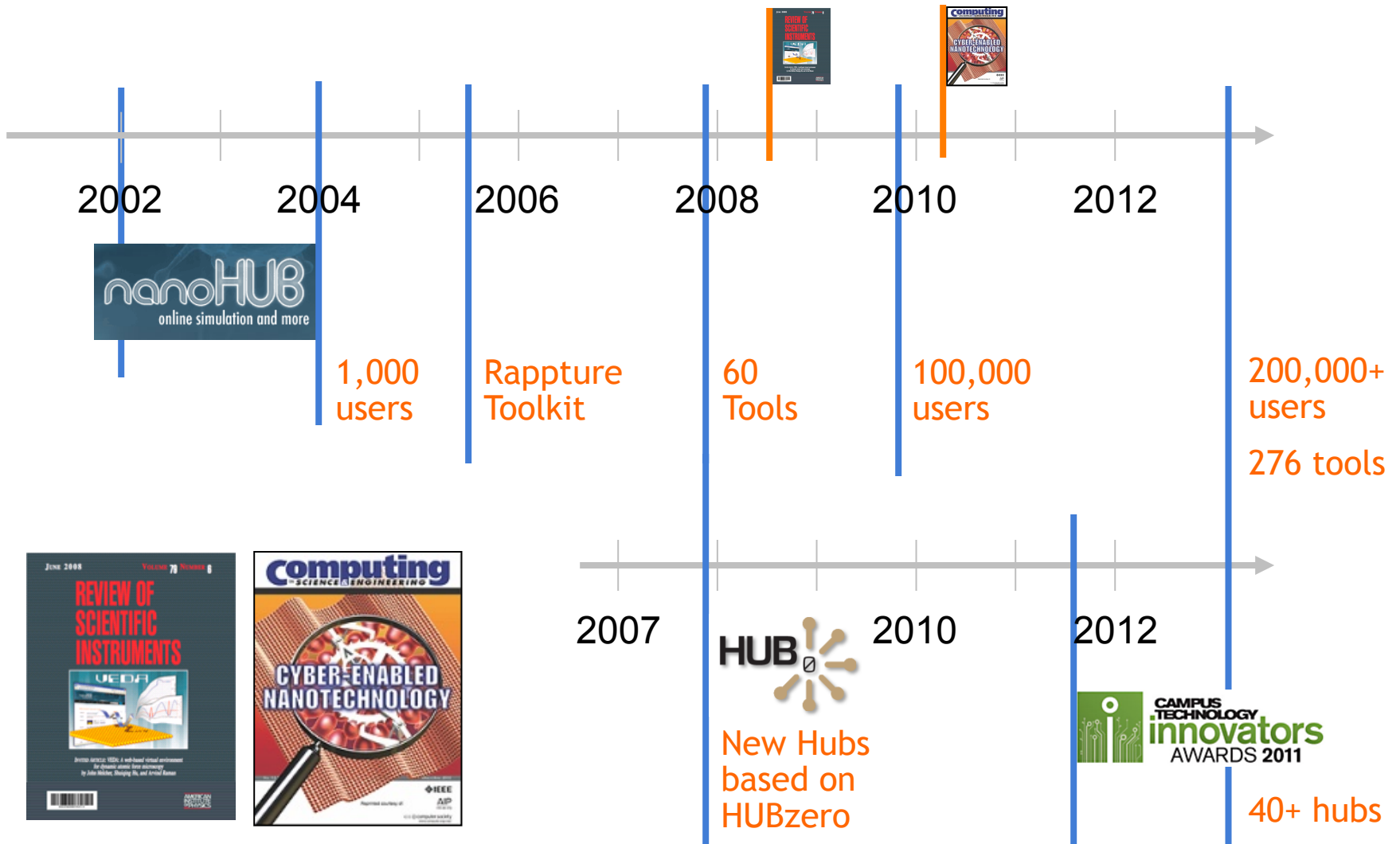




# HUBzero: A Web-based Platform for Research, Education, and Scientific Collaboration

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

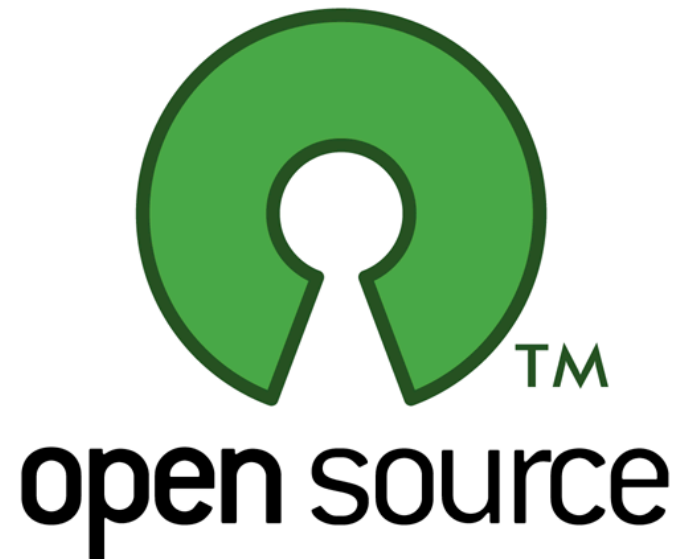
# How This Has Grown and Spread



# What is HUBzero?



A toolbox for building scientific web sites



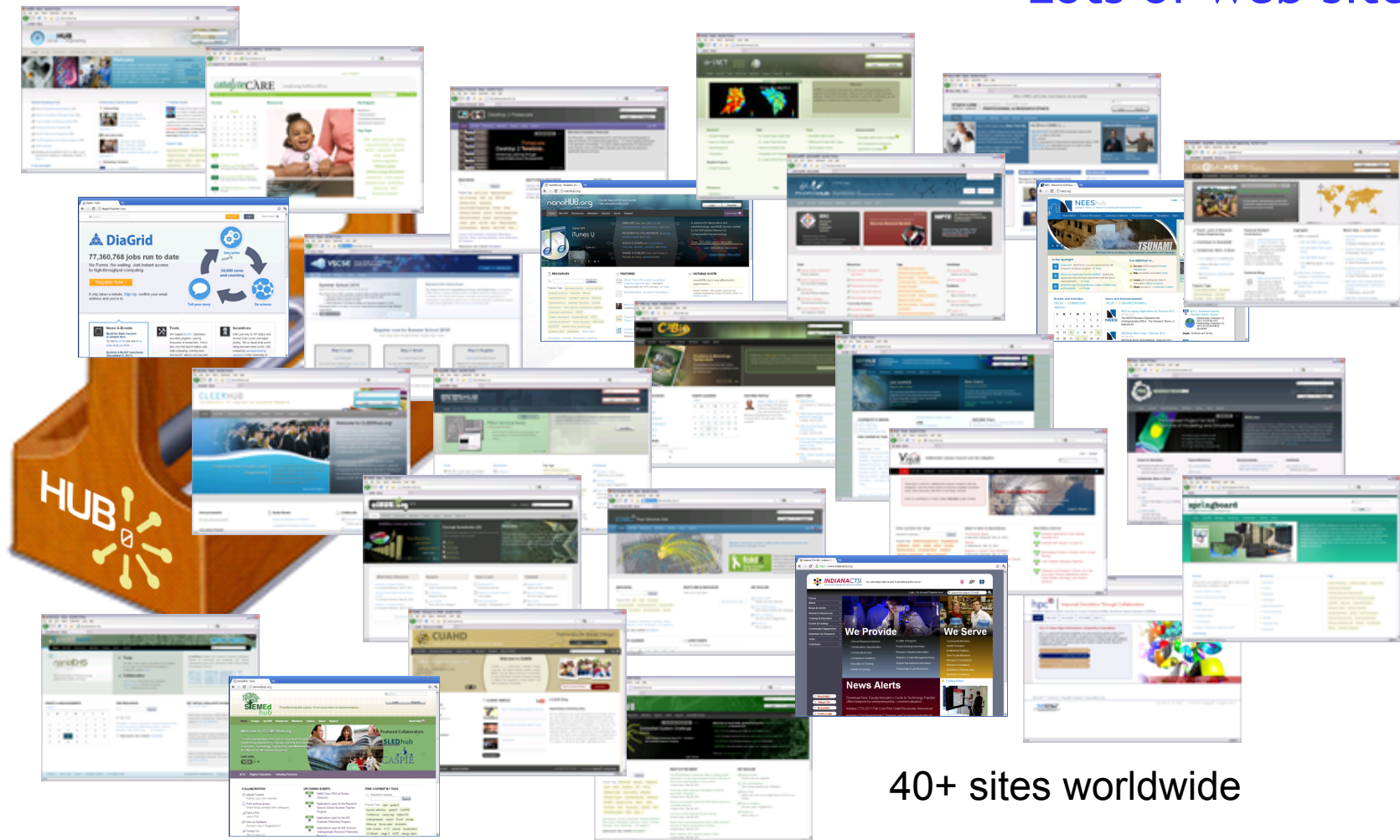
Lesser General Public License, LGPL-3.0  
Linux/Apache/MySQL/PHP

Download: <http://hubzero.org/download>

# What is HUBzero?



Lots of web sites

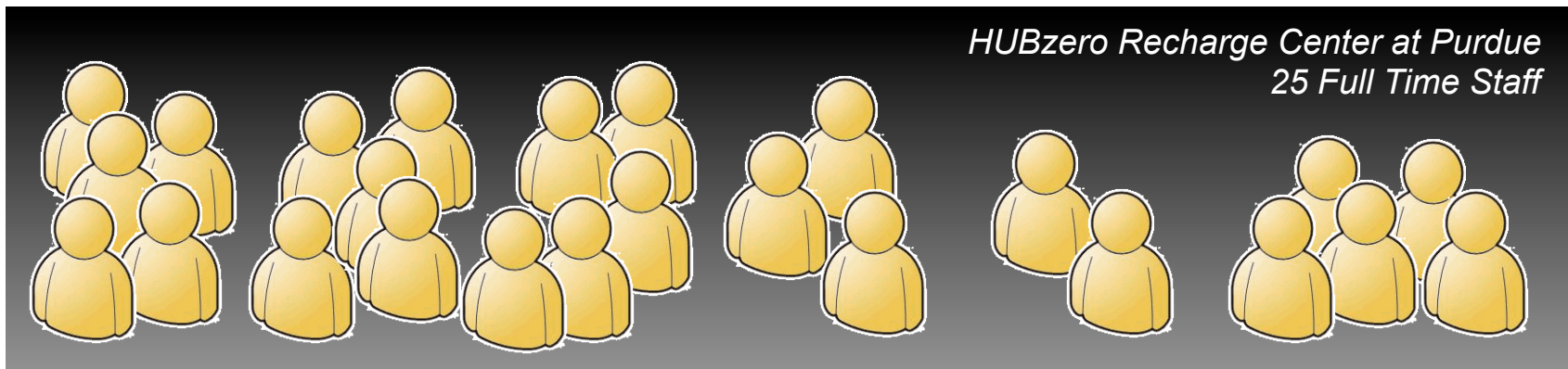
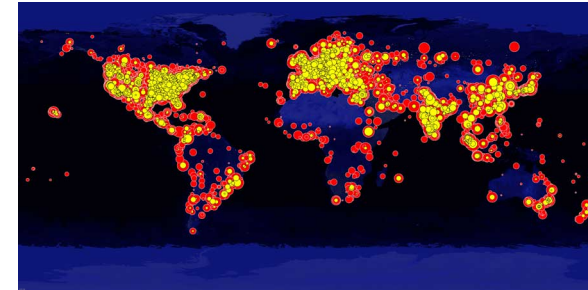


40+ sites worldwide

# Support Staff

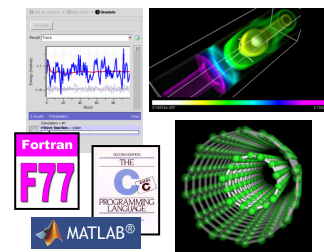
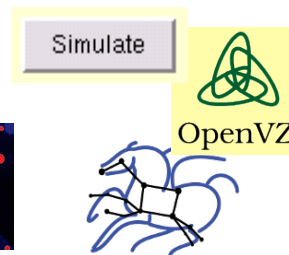
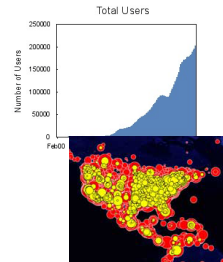
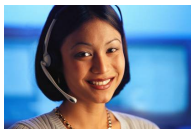


40+ hubs  
850,000 visitors  
hundreds of tools



*HUBzero Recharge Center at Purdue  
25 Full Time Staff*

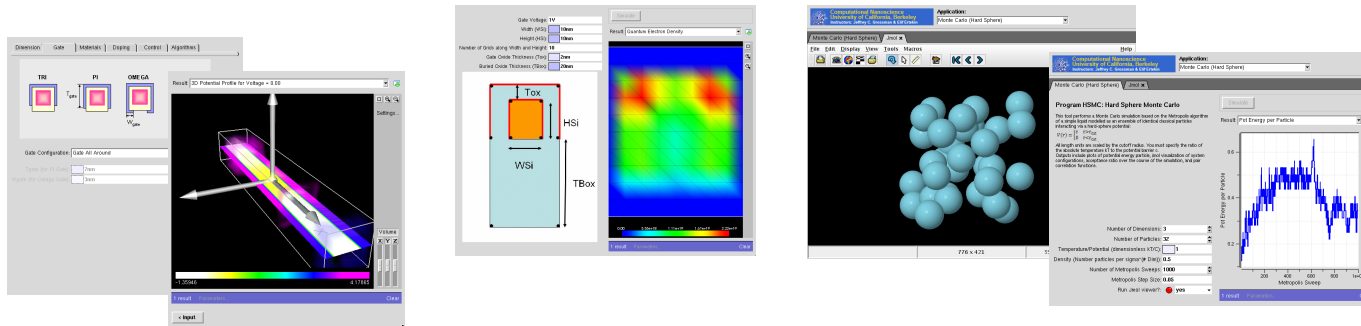
Support/Ops    Web/Databases    Analytics    Middleware    High Perf Computing    Rapture Toolkit





# An “app store” for scientists

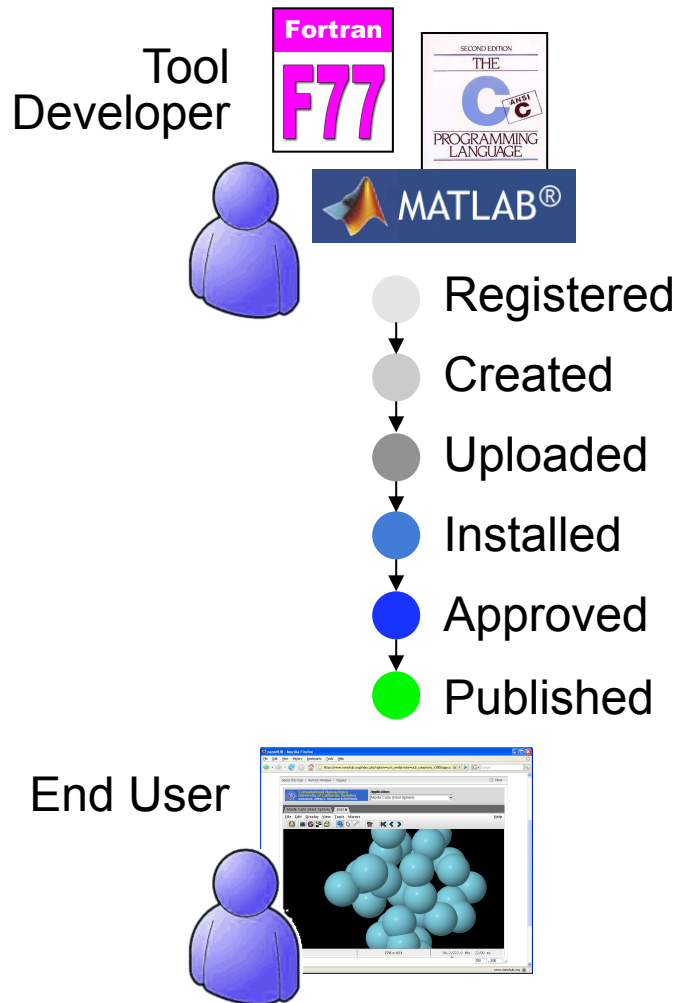
# Powered by Your Community



- Apps created/uploaded by your community
- Accessible from any machine
- Powered by the Cloud
- Intuitive interfaces with integrated visualization
- Easy to push out new versions
- Used in research and education



# Apps created/uploaded by your community



## What's Next?

Your latest code is installed and ready on nanoHUB.org. Please test your tool by clicking the button below to make sure that everything is working properly, as well as verify that the page describing your tool is created and displays correct information:

- ➔ Test your application: **Launch tool**
- ➔ [Review the page describing your tool](#)

## We're waiting for You

Once you tested your tool and verified that it is working properly, click here to let us know:

- ➔ [My tool is working properly. I approve it.](#)

Need to make changes? Once you've checked in your latest fixes, click here to let us know:

- ➔ [I've fixed my code. Please install the latest updates.](#)



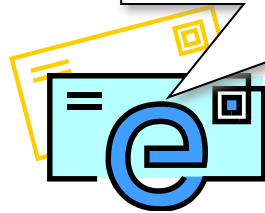


# Accessible from any machine



## Source code bundles

Hello,  
I am grad student from Kazakhstan.  
Your tool not compile for me. I get  
errors. That's a not very nice.



Hey, can you help me?

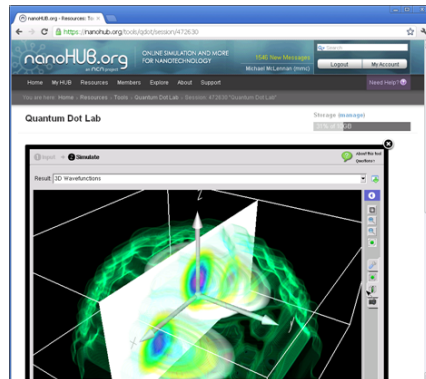
## Binaries



32-bit

64-bit

It doesn't work on my machine!



Live tools accessible  
from any web browser



# Interactive, Graphical Tools

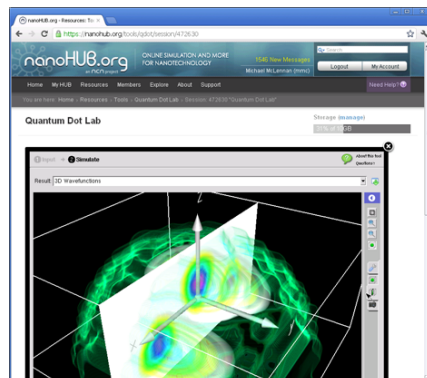
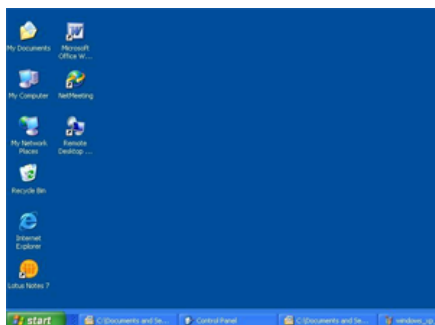


A screenshot of the nanoHUB.org web interface for the CNTbands tool. The browser address bar shows the URL: https://nanohub.org/tools/cntbands-ext/session/567400. The tool title is "CNTbands". The interface includes a "Structure" dropdown menu set to "Carbon Nanotube" and a "Simulation Method" dropdown menu set to "Pz orbital". A "Simulate" button is visible. The "Result" dropdown menu is set to "Molecular structure: overall". The main display area shows a 3D ball-and-stick model of a carbon nanotube, with carbon atoms represented by grey spheres and hydrogen atoms by white spheres. The nanotube is shown in a perspective view, appearing as a cylinder. To the left of the 3D view, there are input fields for "Chirality (n,m)" with values "n: 7" and "m: 0". Below that, "Model parameters" include "Tight Binding Energy" set to "3eV" and "Carbon-carbon spacing" set to "1.42A". A "Length in 3-D view" is set to "40". At the bottom of the interface, there is a "Storage (manage)" indicator showing "42% of 10GB" and a "964 x 594" resolution indicator. A blue play button icon is overlaid on the bottom right corner of the screenshot.

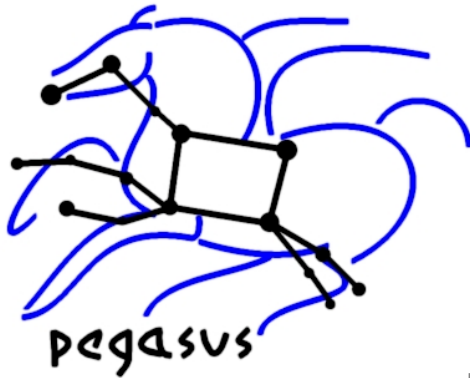
# Powered by the Cloud



Locally  
Installed  
Program



# Scientific Workflows



Ewa Deelman

USC Information Sciences Institute

## *Computational workflows:*

- Manage thousands of runs
- Simplified access to Condor
- “submit” Pegasus workflows
- Integrate into simulation tools



# Real research codes



The image shows a screenshot of the nanoHUB.org website, which is an online simulation and more for nanotechnology. The website features a navigation menu, a search bar, and several sections including 'Resources', 'Featured', and 'Notable Quote'. A 3D molecular simulation of a protein structure is overlaid on the right side of the screenshot.

The image shows a screenshot of the ManufacturingHub website, which is a platform for manufacturing simulation. The website features a navigation menu, a search bar, and several sections including 'Announcements', 'Success Stories', and 'Collaborate, Work, & Share'. A 3D simulation of a mechanical part is overlaid on the right side of the screenshot.

OpenFOAM

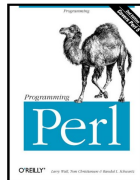
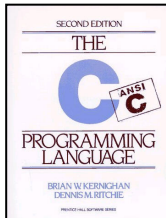
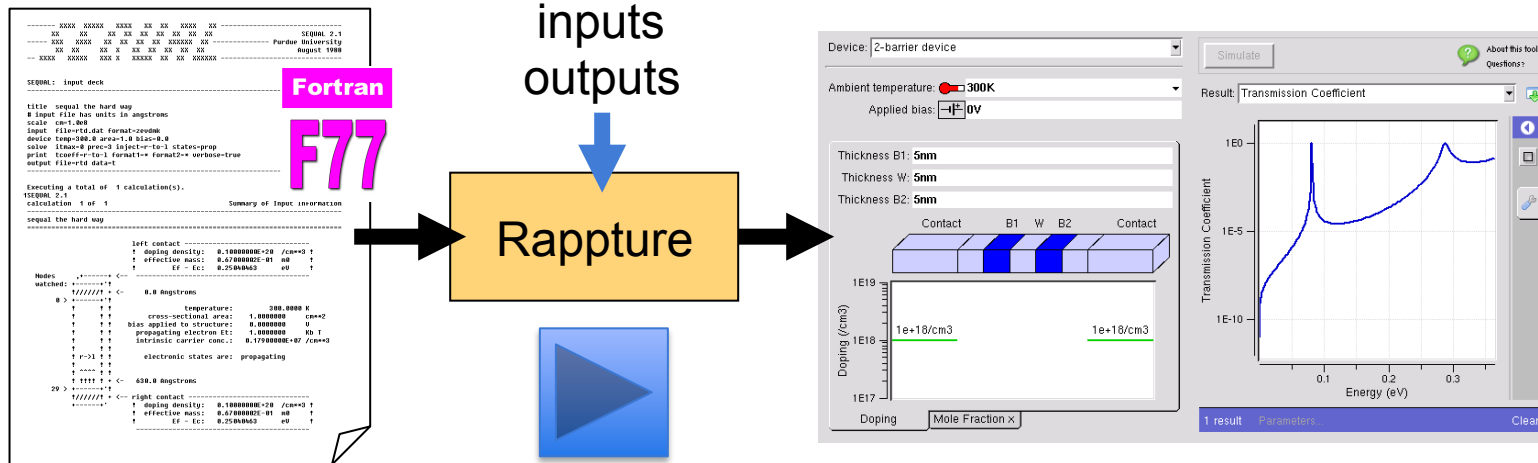
The image shows a screenshot of the NEEShub website, which is a network for earthquake engineering simulation. The website features a navigation menu, a search bar, and several sections including 'In the Spotlight', 'Use NEEShub to...', and 'Events and Activities'. A graph titled 'Floor Displacement Time History under Canoga Park Record' is overlaid on the right side of the screenshot. The graph shows three plots: 'Ground Acc. (g)', 'Disp. (in)' for the 3rd Floor, and 'Disp. (in)' for the 2nd Floor. The x-axis represents time in seconds, ranging from 0 to 25. The y-axis represents acceleration in g and displacement in inches.

OpenSees

The image shows a screenshot of the cceHUB website, which is a collaborative cancer engineering hub. The website features a navigation menu, a search bar, and several sections including 'Shared Modeling Tools' and 'Collaborative Cancer Research'. A graph titled 'Retention time 1 (seconds) versus retention time 2 (seconds)' is overlaid on the right side of the screenshot. The graph shows five data points for different compounds: Tetracosanoic, Tricosanoic, Docosanoic, Heneicosanoic, and Icosanoic. The x-axis represents retention time 2 (seconds) and the y-axis represents retention time 1 (seconds).

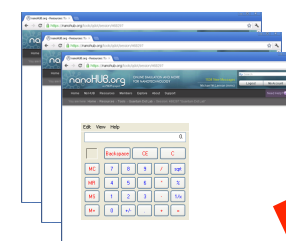
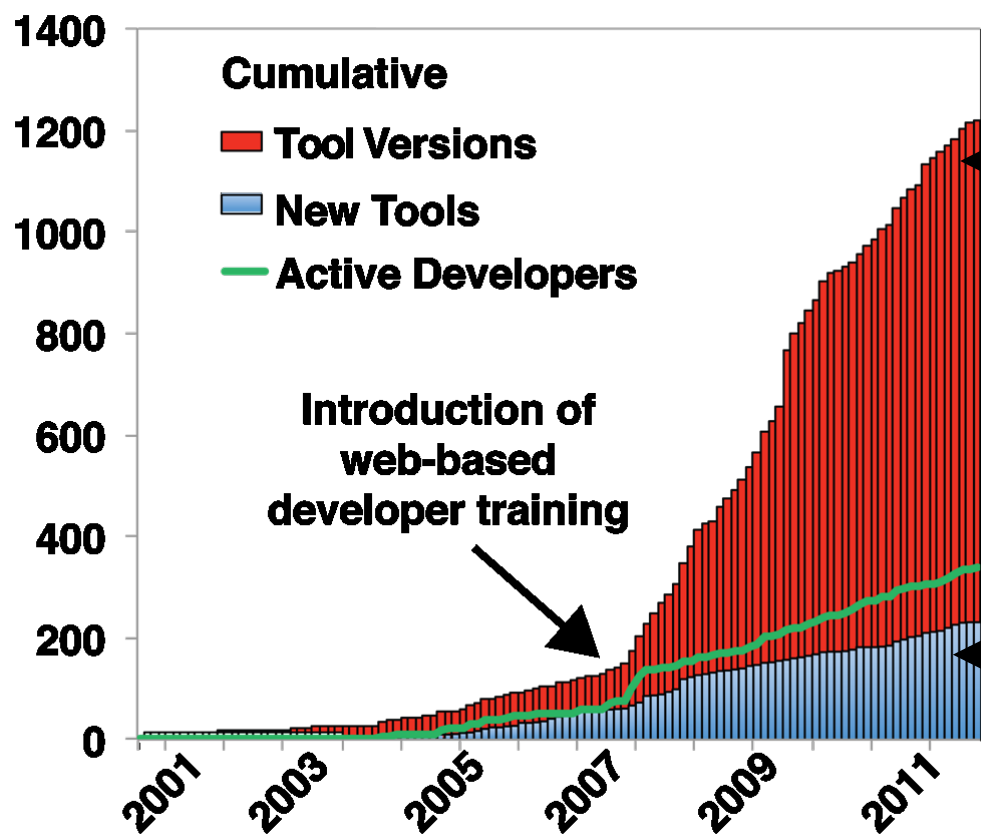
R

# Intuitive Interfaces that are Easy to Build

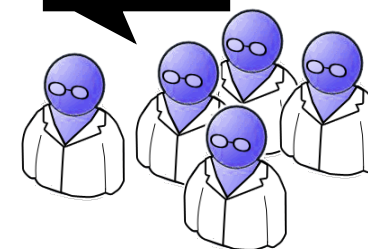
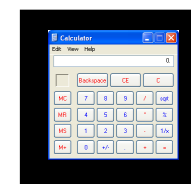


- Rapid Application Infrastructure
- Open Source ([rappture.org](http://rappture.org))
- Interface for real research codes
- Integrated visualization
- Works with your favorite programming language

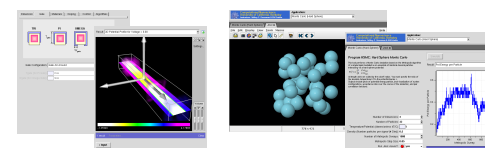
# Easy to push out new versions



New Versions



New Tools



# Used in research and education



52% outside  
NCN

Scaling the High-Performance Double-Gate SOI MOSFET down to 32 nm Technology Node with SiO<sub>2</sub>/sub2/-based Gate Stacks

Device Physicist  
**Enrico Sangiorgi**  
University of Bologna, Italy

Analysis of Scaling Strategies for Sub-30 nm Double-Gate SOI N-MOSFETs

Ultra-thin fully-depleted SOI MOSFETs: Special charge properties and coupling effects

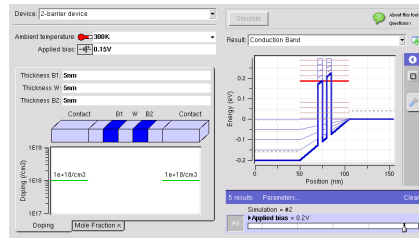
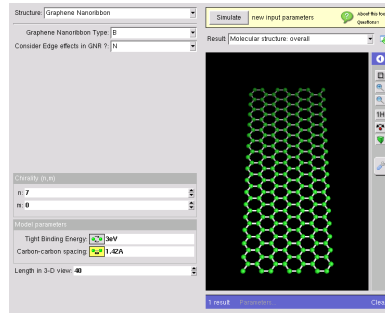
Experimentalist  
**Akiko Ohata**  
IMEP Minatec, France

Electrical characteristics related to silicon film thickness in advanced FD SOI-MOSFETs

|               |     |     |
|---------------|-----|-----|
| ● Research    | 338 | 79% |
| ● Infr./About | 26  | 6%  |
| ● Education   | 37  | 9%  |
| ● Cyberinfr   | 68  | 16% |

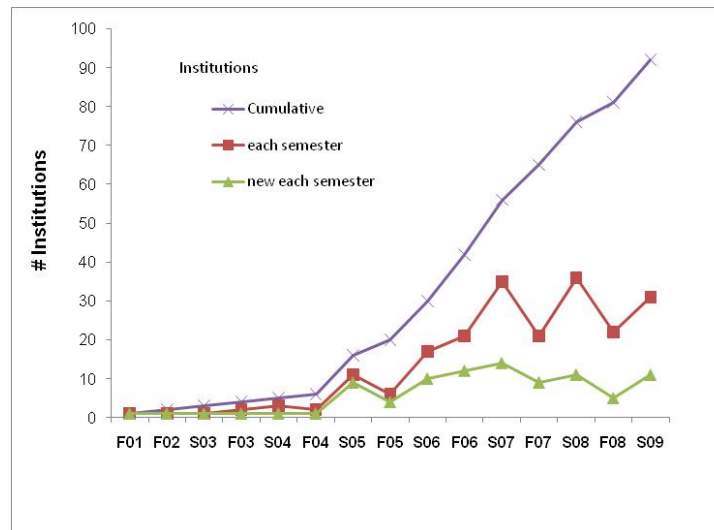
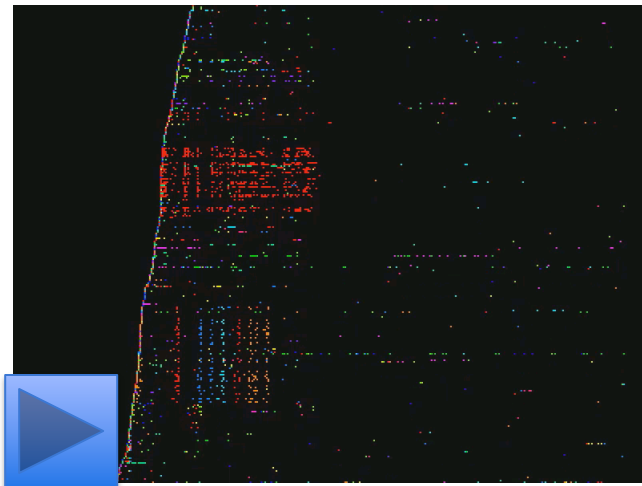


## Simulation/Modeling Tools in the Classroom



- Classroom demonstrations
- Virtual lab assignments
- Senior design projects

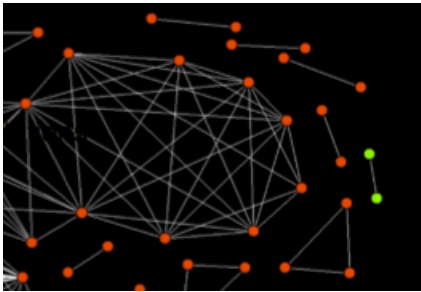
**14,000 students at 185 institutions**



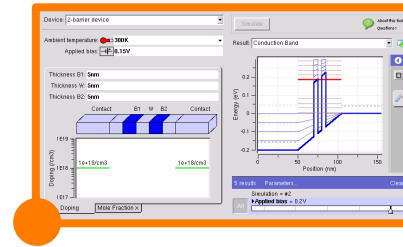
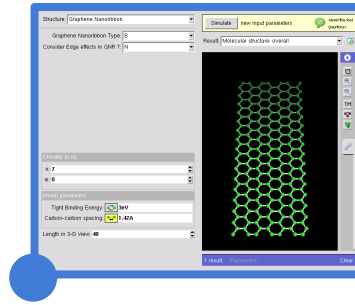
# Tools Span Education and Research



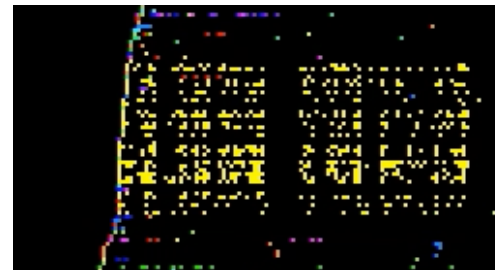
More citations



Research



Education



More  
classroom  
use

# 2

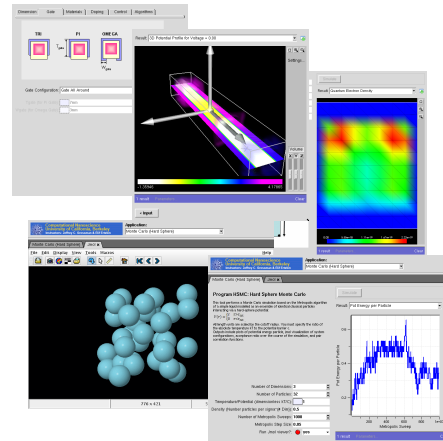
## A repository for data and publications

# Powered by Your Community

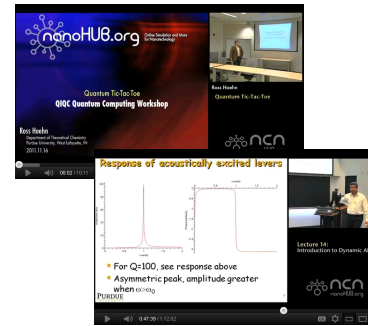


More than just apps

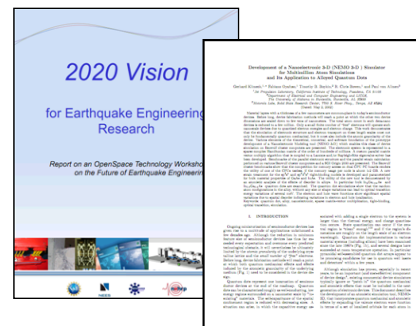
Simulation & Modeling Tools



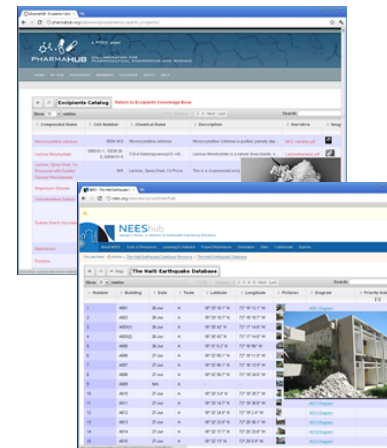
Seminars  
Tutorials



Tech Reports  
Teaching Materials



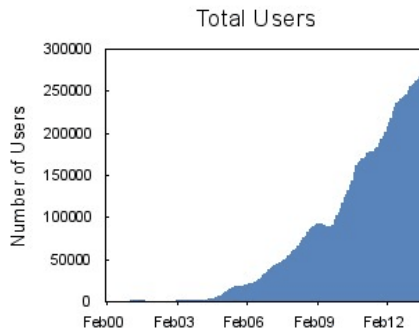
Data from Experiments



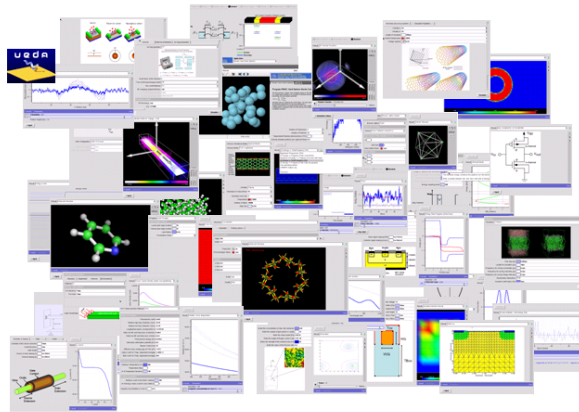
# Example: nanoHUB.org



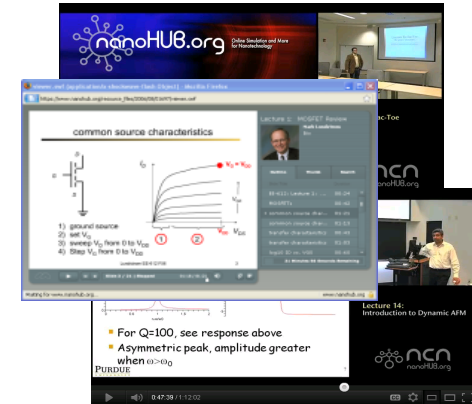
Network for  
Computational  
Nanotechnology  
Established in 2002



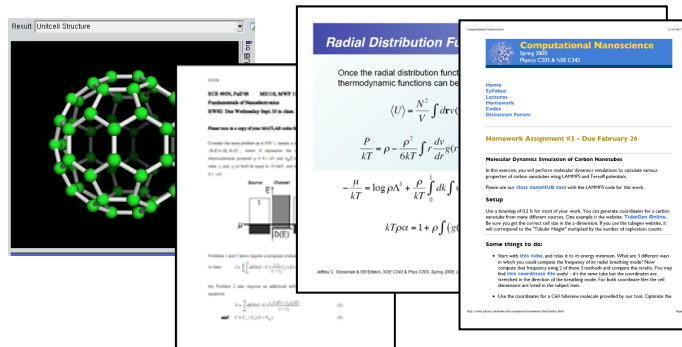
266,000 users



317 simulation tools



3,071 seminars



556 teaching materials

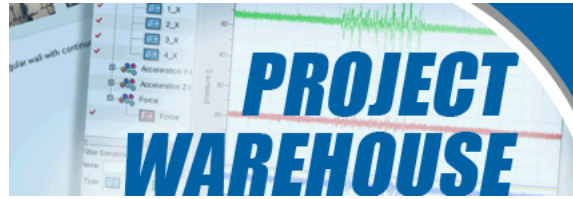


82 courses

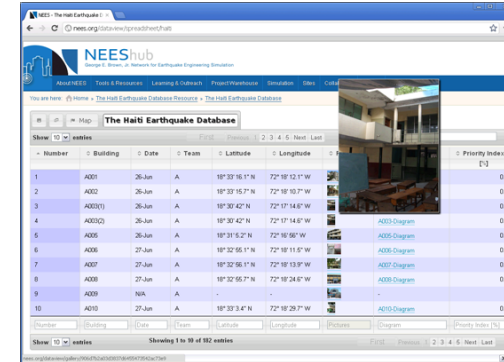
# Example: NEES.org



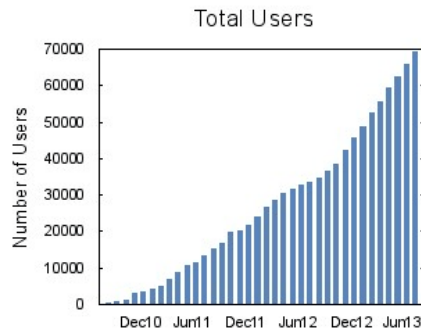
George E. Brown, Jr.  
Network for  
Earthquake Engineering  
Simulation



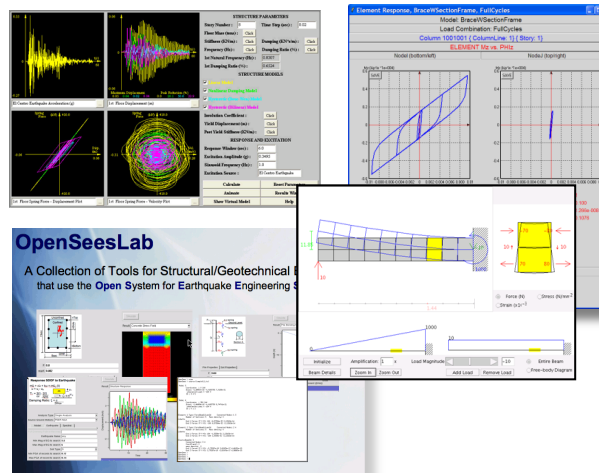
201 projects



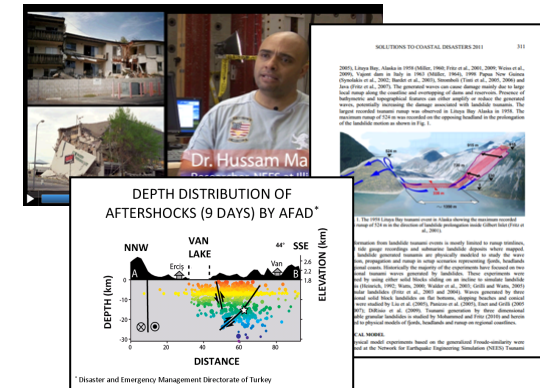
12 databases



69,000 users



66 simulation tools

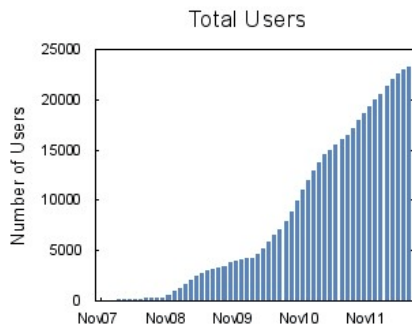


1,456 other

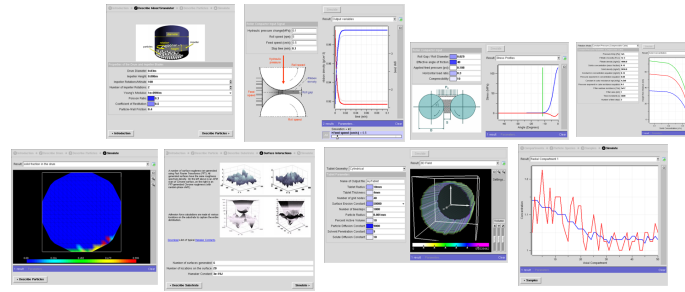
# Example: pharmaHUB.org



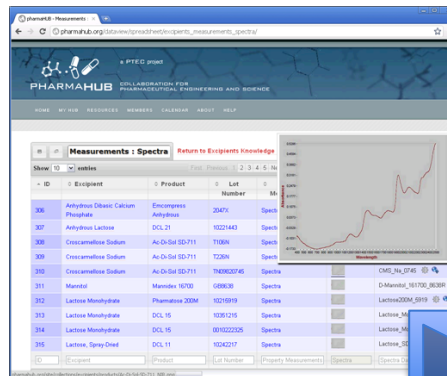
Collaboration for  
Pharmaceutical  
Engineering and Science



23,000 users



22 simulation tools



NIPTE-FDA  
Excipients  
Knowledge Base

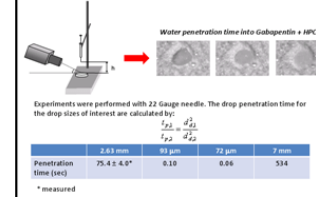
## Visualizing the Interaction of Light & Particles

- No sample preparation in NIR spectroscopy.
- Light interactions with particles.
- Need to learn to visualize the particles and their interaction with light.



Research Article

## Formulation Characterization



## Toward intelligent decision support for pharmaceutical product development

Chunhua Zhao, Arthur Jain, Laxmi Halderman, Prabhu Bhanu, Paramanur Akshay, Ghosh, Sangeeta, Venkat Venkateshwararao, Chaitanya V. Reddy, Ran Morin, and Pravin Bhanu

Intelligent decision support for pharmaceutical product development is a complex process that requires a systematic, and data-driven approach. Information from various sources, including scientific literature, experimental data, and clinical trial data, is used to make informed decisions. This paper presents a framework for intelligent decision support for pharmaceutical product development, which integrates various data sources and uses machine learning techniques to analyze the data and provide intelligent decision support for pharmaceutical product development.

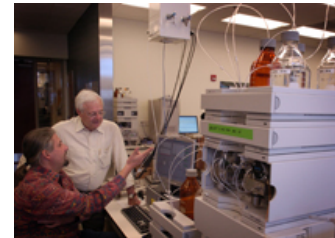
# Example: cceHUB.org



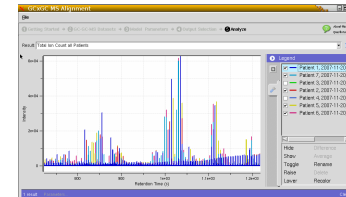
Cancer Care  
Engineering  
Hub



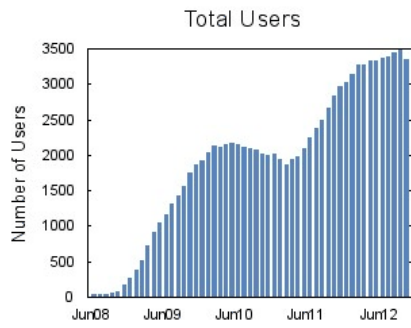
Collect blood samples



Proteomics

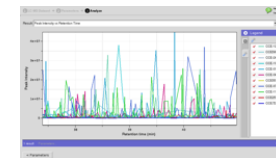
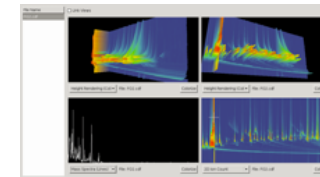
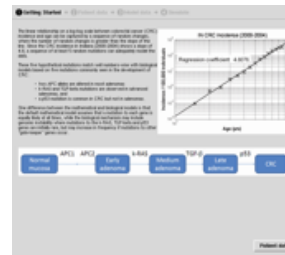


Statistical analysis



3,900 users

| Barcode | Diagnosis Date    | Diagnosis         | Stage    | KRAS Mutation  | Diagnosis TSM | Diagnosis TSM | Diagnosis TSM | Diagnosis TSM | Comments for Diagnosis                          | Transcript |
|---------|-------------------|-------------------|----------|----------------|---------------|---------------|---------------|---------------|---|------------|
| 105     | April 8, 2009     | Colorectal Cancer | Stage IV | Unknown        | 3             | 1             | 1             | 1             |   | No         |
| 109     | March 9, 2009     | Colorectal Cancer | Stage II | Unknown        | 3             | 1             | 0             | 0             |   | No         |
| 111     | November 1, 2007  | Colorectal Cancer | Stage IV | Positive       | 4             | 2             | 1             | 1             |   | Yes        |
| 112     | March 27, 2009    | Colorectal Cancer | Stage IV | Unknown        | 3             | 0             | 1             | 1             |   | Yes        |
| 113     | August 11, 2002   | Colorectal Cancer | Stage IV | Unknown        | 3             | 1             | 1             | 1             |   | Yes        |
| 114     | May 15, 2008      | Rectal Cancer     | Stage IV | Not applicable | 3             | 1             | 1             | 1             |   | No         |
| 115     | April 14, 2009    | Colorectal Cancer | Stage IV | Unknown        | 3             | 0             | 1             | 1             |   | No         |
| 120     | April 28, 2008    | Rectal Cancer     | Stage II | Unknown        | 3             | 2             | 1             | 1             |   | No         |
| 124     | May 9, 2009       | Colorectal Cancer | Stage II | Unknown        | 3             | 1             | 0             | 0             |   | No         |
| 128     | February 9, 2009  | Colorectal Cancer | Stage IV | Positive       | 4             | 2             | 1             | 1             | adjacent chromosome with deletion on 12/12/2008 | Yes        |
| 128     | December 22, 2008 | Colorectal Cancer | Stage IV | Unknown        | 4             | 1             | 1             | 1             | Adjuvant and analysis on 02/10/2009             | Yes        |
| 134     | August 10, 2009   | Colorectal Cancer | Stage IV | Unknown        | 3             | 2             | 0             | 0             |   | No         |
| 132     | December 2, 2009  | Colorectal Cancer | Stage IV | Unknown        | 0             | 0             | 1             | 1             | Immunohistochemistry positive                   | Yes        |
| 139     | November 24, 2009 | Colorectal Cancer |          |                | 2             | 0             | 0             | 0             |   | No         |
| 157     | April 23, 2009    | Rectal Cancer     |          |                | 2             | 1             | 1             | 1             |   | No         |
| 162     | April 15, 2009    | Colorectal Cancer | Stage IV | Positive       | 4             | 2             | 1             | 1             | Not metastatic present                          | Yes        |
| 168     | December 1, 2007  | Colorectal Cancer | Stage IV | Unknown        | 3             | 0             | 1             | 1             |   | Yes        |



17 simulation tools

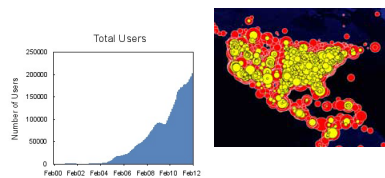
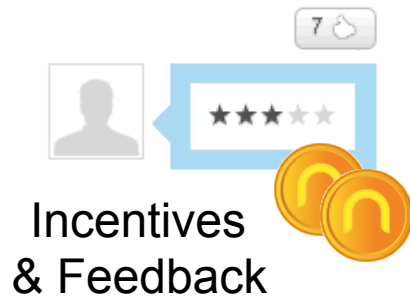
Databases



# 3

A collaboratory for  
team science

# Community / Collaboration Support



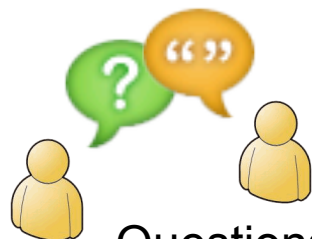
# Tool Development and User Support



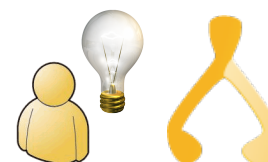
<http://nanohub.org/tools/cntbands-ext>



Collaborative  
Development



Questions  
& Answers



Brainstorming  
& Wish Lists



Bug  
Reports

# Collaboration: Source Code



Collaborative  
Development

Diff r38:40 for trunk -- appor: X

https://nanohub.org/tools/cntbands-ext/changeset?new=40%40trunk&old=38%40trunk

nanohub nanoFORGE

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Wiki Roadmap Browse Source Search Reverse Diff

### Changes in trunk [38:40]

Location: trunk/rappture  
Files: 3 modified

- cnbandswr (1 diff)
- cnbandswr\_matlab (1 diff)
- examples/CNT.xml (1 diff)

Unmodified  Added  Removed

trunk/rappture/cnbandswr

```
r38 r39
38 38 # BEGIN :: the following portion changed by DA
39 39 if (${structure} == "Graphene Nanoribbon") {
40 40   if (${typeN} == ${typeM} && ${typeN} > 1 && ${typeN} < 101) {
41 41     set flag_valid 1
42 42   } elseif (${typeM} == 0 && ${typeN} > 1 && ${typeN} < 101) {
43 43     set flag_valid 1
44 44   } else {
45 45     set flag_valid 0
46 46     foft put output.log "Invalid input of (n,m)\n\nFor graphene nanoribbon,\nthe following restrictions are enforced:\n(1) (n,n) or\n(2) (n,0),\nwhere n
is within interval [2, 100].\n"
47 47     set tempStr {(2,100)}
48 48     foft put output.log "Invalid input of (n,m)\n\nFor graphene nanoribbon,\nthe following restrictions are enforced:\n(1) (n,n) or\n(2) (n,0),\nwhere n
is within interval $tempStr.\n"
49 49   } elseif (${structure} == "Carbon Nanotube") {
50 50     if (${typeN} + ${typeM} > 3) {
51 51     if ([expr ${typeN} + ${typeM}] > 3) {
52 52       set flag_valid 1
53 53     } else {
```

trunk/rappture/cnbandswr\_matlab

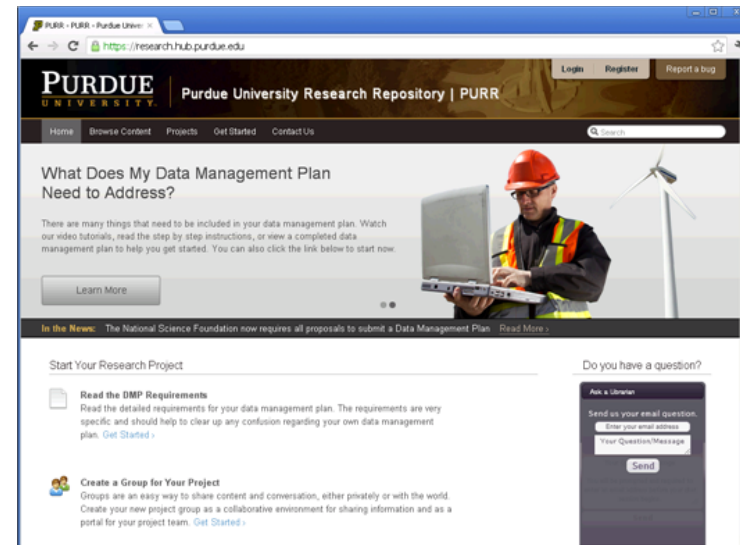
```
r38 r39
36 36 # BEGIN :: the following portion changed by DA
37 37 if (${structure} == "Graphene Nanoribbon") {
```

View of source code differences in project repository

# New applications: Data Management



**P**urdue  
**U**niversity  
**R**esearch  
**R**epository



<http://purr.purdue.edu>

- Data management solution for the masses
- Team effort: Purdue Libraries, Sponsored Programs, VPR, HUBzero
- HUBzero project areas for private collaboration
- Publication process with Digital Object Identifiers
- Seeking ISO 16363 Certification for Trustworthy Digital Repositories

# 4

## Education, Outreach, and Training

# Analytics to Study Impact



World usage  
Location of all "CNTbands" Users Since its Posting

Simulation Users  
**4,150**  
Jun 2013

Monthly Yearly Cumulative

Zoom 3m 6m 1y All

Resource usage metrics

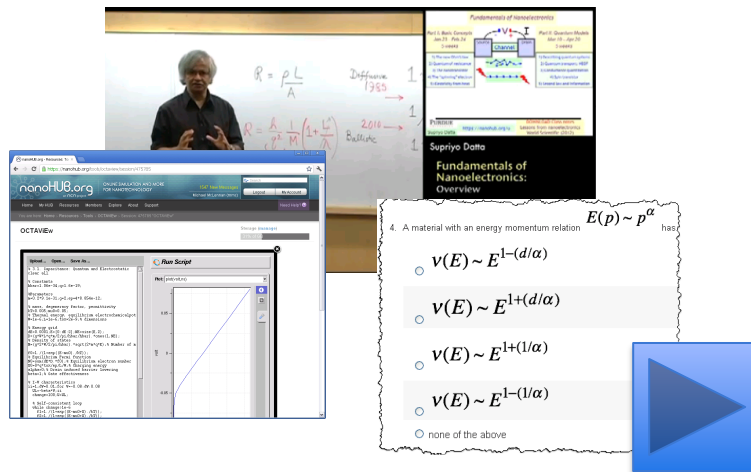
Contributor impact

| # | Tool Name   | Users served in last 12 months | Simulation Runs in last 12 months | Total users served | Total Simulation Runs | Citations | Published On |
|---|---|--------------------------------|-----------------------------------|--------------------|-----------------------|-----------|--------------|
| 1 | OCTAVIEW  | 355                            | 1,495                             | 527                | 2,726                 | -         | 15 Feb 2012  |
| 2 | Thermoelectric Generator Module with Convective Heat Transfer | 31                             | 433                               | 116                | 1,413                 | 1         | 12 Jul 2010  |

|       |       |        |        |         |
|-------|-------|--------|--------|---------|
| total | 3,106 | 48,719 | 14,069 | 424,012 |
|-------|-------|--------|--------|---------|



<http://nanohub.org/u>



- ▶ Fundamentals of Nanoelectronics, Part 1: Basic Concepts
- ▶ Fundamentals of Nanoelectronics, Part 2: Quantum Models
- ▶ Fundamentals of Atomic Force Microscopy, Part 1: Fundamental Aspects of AFM
- ▶ Fundamentals of Atomic Force Microscopy, Part 2: Dynamic AFM Methods
- ▶ Nanoscale Transistors
- ▶ Thermal Energy at the Nanoscale
- ▶ From Atoms to Materials: Predictive Theory and Simulations



So...

# Why HUBzero?

# Why HUBzero?



*Broad feature set targeted for science/engineering*

|                               | Open Course Ware | Drupal / CMS | Sharepoint | MyExperiment | nanoHUB.org |
|-------------------------------|------------------|--------------|------------|--------------|-------------|
| Seminars & Teaching Materials | ✓                | ✓            |            |              | ✓           |
| Discussion Forums             |                  | ✓            | ✓          | ✓            | ✓           |
| Community Wiki                |                  | ✓            | ✓          |              | ✓           |
| Calendars & Events            |                  | ✓            | ✓          |              | ✓           |
| Wish Lists                    |                  |              |            |              | ✓           |
| Support Tickets               |                  | ✓            |            |              | ✓           |
| User Groups                   |                  | ✓            | ✓          | ✓            | ✓           |
| Simulation/Modeling Tools     |                  |              |            | ✓            | ✓           |
| Scientific Workflows          |                  |              |            | ✓            | ✓           |
| High-Performance Computing    |                  |              |            | ✓            | ✓           |
| Scientific Visualization      |                  |              |            |              | ✓           |
| Usage Metrics / Assessment    |                  |              |            | ✓            | ✓           |
| Data Sharing                  |                  |              | ✓          | ✓            | ✓           |
| DOIs, Library Standards       |                  |              |            | ✓            | ○           |
| Uncertainty Quantification    |                  |              |            |              | ○           |
| Integrated Data & Tools       |                  |              |            |              | ○           |
| Data Provenance               |                  |              |            |              | ○           |
| Peer-Review                   |                  |              |            |              | ○           |

Collaboration  
Data Management  
Integrated Analysis

|   |   |
|---|---|
| ✓ | ○ |
| ✓ | ○ |
|   | ○ |
|   | ○ |
|   | ○ |

# 40+ Hubs for many disciplines



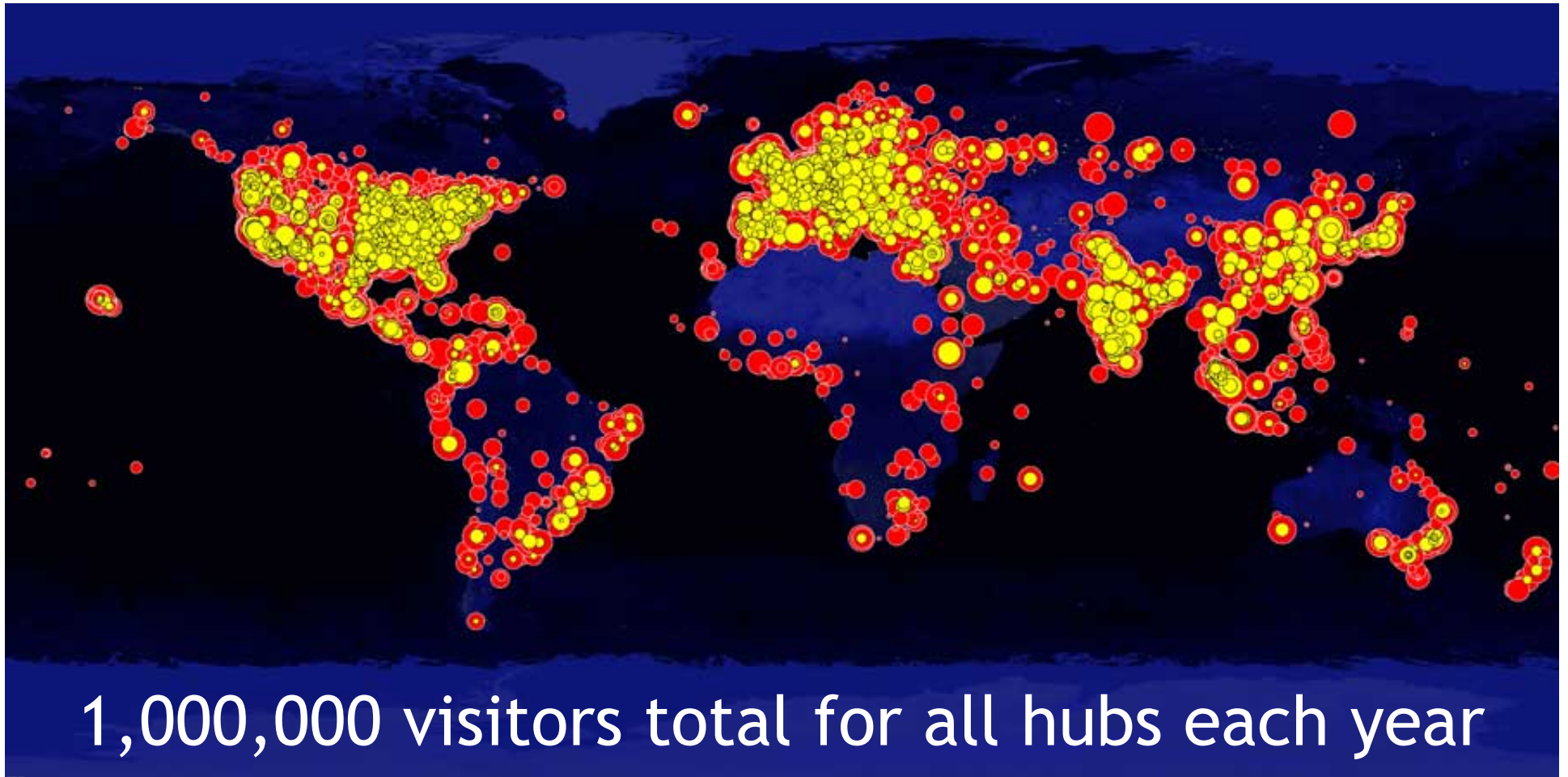
**~1,000,000**  
visitors total

| visitors | users   | Hub Logo | Hub Name         |
|----------|---------|----------|------------------|
| 540,063  | 258,791 |          | nanoHUB.org      |
| 230,698  | 59,175  |          | nees.org         |
| 59,659   | 29,965  |          | GlobalHUB.org    |
| 32,700   | 22,651  |          | pharmaHUB.org    |
| 32,314   | 11,199  |          | vhub.org         |
| 37,414   | 3,132   |          | HABRIcentral.org |
| 15,898   | 3,933   |          | cceHUB.org       |
| 14,977   | 5,797   |          | ciHUB.org        |
| 12,304   | 3,510   |          | StemEdHub.org    |
| 11,754   | 1,907   |          | iemhub.org       |
| 10,995   | 1,863   |          | C3Bio.org        |
| 7,317    | 1,246   |          | cleerHUB.org     |

# Why HUBzero?



*Works for many users*



## More information



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<http://hubzero.org/pressroom>

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