

State of the Hub: 2013



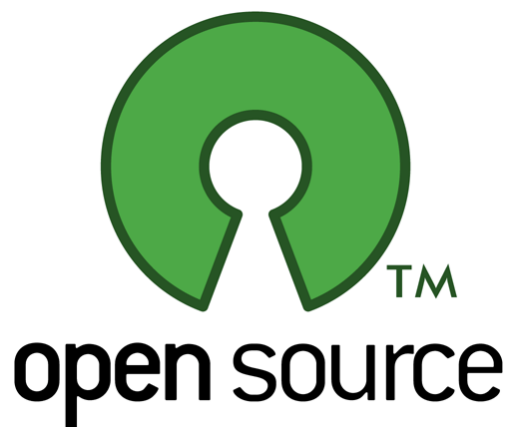
Michael McLennan, Ph.D.

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Purdue University

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What is HUBzero?



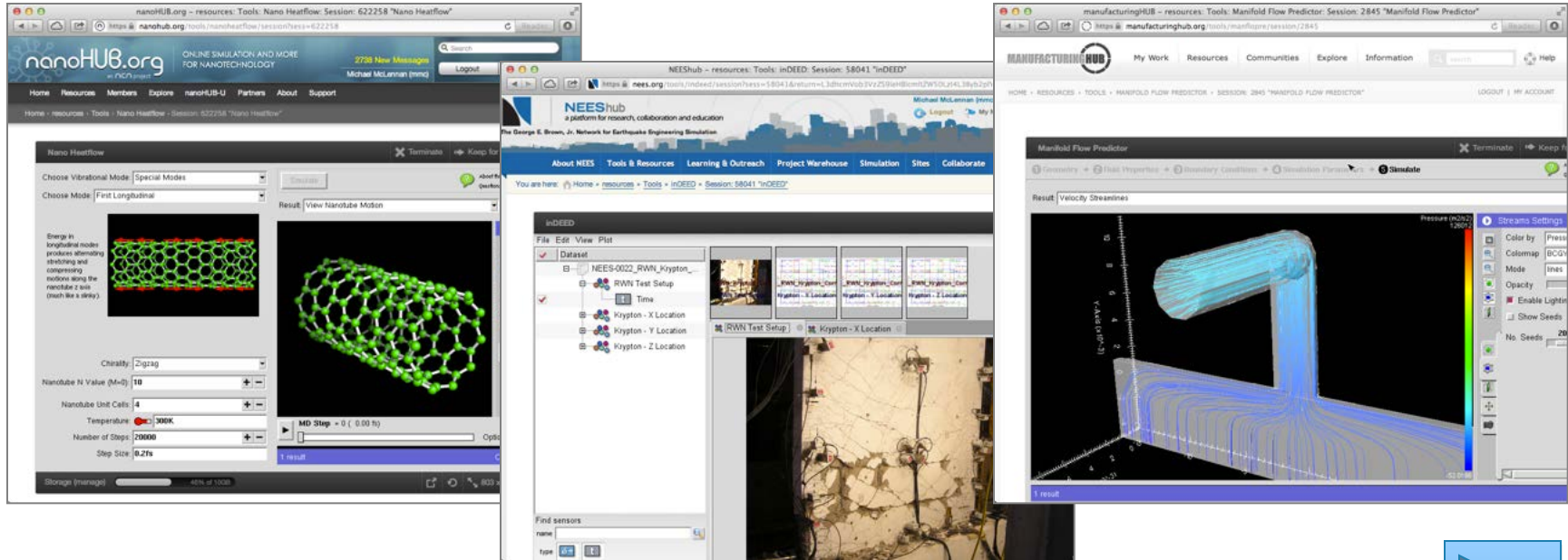
Open source software platform
used for building

“Science Gateways”

“Collaboratories”

“Hubs”

HUBzero: Simulation/Modeling Tools



- ✓ Powerful research codes
- ✓ Uploaded by researchers in the community
- ✓ Run on cloud/grid/cluster resources
- ✓ Integrated visualization



HUBzero: Databases and Digital Assets



Number	Building	Date	Team	Latitude	Longitude
A001		26-Jun	A	18° 23' 16.1" N	72° 18' 32.1" W
A002		26-Jun	A	18° 33' 15.7" N	72° 18' 10.7" W
A003(1)		26-Jun	A	18° 30' 42" N	72° 17' 14.6" W
A003(2)		26-Jun	A	18° 30' 42" N	72° 17' 14.6" W
A005		26-Jun	A	18° 31' 5.2" N	72° 16' 56" W
A006		27-Jun	A	18° 32' 55.1" N	72° 18' 11.5" W
A007		27-Jun	A	18° 32' 56.1" N	72° 18' 13.9" W

IS Number	Chemical Name	Description
11-1, 15039-26-5, 84044-81-6	O-β-D-Galactopyranosyl-(1→4)-D-Glucose	Lactose Monohydrate is a natural disaccharide, consisting of a galactose unit linked to a glucose unit.
9004-34-6	Microcrystalline cellulose	A colloid-forming, attrited mixture of Microcrystalline cellulose.
N/A	Lactose, Spray-Dried, Co-Processed	This is a co-processed excipient composed of spray-dried lactose and microcrystalline cellulose.
557-04-0	Octadecanoic acid magnesium salt	A compound of magnesium with a mixture of octadecanoic acid and stearic acid.
74811-65-7	Cellulose, carboxymethyl ether, crosslinked	Crosslinked Cellulose is the sodium salt of a carboxymethylated cellulose.
9083-38-1	Sodium carboxymethyl starch	Sodium Carboxymethyl Starch is a derivative of starch.
9050-36-6	Maltodextrin	Maltodextrin is a non-sweet, nutritive saccharide.



..... Additional materials available (5)

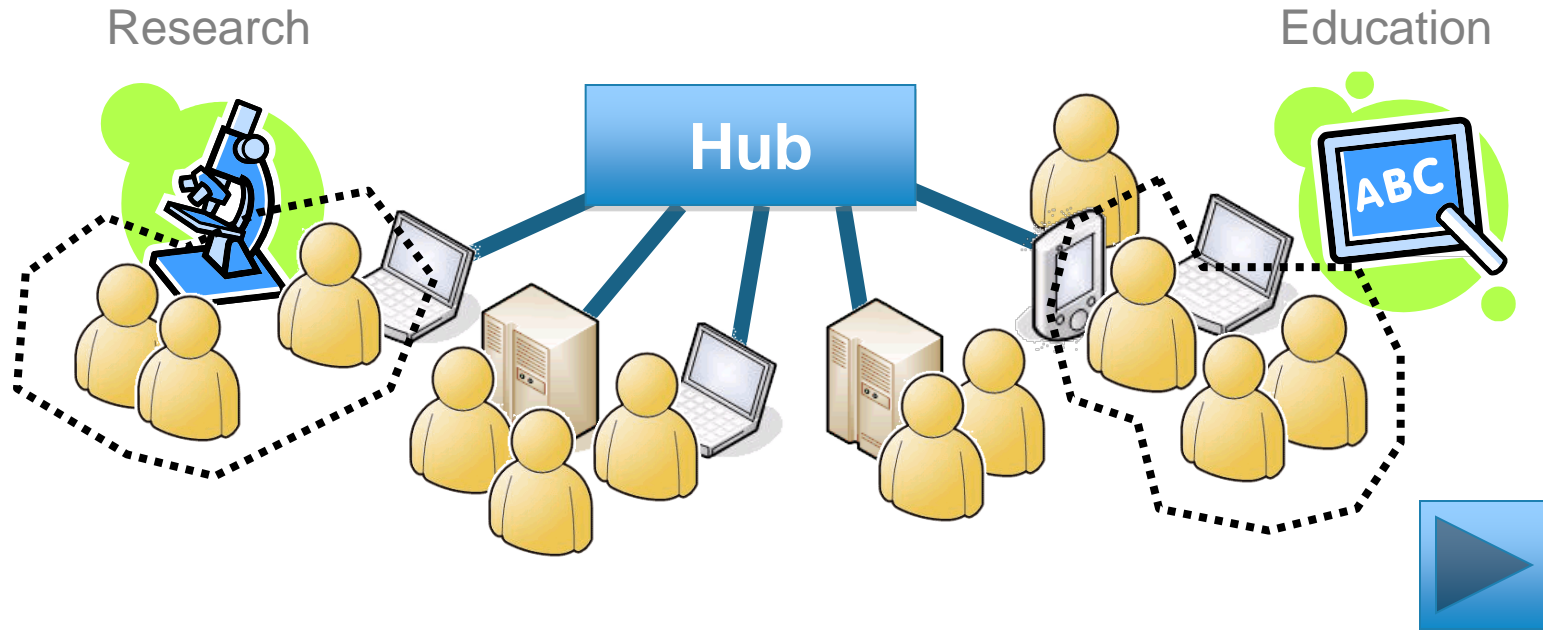
Version 1.0 - published on May 09, 2013
doi:10.4231/D32J68452 - cite this

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- ✓ Databases and digital publications
- ✓ Uploaded by researchers in the community
- ✓ Digital Object Identifiers and license options
- ✓ Data ↔ tools for analysis

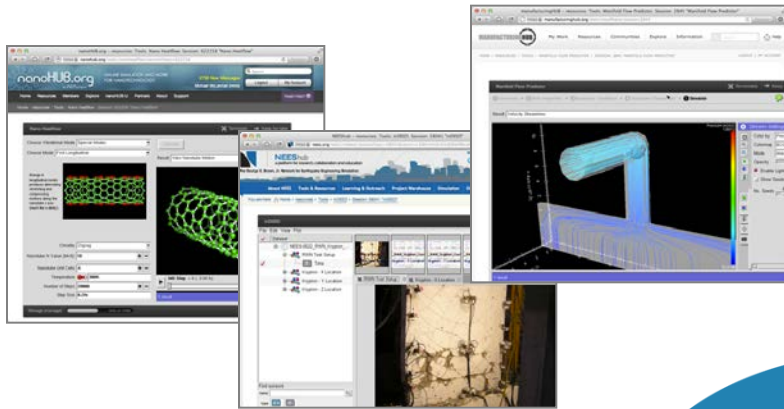


HUBzero: Group/Project Collaboration



- ✓ Private groups/projects for collaboration
- ✓ Messages, wikis, blogs, calendars
- ✓ Data repository with versioning

Platform for Scientific Collaboration



Computational Tools



Databases / Publications



Group/Project Collaboration

50+ Hubs for many disciplines



~1,000,000
visitors total

visitors	users
554,223	266,292
249,187	69,232
58,690	28,972
36,660	23,143
35,807	12,380
44,478	3,539
17,037	3,923
16,211	5,523
13,592	4,278
12,198	2,185
14,184	2,129
7,501	1,272



nanoHUB.org



nees.org



GlobalHUB.org



pharmaHUB.org



vhub.org



HABRIcentral.org



cceHUB.org



ciHUB.org



StemEdHub.org



iemhub.org



C3Bio.org



cleerHUB.org



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

Join the HUBzero Foundation



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

hubzero
PRINCIPAL



PARTICIPANT IN THE
HUBZERO FOUNDATION

PURDUE
UNIVERSITY

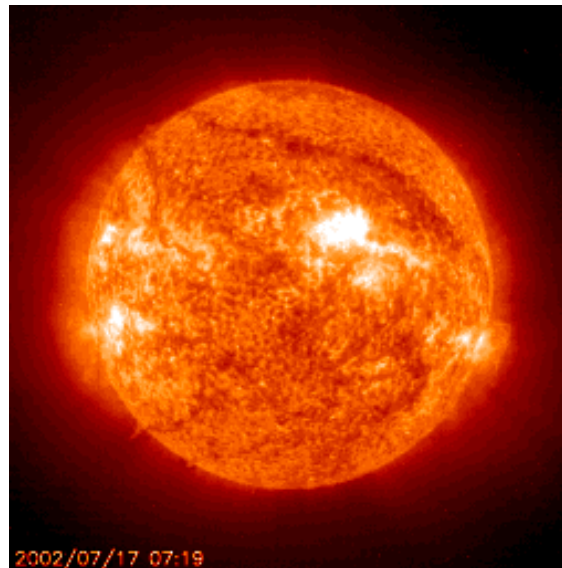


INDIANA UNIVERSITY

know innovation

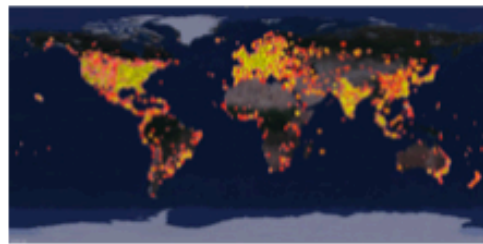
- ✓ Up-to-the-minute access to HUBzero enhancements
- ✓ Inside track on HUBzero development plans
- ✓ Participation in regular technical meetings
- ✓ Special recognition as “HUBzero Principal”

What's New?



February 5, 2013

Purdue researchers win \$14.5 million NSF grant to take nanoHUB.org to next level



Nearly 250,000 users participate in nanoHUB, an online meeting place for simulation, research, collaboration, teaching, learning and publishing. The red dots indicate users of online lectures, seminars, courses and teaching materials, while yellow dots indicate simulation users. (Photo illustration by Office of the Vice President for Research)

[Download Photo](#)

WEST LAFAYETTE, Ind. - Purdue University researchers have received a five-year \$14.5 million National Science Foundation grant to expand its widely used nanoHUB.org online science gateway.

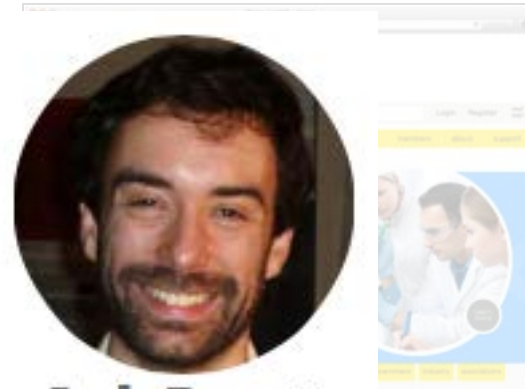
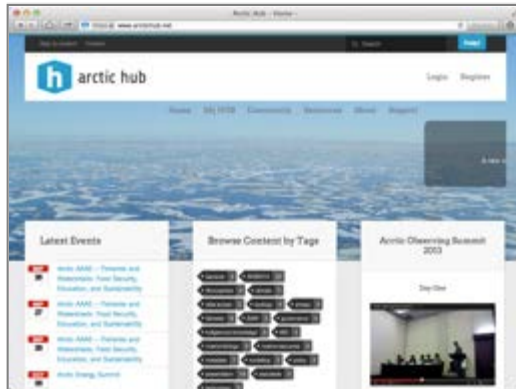
The Purdue-led Cyber Platform, a **for Computational Nanotechnology**, will assist researchers across the globe by developing a virtual society that shares simulation software, data and other innovative content to provide engineers and scientists with the fundamental knowledge required to advance nanoscience into nanotechnology.

"Thousands of times a day the leading researchers 'come' to Purdue through the globally unique nanoHUB," Purdue President Mitch Daniels said Tuesday (Feb. 5) in announcing the grant. "The new NSF investment is an affirmation of the brilliance of

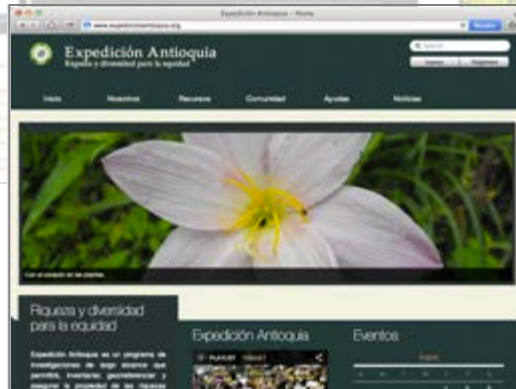
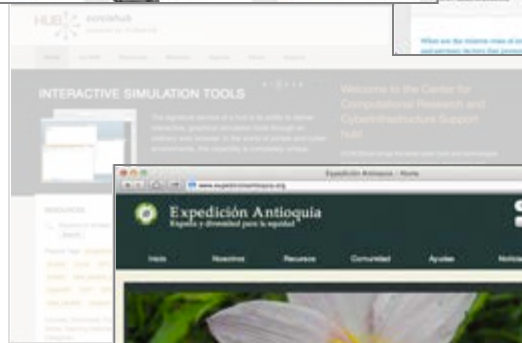


554,223 Visitors
266,292 Users
4,593 Resources
1,054 Citations

14 New Hubs!



Andy Burnett



Leidy Lorena Alzate-Vargas



Hear more from conference speakers

New Release!

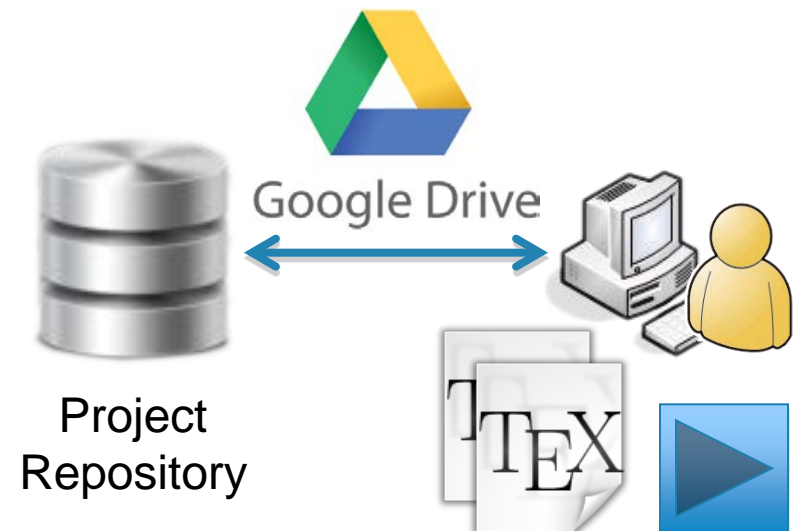


More than 60 new features!

New Feature: Data Management



- ✓ Sync repository with Google Drive
- ✓ Compile/preview LaTeX documents



New Feature: Data Publication



- ✓ Create interactive databases
- ✓ Publish digital assets that can be cited



New Feature: Learning Mgmt System



- ✓ Drag-and-drop builder for new courses
- ✓ Lectures, quizzes, homeworks, exams
- ✓ Hands-on activities with simulation tools
- ✓ Discussion forum for instructor interaction



<http://nanohub.org/u>

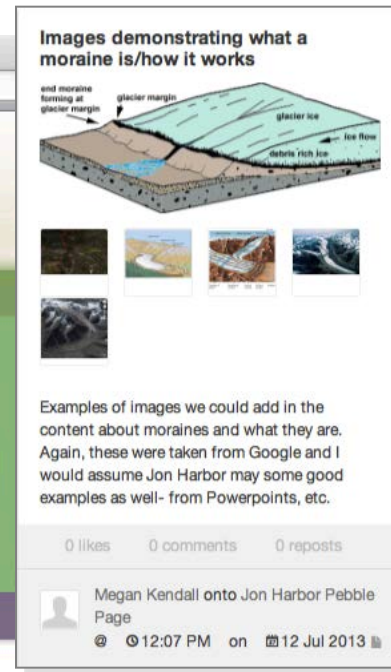


<http://purduenext.purdue.edu>

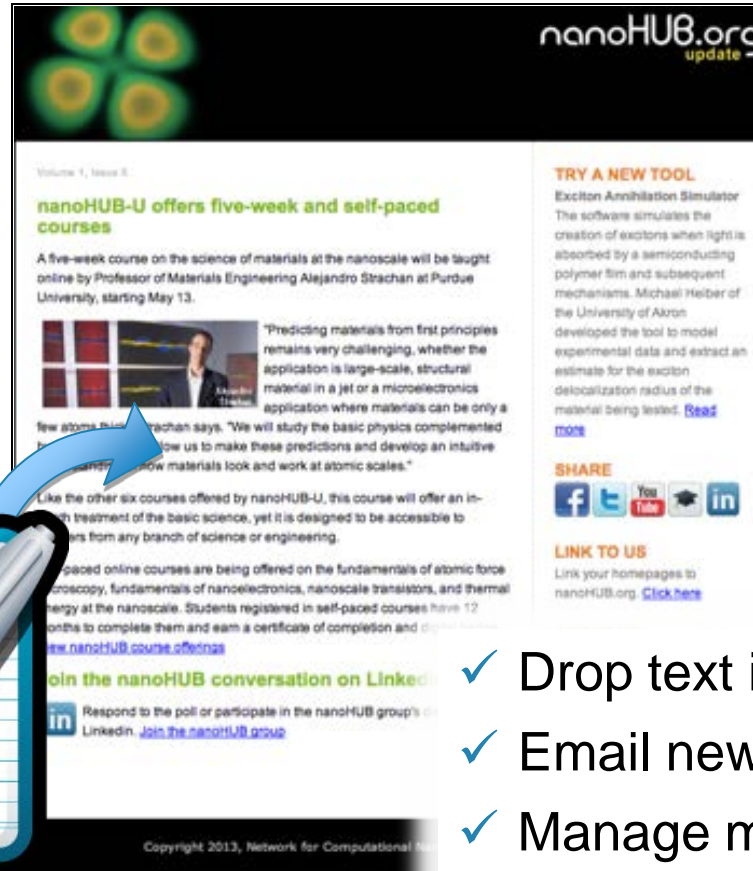
New Feature: Collections



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



New Feature: Newsletters



- ✓ Drop text into HTML templates
- ✓ Email newsletters to mailing lists
- ✓ Manage multiple mailing lists
- ✓ Easy “unsubscribe” option

Much, Much More



Calendar Aggregation

New Wiki Parser

Joomla 2.5 Upgrade

Member Stats

Rapture Runtime Collection

Vtk Plotting Modes

Support Ticket Watch List

Citation Detail View



Internal Wiki Search

iCal Import

Video Time Tracking

Parameter Sweeps

SGE Job Protocol

Multi-File Upload in Projects

Cron Framework

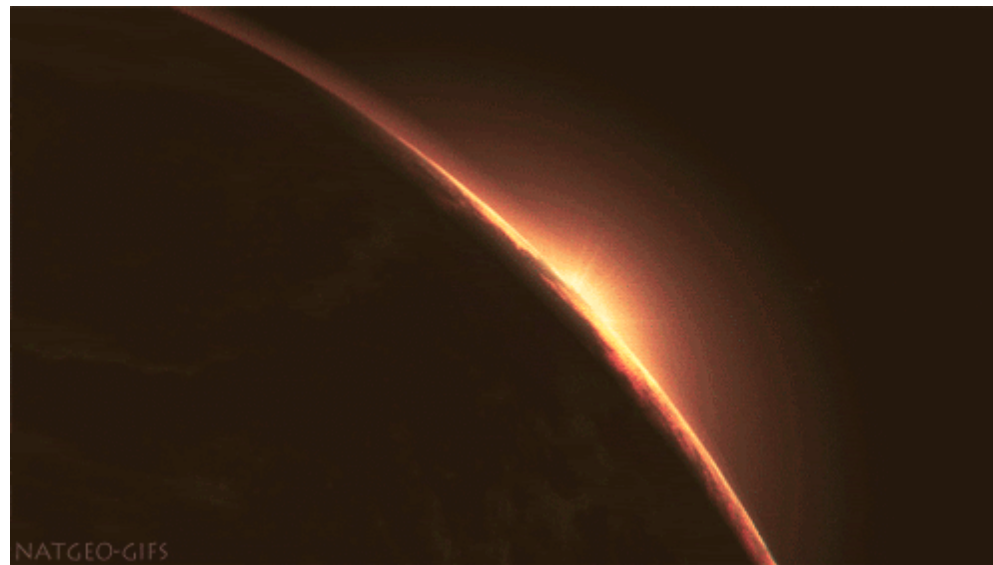
Job Notification Email

<http://hubzero.org/download>

VMware virtual machine images

Debian packages

What's Next?



BOINC: Volunteer Computing

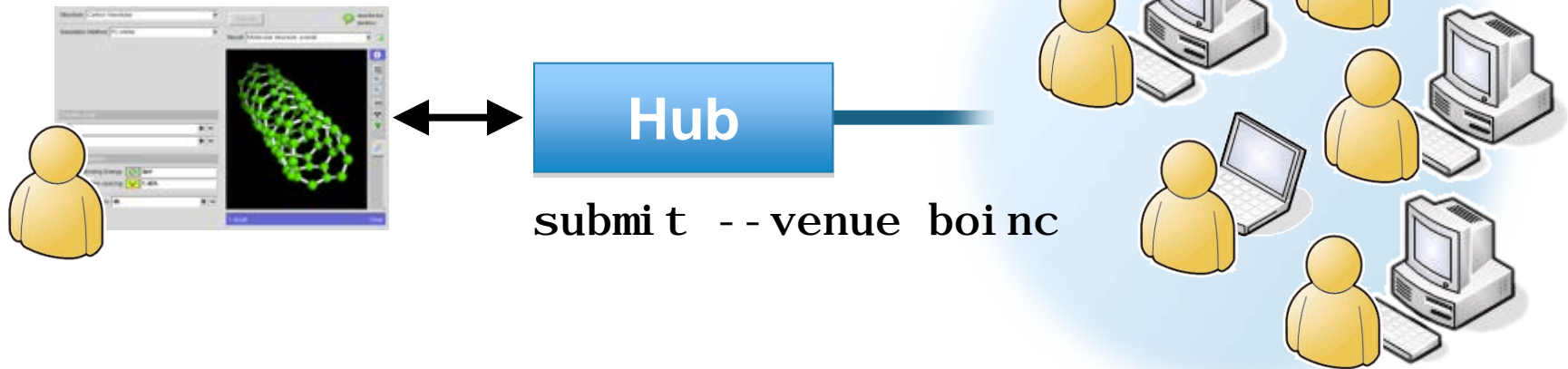


David Anderson

- ✓ New “submit” venue for computation
- ✓ Dispatch thousands of jobs via one command



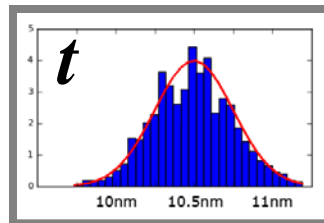
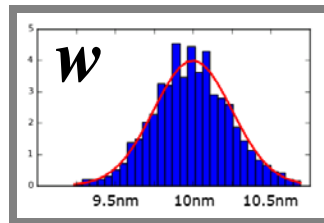
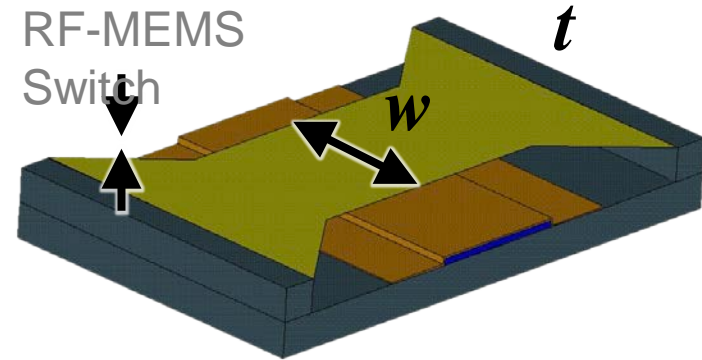
Volunteer Network



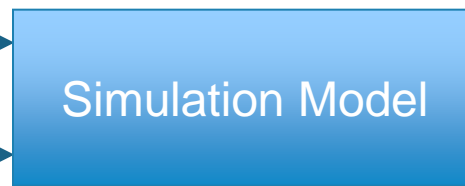
Uncertainty Quantification



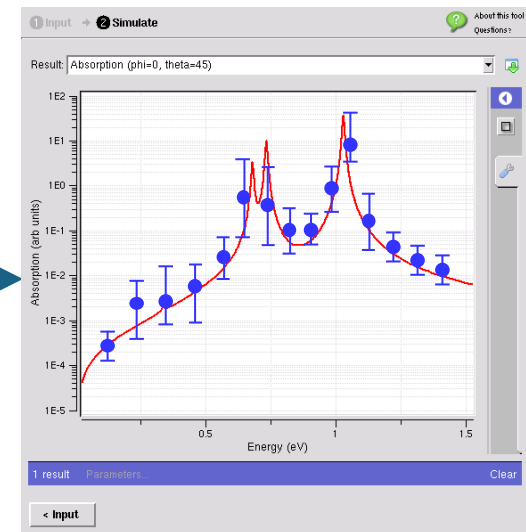
Alejandro Strachan



Variation in input parameters



Stochastic Collocation



Uncertainty in Outputs

International Hosting Sites



- ✓ “Content Delivery Network” for tool sessions
- ✓ Amazon for hosting services and execution hosts

Just for Fun



iPad App
for nanoHUB
Download
from the
iTunes Store

Hub-in-a-Box
running on Raspberry Pi
Stop by and check out
the demo



Raspberry Pi™



Price: **\$35.00**

Get Involved!



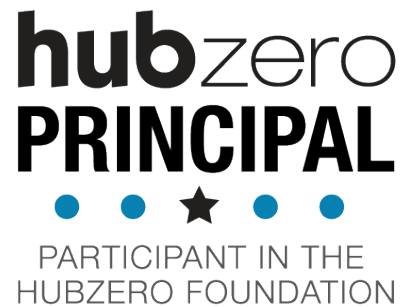
1

Download and
have at it!



2

Join the
Foundation



3

Consulting and
Hosted Solutions



Thursday

Plenary Session

Ale Strachan, Michael Zentner,
Meredith Drosback, Gerry McCartney,
Chris Dagdigan

Lunch

Applications
and
Experiences

Configuring
& Using
Hubs

Building
Scientific
Tools

Banquet Dinner
Gameshow



Friday

Plenary Session

David Anderson, Andy Burnett,
Mark Lundstrom, Supriyo Datta,
Ann Christine Catlin, Eric Letvin

Lunch

Hub Owners' Meeting

Data
Management
and
Publication

HUBzero
Web
Development

Demos
Q&A with
HUBzero
Team