

 @hubzeroplatform

 hubzero

HUBzero:

A Platform for Scientific Research, Education, and Collaboration

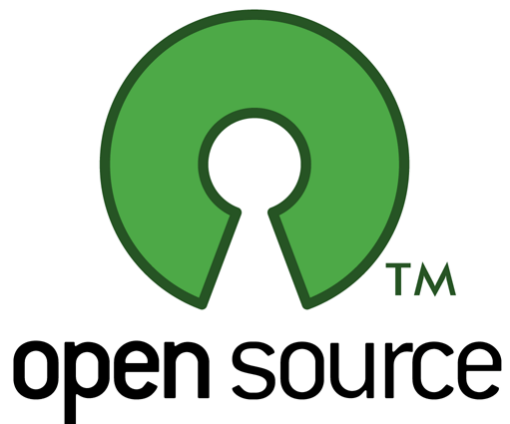
Michael McLennan, Ph.D.

Director, HUBzero® Platform for Scientific Collaboration

Purdue University

mmclennan@purdue.edu

What is HUBzero?



Open source software platform
used for building

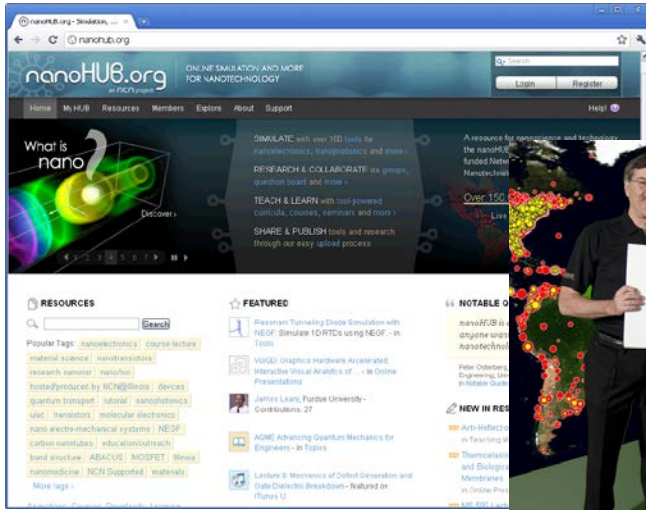
“Science Gateways”

“Collaboratories”

“Hubs”



Started with nanoHUB.org



Network for
Computational
Nanotechnology
Established in 2002

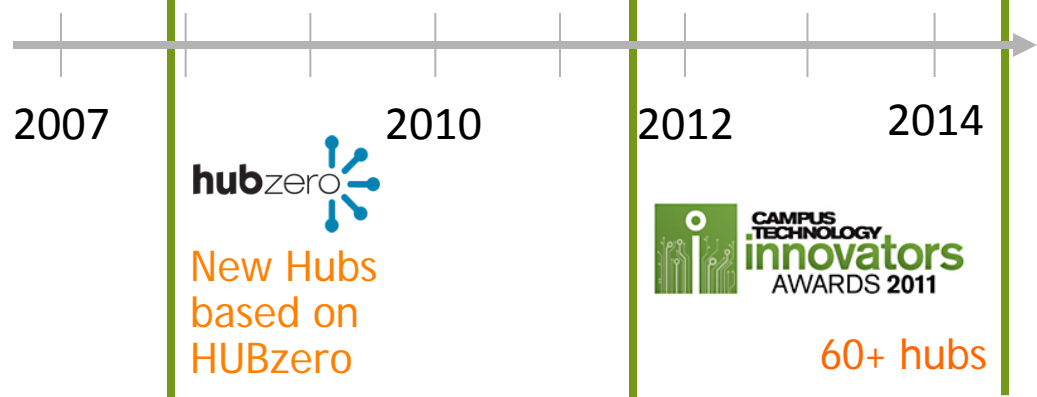
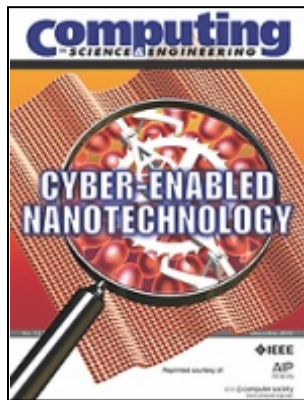
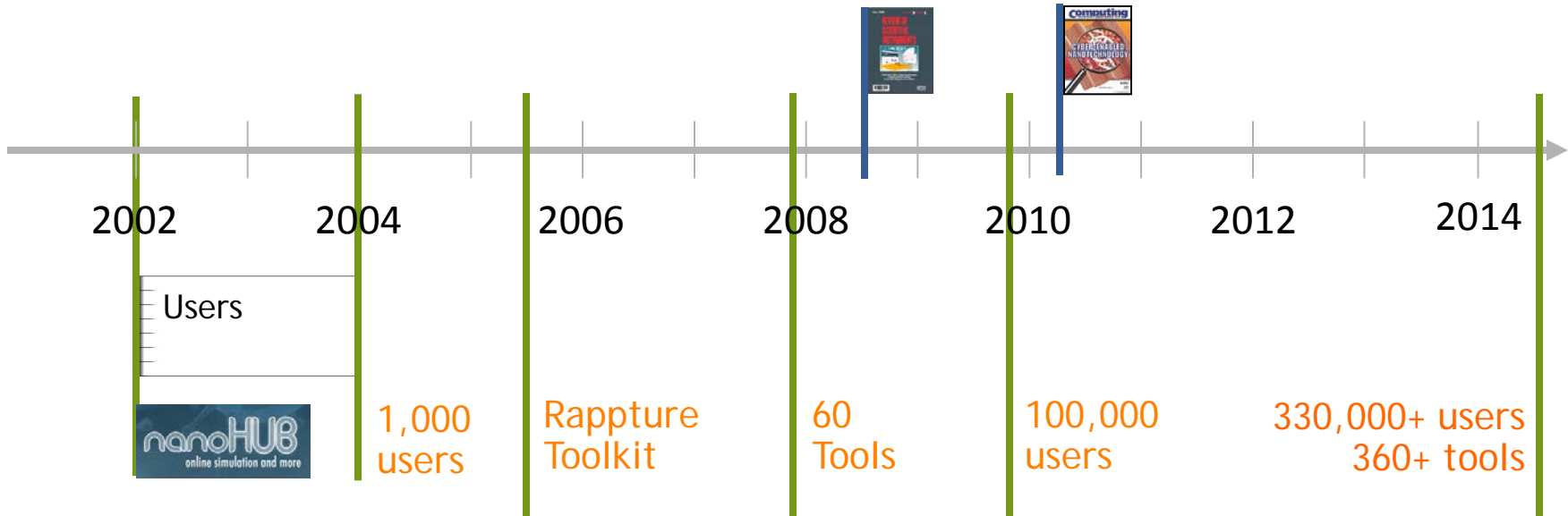


Awards
EEC-0228390
EEC-0634750
OCI-0438246
OCI-0721680

730,877 Visitors
324,560 Users
362 Simulation Tools
4,651 Resources
1,191 Citations
22,649 Students at 185 Institutions



How This Has Grown and Spread



60+ Hubs for many disciplines



~1,800,000
visitors total

visitors	users
730,877	324,560
422,031	137,460
65,389	8,645
63,419	23,725
62,918	7,468
53,422	26,432
51,771	11,267
42,710	5,052
40,234	9,817
37,957	9,416
36,588	4,386
34,879	3,315



nanoHUB.org



nees.org



HABRIcentral.org



GlobalHUB.org



ciHUB.org



pharmaHUB.org



molecularHUB.org



iemhub.org



vhub.org



cceHUB.org



PURR



DiaGrid.org

Global community

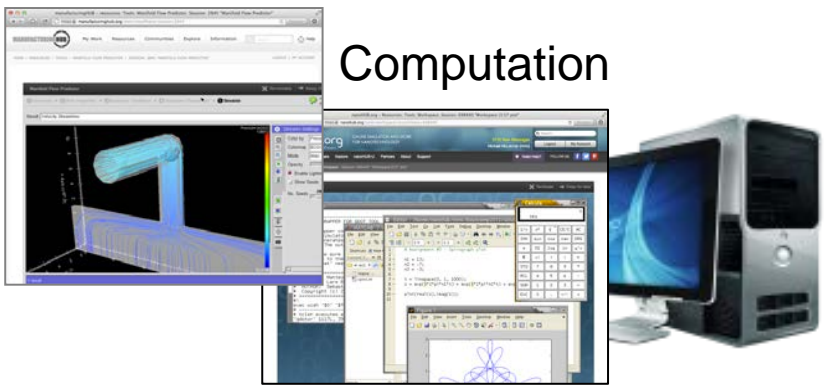
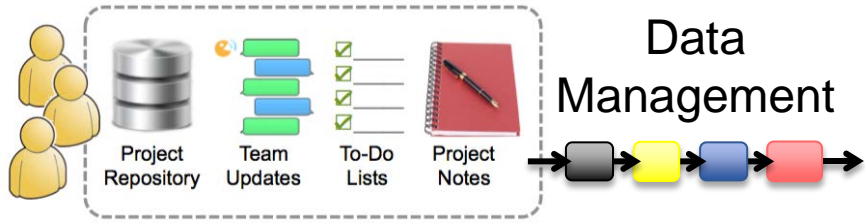


- Non-profit organization
- Independent owner of HUBzero code
- Promotes dissemination and outreach
- Coordinates software contributions

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

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

Built for the Academic Mission



A collage of educational content including a video lecture with a whiteboard, a slide titled 'Fundamentals of Nanoelectronics: Overview', and a quiz question.

4. A material with an energy momentum relation $E(p) \sim p^{\alpha}$ has

- $v(E) \sim E^{-1-(d/\alpha)}$
- $v(E) \sim E^{1+(d/\alpha)}$
- $v(E) \sim E^{1/(1/\alpha)}$
- $v(E) \sim E^{-1/(1/\alpha)}$
- none of the above

Research

Education

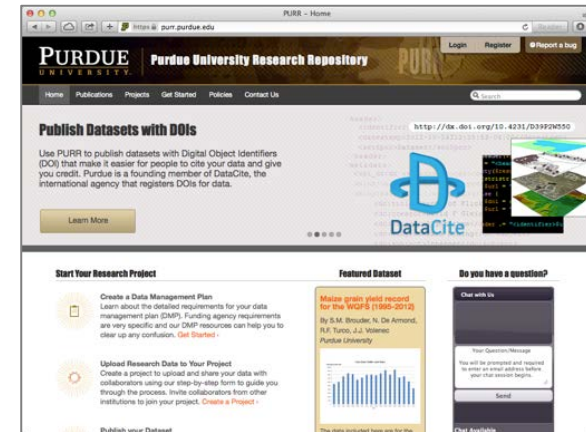
Case Study: PURR



Michael Witt



Purdue University Research Repository



<http://purr.purdue.edu>

- 1,300+** Proposals using PURR as data mgmt solution
- 469** Total projects
- 1,156** Active researchers (average team size: 5)
- 51,765** Total files

Integrating Data and Tools

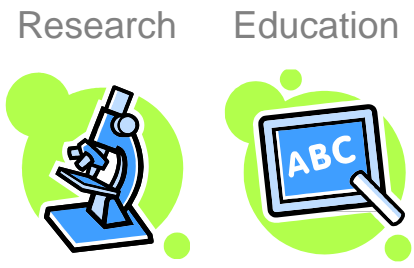


DOI resolver
Resolve a DOI string (e.g. 10.5284/1000164) by entering it below:

Submit

DOI
10.4231/D3F76671Z

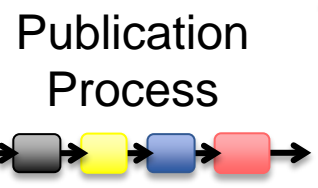
[http://nanohub.org/tools/mdshowcase/...](http://nanohub.org/tools/mdshowcase/)



Published Digital Assets

Publication Process

Project Repository Team Updates To-Do Lists Project Notes



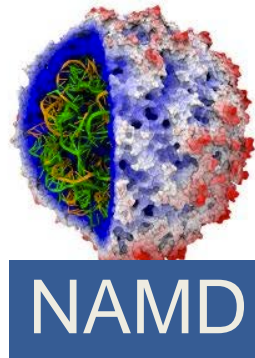
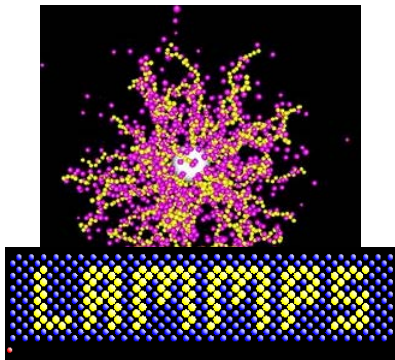
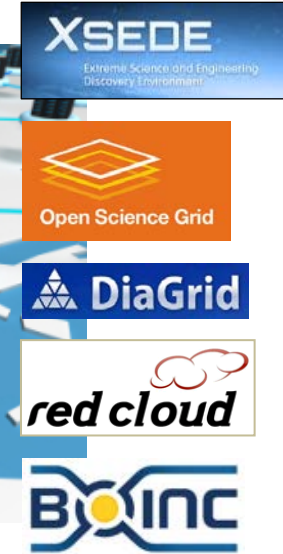
Molecular Dynamics Trajectory

10.4231/D3F76671Z

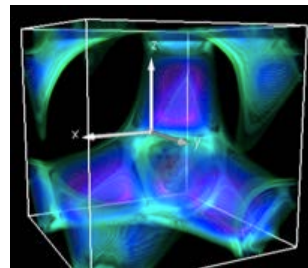
DOI DOI

Many people,
many projects

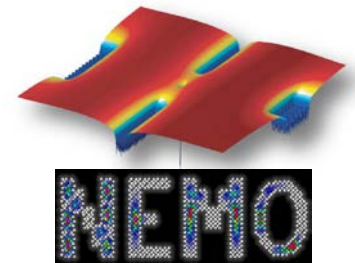
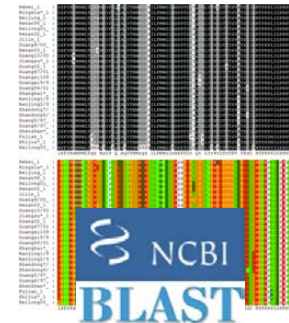
Research Computing



NAMD

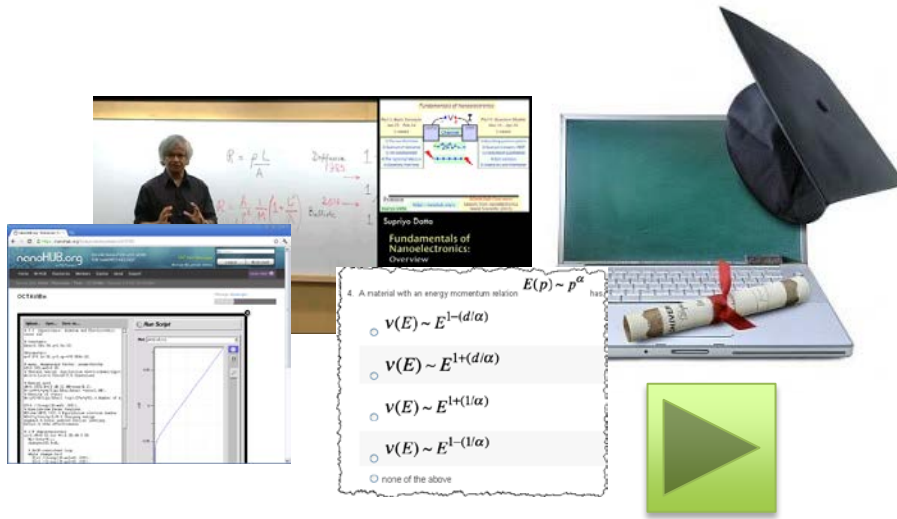


abinit



Access research codes and remote supercomputers

HUBzero: Online Education



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

Two Projects Using This Framework:



<http://nanohub.org/u>

13 nanotechnology courses



<http://purduenext.purdue.edu>

24 courses



How is HUBzero Developed?

Starting a New Hub

1

Download and have at it!



2

Join the Foundation



3

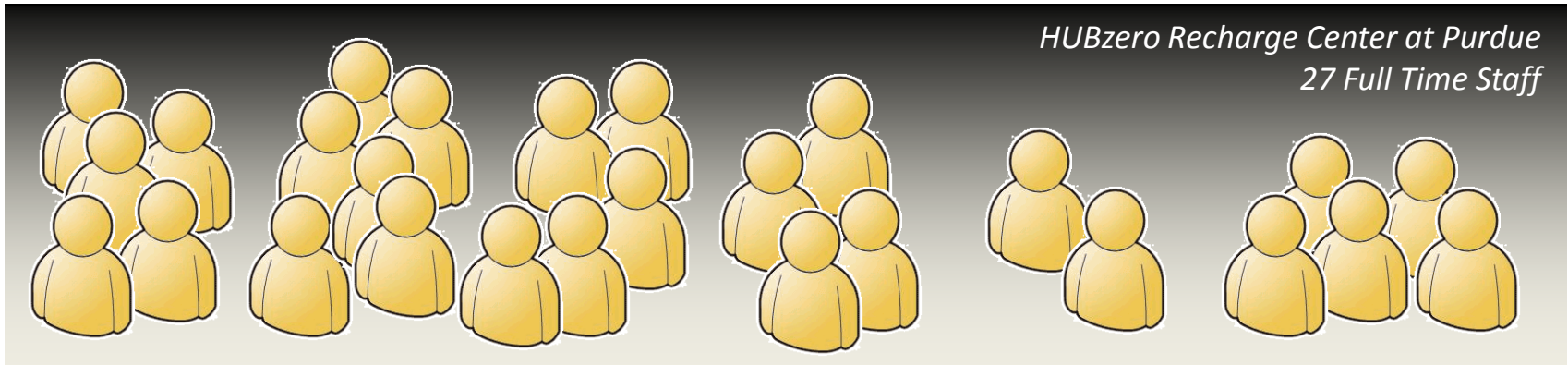
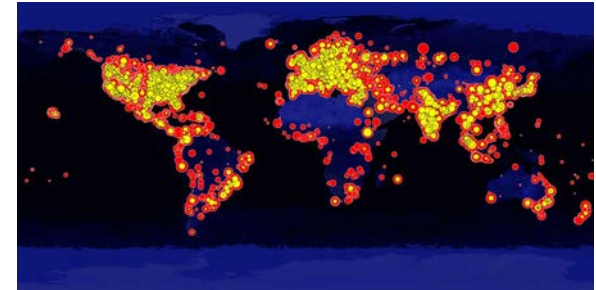
Consulting and Hosted Solutions



Support Staff

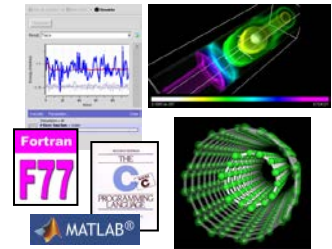
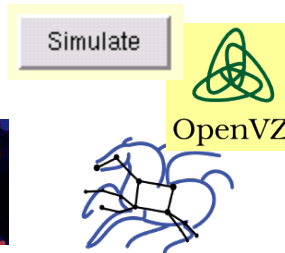
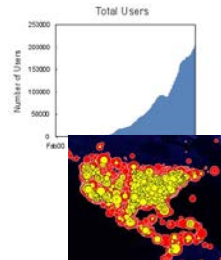


60+ hubs
1,800,000 visitors
hundreds of tools



HUBzero Recharge Center at Purdue
27 Full Time Staff

Support/Ops Web/Databases Analytics Middleware High Perf Computing Rapture Toolkit



How is HUBzero developed?



1 According to the goals of various hub projects



How is HUBzero developed?



2 By specific sponsored research projects



Carol Song

DIBBs: Integrating Geospatial Capabilities into HUBzero

PI: **Carol Song**

NSF #1261727, \$3.4M



Ann Christine Catlin

DIBBs: Building a Modular Cyber-Platform for Systematic Collection, Curation, and Preservation of large Engineering and Science Data

PI: **Santiago Pujol**, co-PI: **Ann Christine Catlin**

NSF #1443027, \$1.5M



Michael Zentner

Collaborative Research: The Science Gateway Institute (SGW-I) for the Democratization and Acceleration of Science

co-PI: **Michael Zentner**

NSF #1216870, \$225k



How is HUBzero developed?



3 By anyone in the open source community

HUBzero®
Individual Contributor License Agreement
("Agreement") V1.1

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Full name: _____ E-Mail: _____
Address: _____ Telephone: _____
City: _____ Fax: _____
Country: _____

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Get more
developers
involved



hubzero
FOUNDATION

HUBbub 2014

the 5th Annual HUBzero User Conference

Sept 29-Oct 1, 2014

Sheraton Indianapolis City Centre Hotel, Indianapolis, Indiana

<http://hubzero.org/hubbub>



Plenary Talks ♦ Hands-On Training ♦ Hub Case Studies



Victoria Stodden



David Lifka



Von Welch



Laura Paglione



Michael McLennan

Director, HUBzero® Project
mmclennan@purdue.edu

<http://hubzero.org/pressroom>

 @hubzeroplatform

 hubzero

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