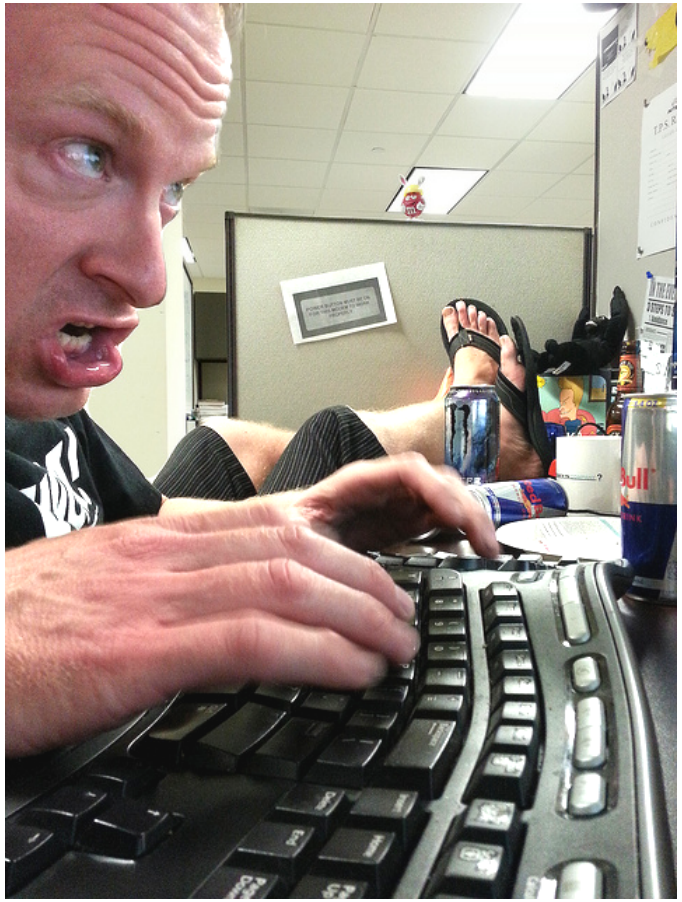
Turn that MATLAB script into something that other people can use.

Deploying Live Tools for Others To Use

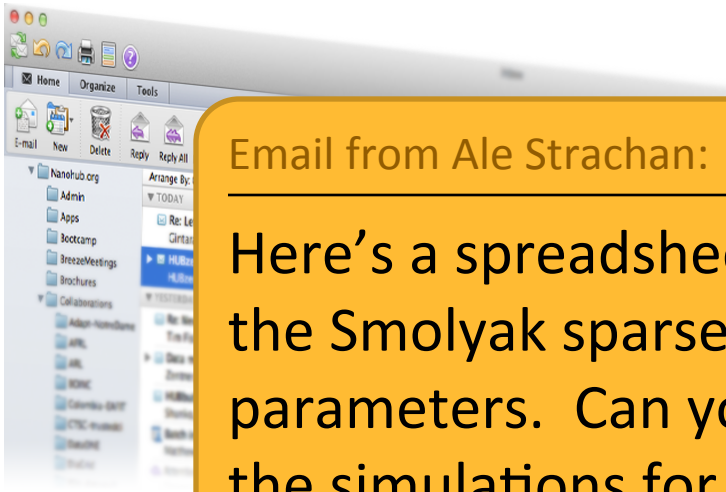
Magnetic Tape: $10



Live Tool: Priceless



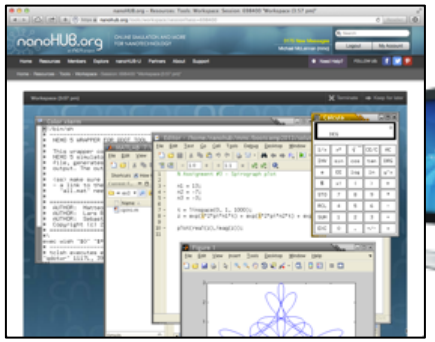
3:20pm



Email from Ale Strachan:

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

Research Computing

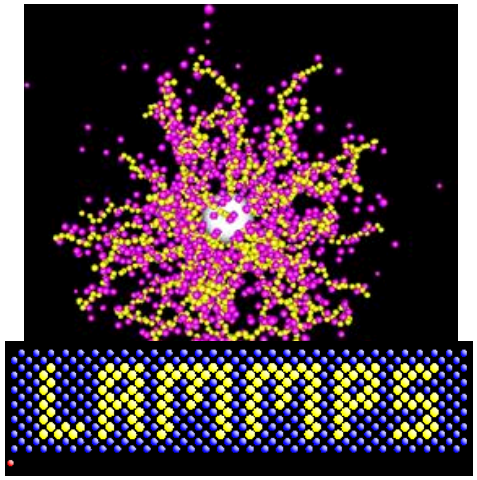


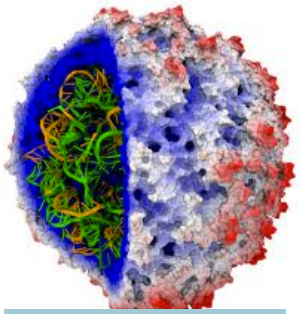
XSEDE
Extreme Science and Engineering Discovery Environment

Open Science Grid

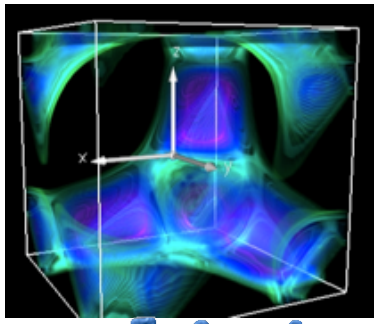
DiaGrid

red cloud

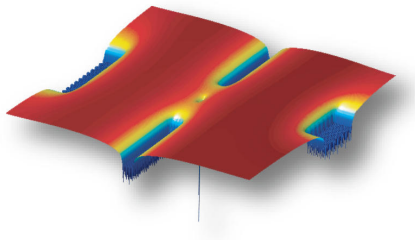




NAMD



abinit



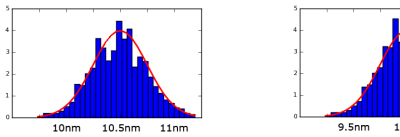
NEMO

Access research codes and remote supercomputers

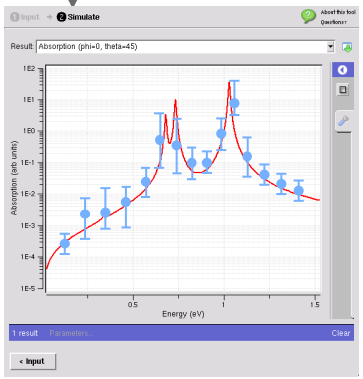
Powerful Computational Support

Uncertainty Quantification

Parameter Probability Distributions



Simulation Model

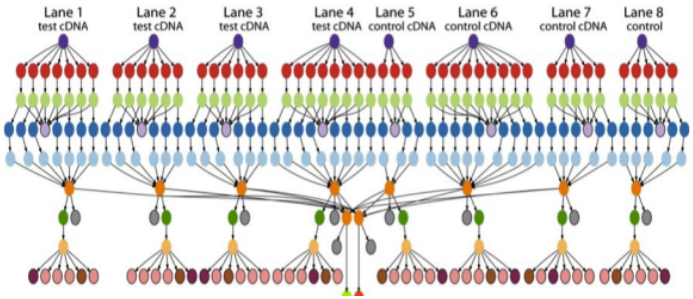


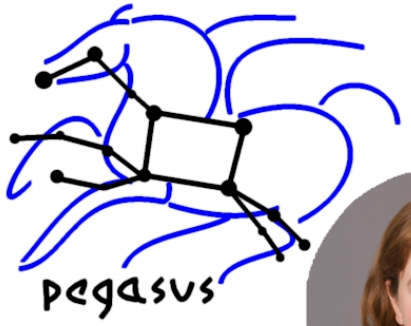
Uncertainty in Outputs

Alejandro Strachan

Automated Workflow

Pegasus "DAX" Workflow





Ewa Deelman

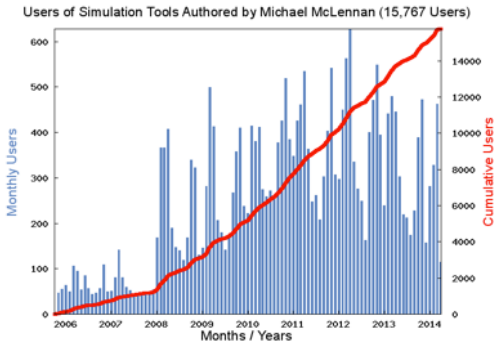
5:42pm

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

Dissemination and Digital Publication

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

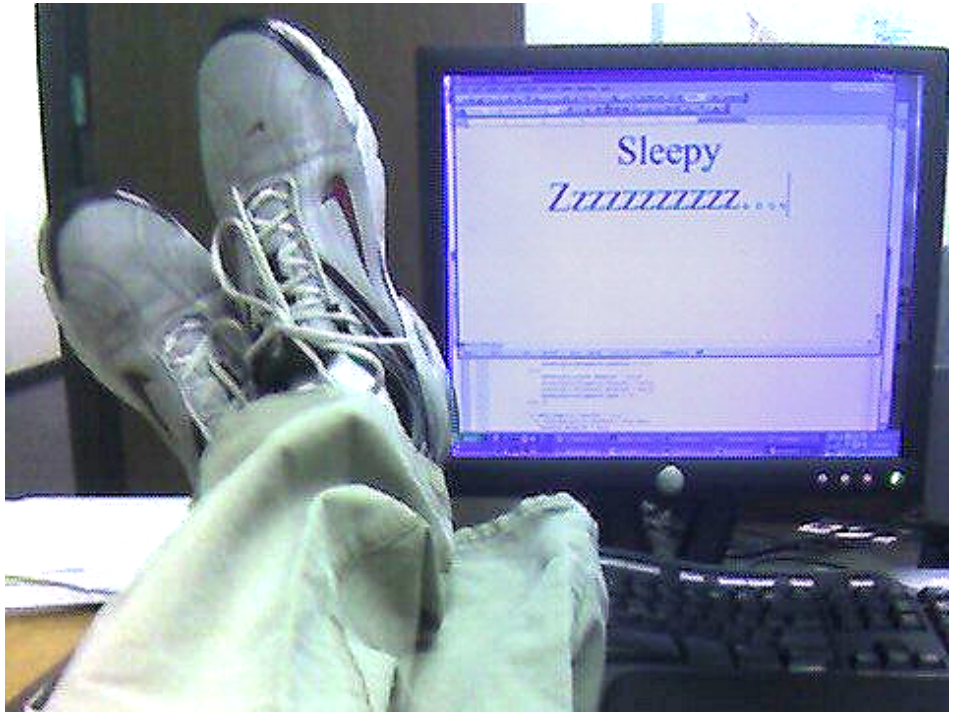
nanoHUB.org
an NCN project



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	nanoHUB.org
364,304	118,016	nees.org
63,487	32,236	pharmaHUB.org
62,495	5,492	HABRIcentral.org
53,507	13,487	vhub.org
49,559	23,168	GlobalHUB.org
47,972	6,976	ciHUB.org
47,085	12,788	cceHUB.org
46,083	5,166	PURR
45,833	5,473	iemhub.org
45,176	9,069	molecularHUB.org
41,048	8,078	StemEdHub.org

Global community

hubzero FOUNDATION

- 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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mmclennan@purdue.edu

http://hubzero.org/pressroom

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