

nanoHUB.org and the Delivery of Value to Authors and Users

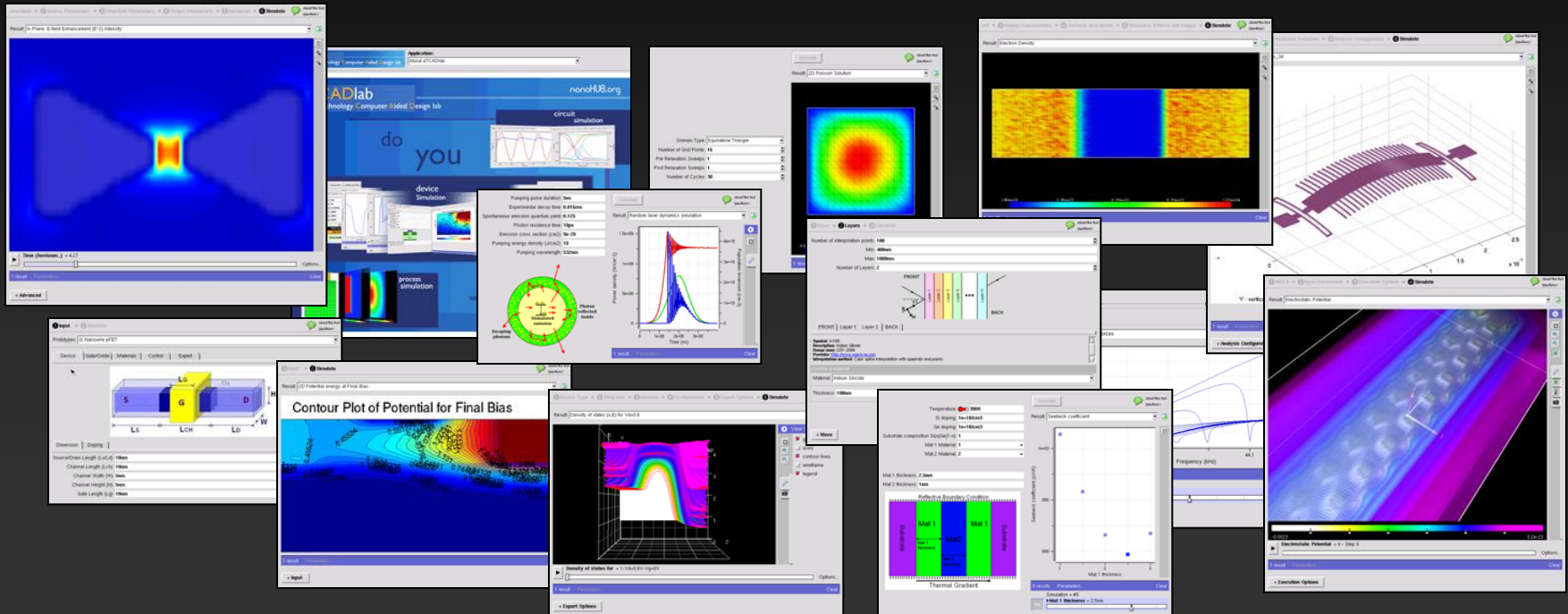
George B. Adams III

Network for Computational Nanotechnology

Purdue University

nanoHUB.org

MISSION: Support the National Nanotechnology Initiative by designing, constructing, deploying, and operating a national cyber-resource for nanotechnology theory, modeling, and simulation.



It Happens Here

The screenshot shows the nanoHUB.org website in a web browser. The header includes the logo, navigation links (Home, My HUB, Resources, Members, Explore, About, Support), and a search bar. The main banner features an iTunes U logo and text about online simulation and collaboration. Below the banner, there are three columns: Resources with a search bar and popular tags; Featured resources with icons and titles; and a Notable Quote section. The bottom of the page includes a link to upload content and a list of recent resources.

nanoHUB.org ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

Home My HUB Resources Members Explore About Support Help

now on iTunes U

SIMULATE with over 160 tools for nanoelectronics, nanophotonics and more

RESEARCH & COLLABORATE via groups, question board and more

TEACH & LEARN with tool-powered curricula, courses, seminars and more

SHARE & PUBLISH tools and research through our easy upload process

A resource for nanoscience and technology, the nanoHUB was created by the NSF-funded Network for Computational Nanotechnology.

Over 100,000 users annually

RESOURCES

Popular Tags: nanoelectronics, course lecture, material science, nanotransistors, research seminar, nano/bio, hosted/produced by NCN@Illinois, devices, quantum transport, tutorial, molecular electronics, nano electro-mechanical systems, transistors, NEGF, nanophotonics, carbon nanotubes, education/outreach, quic, nanomedicine, Illinois, ABACUS, NCN Supported, band structure, MOSFET, materials

FEATURED

- Drift Diffusion Lab: Simulate single semiconductor characteristics - in Tools
- Illinois ECE 450 Optical Imaging, Chapter 3: Imaging - in Teaching Materials
- James Leary, Purdue University, West Lafayette - Contributions: 26, Average resource ranking: 8.38
- ANTS-Assembly for Nanotechnology Survey Courses - in Topics
- ECE 495N: Fundamentals of Nanoelectronics - featured on iTunes U
- Why is Fermi level referred to as electrochemical potential - asked by Anonymous, in Answers

NOTABLE QUOTE

All of the tools on nanoHUB are easy to use, amazingly comprehensive and accurate.

Chris Ates, Graduate Student, Arizona State University - in Notable Quotes

NEW IN RESOURCES

- Overview of How People Learn Framework to Support Instructional Design in Online Presentations, Apr 19, 2010
- PN junction in Animations, Apr 17, 2010
- Local density of states in Animations, Apr 17, 2010

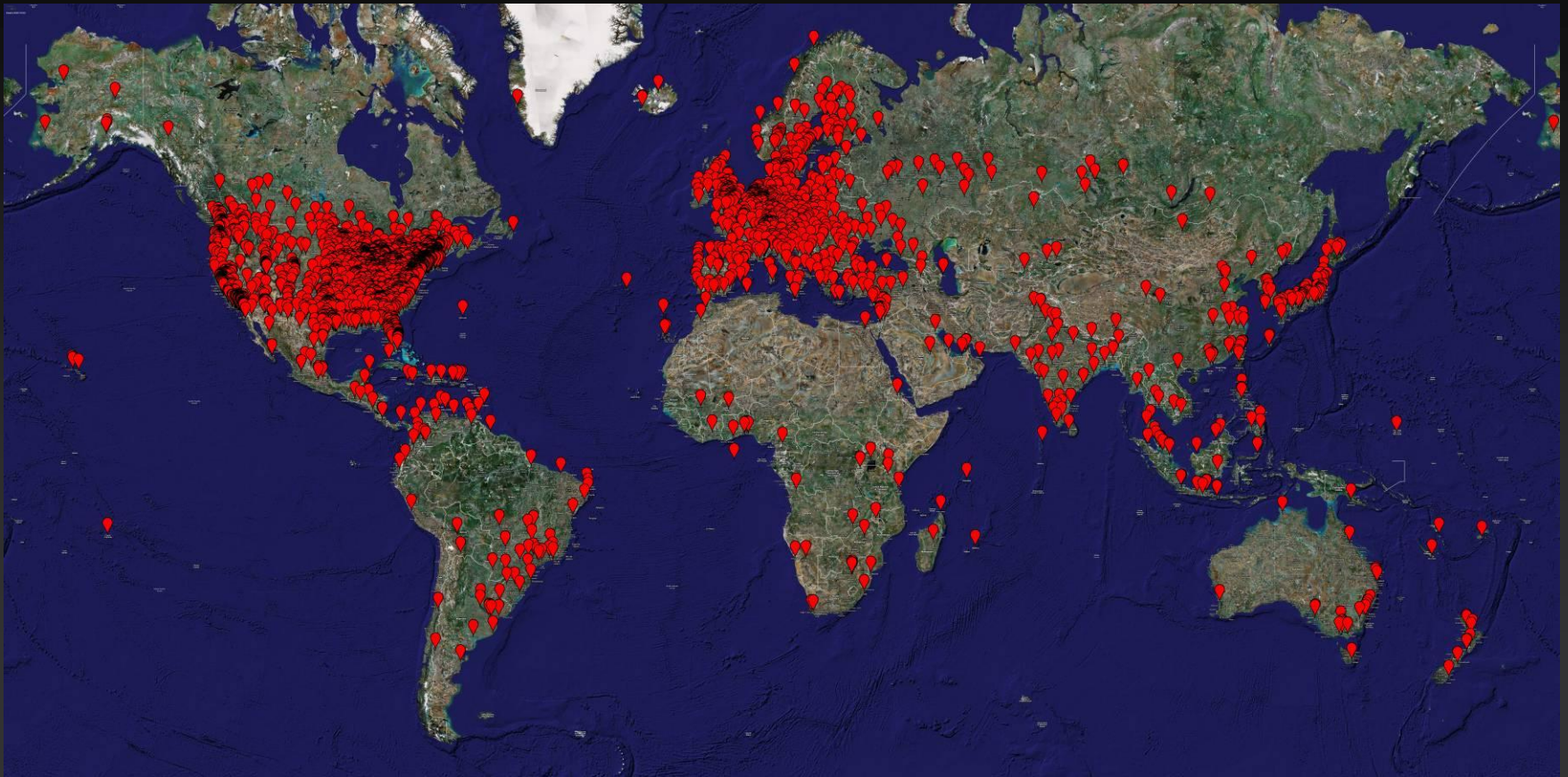
See what else is new

Animations, Courses, Downloads, Learning Modules, Notes, Online Presentations, Publications, Series, Teaching Materials, Tools, Workshops... All Categories

Upload your own content! Get started

nanoHUB.org stats

- 180 simulation tools
- 2300 total resources
- 161,000 users past 12 months



A dense collage of various scientific and engineering software interfaces, including plots, 3D models, and data visualizations, representing the field of computational science. The interfaces show a wide range of data analysis tools, from spectral plots and time-series graphs to complex 3D molecular models and finite element analysis visualizations. Some windows display circuit diagrams, while others show detailed material property data or simulation results. The overall theme is the integration of different computational methods to solve complex scientific problems.

Do you Teach?

AQME
Quantum Mechanics for Engineers

More »

SIMULATE with over 160 tools for nanoelectronics, nanophotonics and more »

RESEARCH & COLLABORATE via groups, question board and more »

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[Detailed statistics](#) | [Who's online?](#)

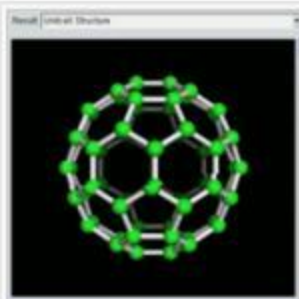
- Past 12 months' user activity
 - 138,000 downloaded content
 - 49,000 interacted with site more than 15 minutes
 - 9,800 ran 364,000 simulation jobs
- 575 scientific papers cite nanoHUB.org
- 379 courses at 131 institutions have used nanoHUB.org
- Powered by HUBzero™

Wikipedia Contributions

ਨੈਨੋਤਕਨੀਕ

Punjabi

ਨੈਨੋਤਕਨੀਕ ਜਾਂ ਨੈਨੋਪ੍ਰੋਟੋਗੀਕੀ, ਵਿਵਹਾਰਕ ਸੀਮਾ ਦੇ ਅੰਦਰ ਵੈੱਬ ਨੈੱਟਵਰਕ ਦੇ ਰੂਪ ਵਿੱਚ ਹੈ ਅਣੂਆਂ ਦੇ ਗੈਰ ਕੋਵਲੈਂਟ ਪ੍ਰਭਾਵ ਤੇ ਕੇਂਦਰਤ ਹੈ। ਇਨ੍ਹਾਂ ਦਿਸ਼ਾਵਾਂ ਵਿੱਚ ਖੋਜ ਦੇ ਕੀ ਨਤੀਜੇ ਹੋਣਗੇ C₆₀, ਜਿਨ੍ਹਾਂ ਬਕਿਬਾਲ ਵੀ ਕਹਿੰਦੇ ਹਨ, ਜੋ ਕਾ

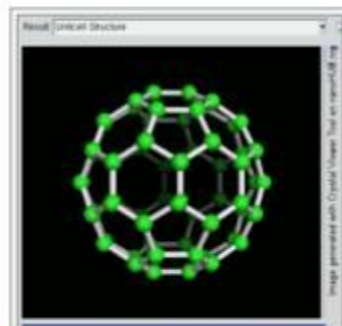


ਬਕਮਿਨਿਸਟਰ ਫੁੱਲਰੀਨ C₆₀ ਦਾ ਘੁੰਮਦਾ ਦ੍ਰਿਸ਼

Dalla grafite al C₆₀

Italian

Nei **polimeri**, le molecole organiche classiche sono composte da azoto, cloro e zolfo). Essi sono ottenuti dalla benzina e sono parte di queste molecole sono isolanti quando superano la loro conduttività, in particolare la grafite (recuperata dal carbone) è un **semi-metallo**, una categoria compresa fra metalli e semiconduttori. Fra ogni *foglio*, le interazioni sono abbastanza deboli.



Veduta ruotante di cristallo C₆₀ di Fullerene Buckminster.

L'adattamento del fullerene a nanometriche rimane un campo di ricerca chimici hanno esplorato che potrebbero essere utilizzati in interstellari dove il carbonio è presente. Smalley (Rice University) ha vaporizzato mediante laser un cluster contenente sei atomi di 60 atomi. Harry Kroto (Cambridge) ha una geometria possibile. Denominati buckminsterfullerene, questi oggetti furono rapidamente

Nanotubi di carbonio

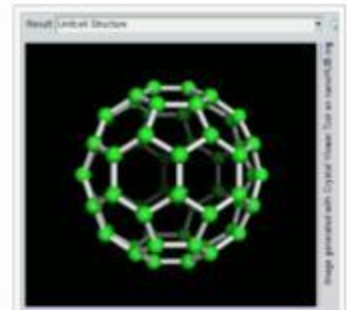
Fullerene

German

Als **Fullerene** (Einzahl: *Fulleren*) werden sphärische **Moleküle** aus **Kohlenstoffatomen** (mit hoher **Symmetrie**, z. B. *I_h*-Symmetrie für C₆₀) bezeichnet, welche weitere Modifikationen des chemischen Elements Kohlenstoff (neben **Diamant** und **Graphit**) darstellen.

Inhaltsverzeichnis [Verbergen]

- 1 Geschichte
- 2 Name
- 3 Herstellung
- 4 Eigenschaften
 - 4.1 Nomenklatur
 - 4.2 Struktur und Stabilität
 - 4.3 Reaktionen von C₆₀
- 5 Literatur
- 6 Weblinks
- 7 Einzelnachweise



rotierende Struktur von C₆₀



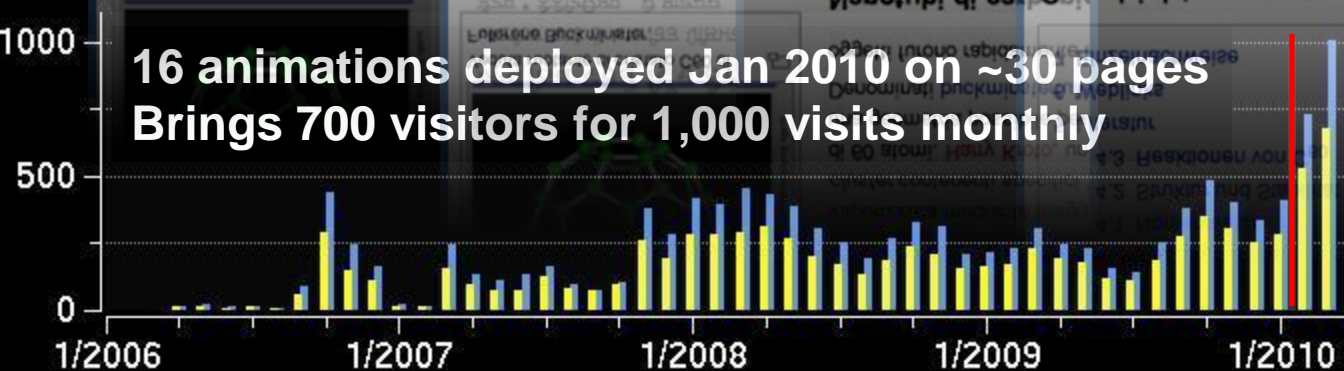
Geschichte [Bearbeiten]

Geschichte [Bearbeiten]

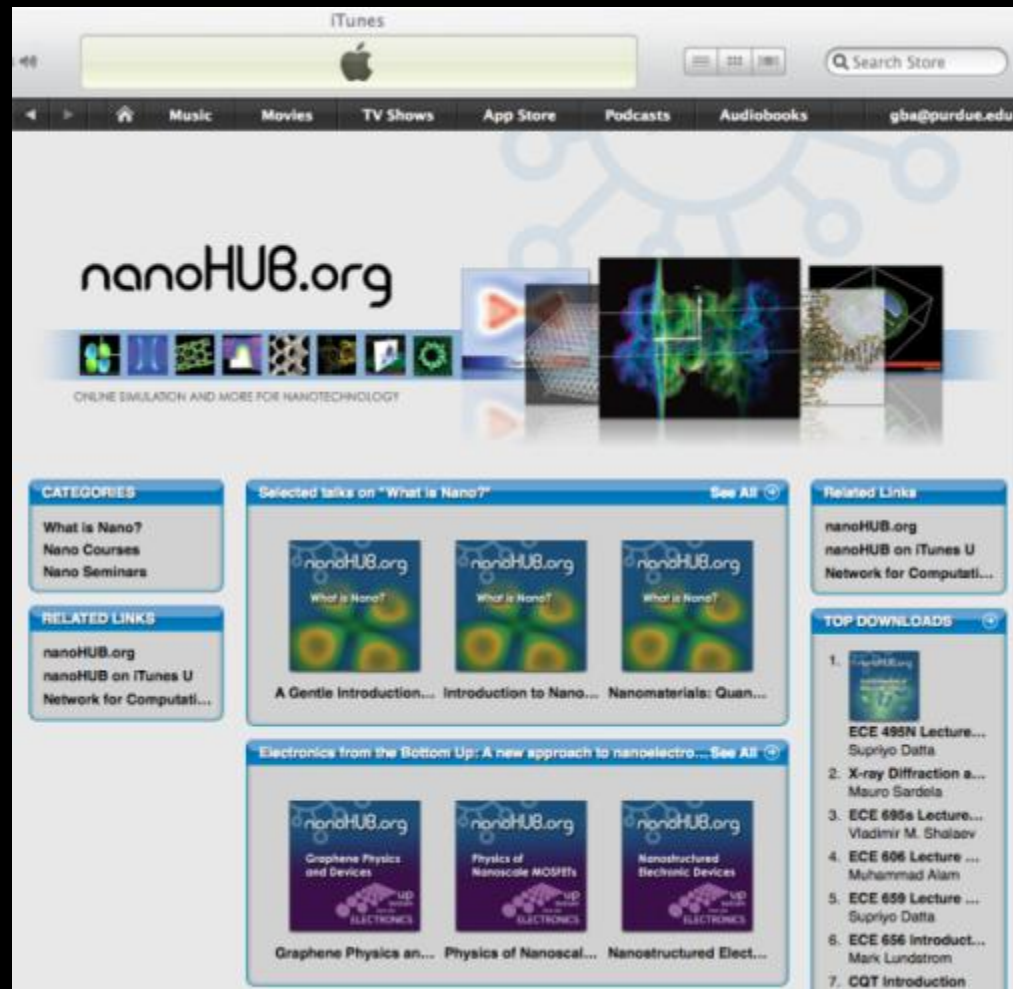


rotating view of Buckminster fullerene

16 animations deployed Jan 2010 on ~30 pages
Brings 700 visitors for 1,000 visits monthly



nanoHUB.org on iTunes U

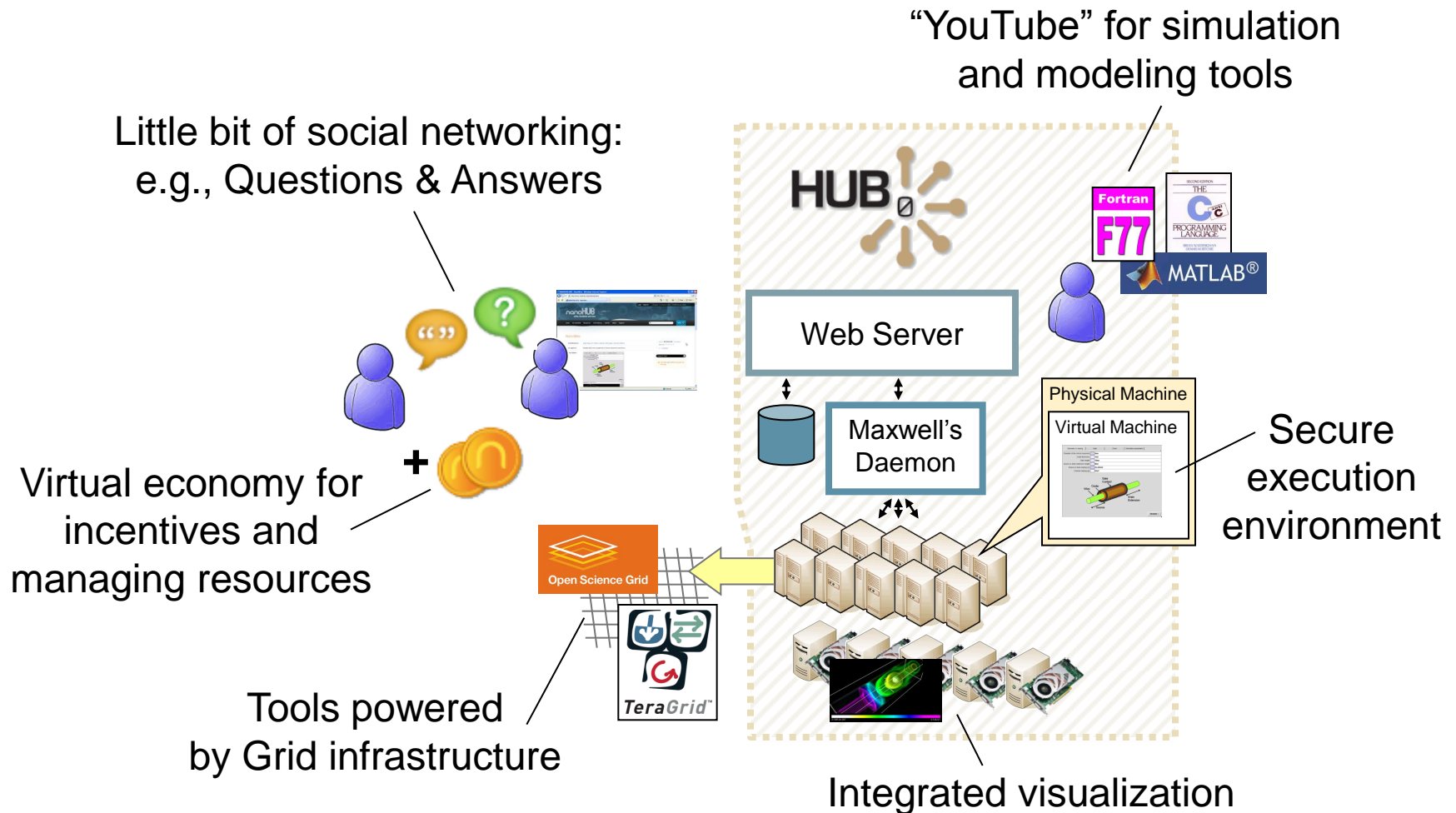


One of 68 “institutions”
allowed in
iTunes U Beyond Campus

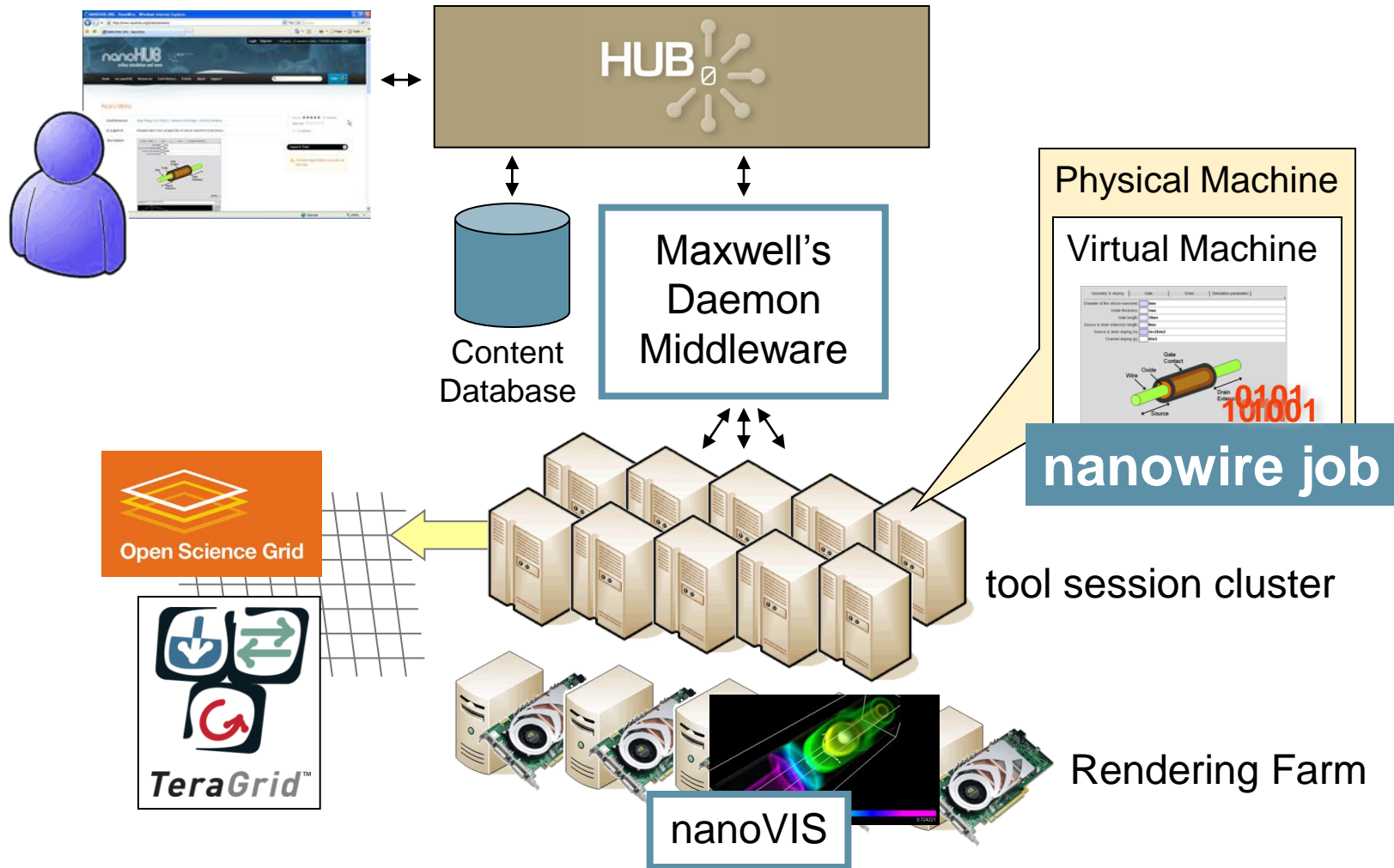
Alongside:
MoMA,
The New York Public Library,
Public Radio International,
PBS stations

Deployed
350 content items
10,000 downloads / month

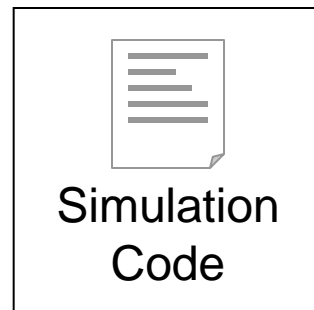
Platform for Scientific Collaboration



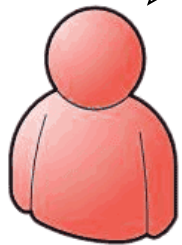
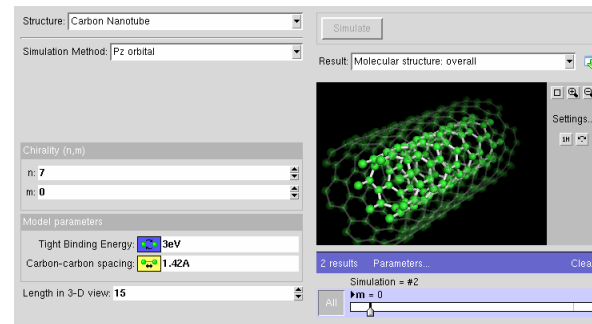
Cyberinfrastructure for Running Tools



Rappture: Rapid Application Infrastructure



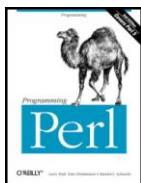
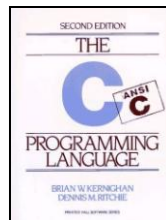
Rappture



Scientist



Fortran
F77



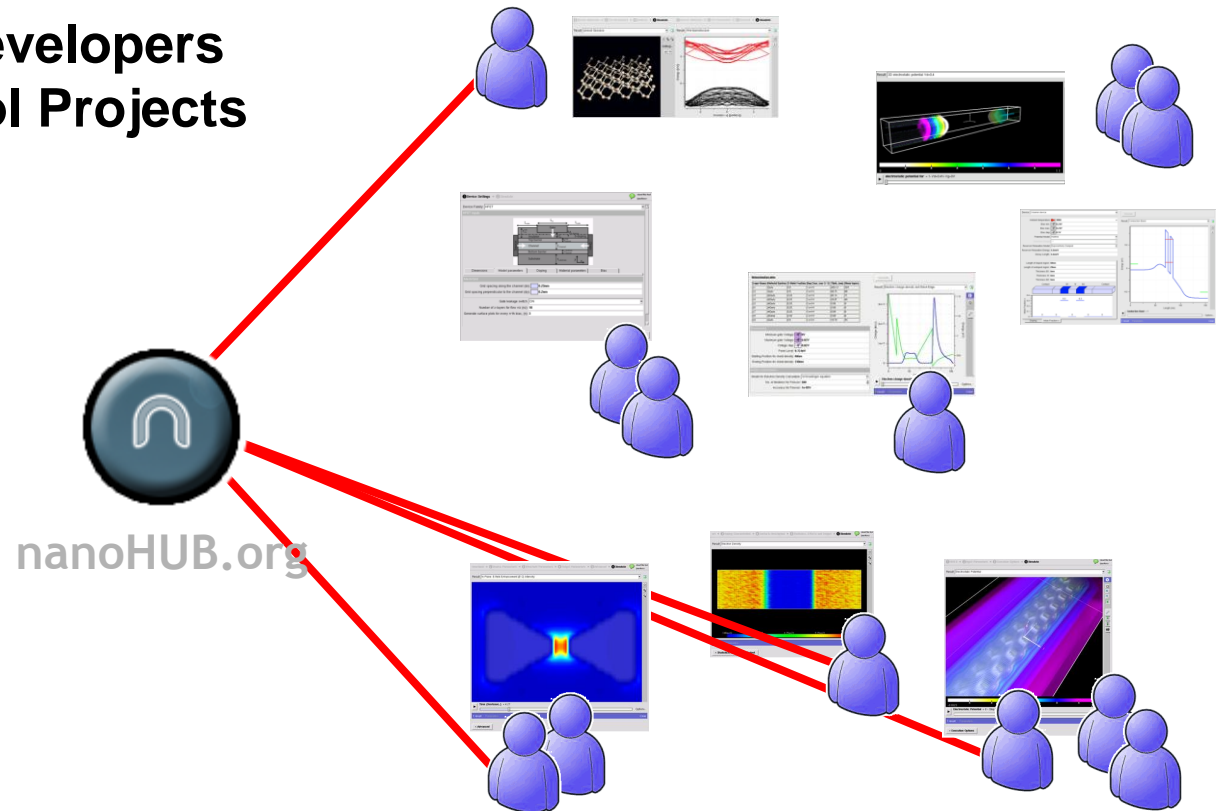
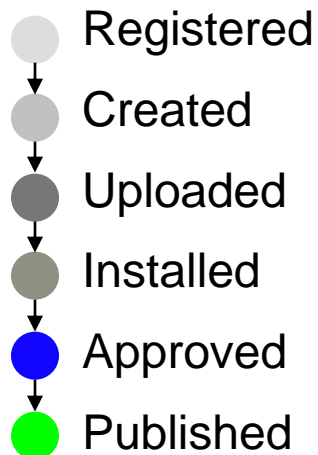
Ruby



- Works with your favorite programming language
- Open Source
- Online at <http://rappture.org>
- Used by 180 projects and 200 developers

Supporting hundreds of projects

Hundreds of Developers
Hundreds of Tool Projects



281 Tool Projects

Year of Development >>

Automated infrastructure is easy to manage



HUBzero Team

Hubs 'R Us



- Feb 2007: 1 hub
- Feb 2008: 5 hubs
- Feb 2009: 8 hubs
- Feb 2010: 21 hubs

Each hub has its own funding stream



HUBzero: an organization with Recharge Center

HUBzero Consortium



- Four founding members
- Ongoing development of HUBzero core
- Documentation: <http://hubzero.org/documentation>
- Dissemination and support, yearly conference

Recent Workshop

**April 13-14, 2010
Indianapolis, IN**

Open Source Release!

Tutorial Tracks:

- Setting up a new hub
- Managing hub content
- Creating and publishing scientific tools
- Extending hub functionality through PHP/web programming

<http://hubzero.org/hubbub2010>



Value proposition for publishing

- In Isaac Newton's day researchers communicated their ideas and results to the community via exchange of letters
- Evolved to the Journals, Proceedings we use today
- Value proposition to authors (contributors):
 - Community recognition
 - Citations by others in the community
 - Promotion of career
- Value proposition to readers (users):
 - Access to vetted content

HUBzero value proposition

- HUBzero generalizes the concept of publishing
- Value to **authors** (contributors):
 - Share more than ideas and results – share tools, educational materials, and data (can imagine)
 - Citations by others in the community
 - Wider use of tools accelerates research, learning, and career (with attitude and culture change)
 - Promotion of career (with culture change)
- Value to **users**:
 - Access to vetted (with community participation) content
 - Ability to vet simulation-based research

A New Way of Publishing

nanoHUB.org - Resources: Band Structure Lab - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://nanohub.org/resources/bandstrlab

nanoHUB.org - Resources: Ban...

zotero

nanoHUB.org
an NCN project

ONLINE SIMULATION FOR NANOTECHNOLOGY

Home My HUB Resources Members Explore About

You are here: Resources > Tools > Band Structure Lab > About

Band Structure Lab

By [Abhijeet Paul¹](#), [Mathieu Luisier¹](#), [Neophytos Neophytou²](#), [raseong kim¹](#), [Michael McLennan¹](#), [Mark Lundstrom¹](#), [Gerhard Klimeck¹](#)

1. *Purdue University, West Lafayette*; 2. *Technical University of Vienna*;

Computes the electronic structure of various materials in the spatial configuration of bulk (infinitely periodic), quantum wells (confined in one dimension, infinitely periodic in 2 dimensions), and wires (confined in 2 dimensions and infinitely periodic ...)

Launch Tool

Version **2.0.8** - published on 26 Jan 2010
DOI: 10254/nanohub-r1308.12 [cite this](#)
This tool is closed source.

[First-Time User Guide](#)
[View All Supporting Documents](#)

10.0 RANKING

★ NCN Supported

2756 user(s), detailed usage

23 questions (Ask a question)

5 review(s) (Review this)

13 wish(es) (Add a new wish)

23 citations

Share: [f](#) [t](#) [g+](#) ...

SEE ALSO

Band Structure Lab

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Done



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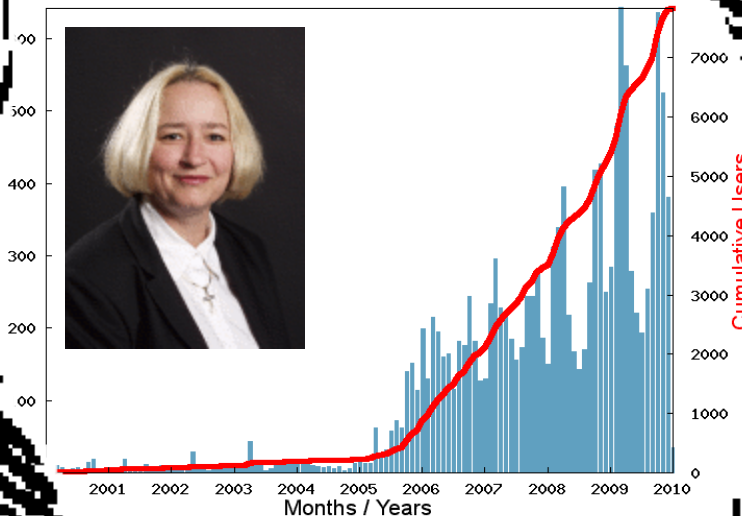
23 citations

Share: [f](#) [t](#) [g+](#) ...

Faculty Incentive

Dragica Vasileska

Users of Simulation Tools Authored by Dragica Vasileska (7,835 Users)



Tool usage \approx
reading papers

7,835 users

Proof of Impact!
Great in Proposals!

Expose quality

Schred 97 citations – listed with tool information

About Usage Questions Reviews Wish List Versions Citations Supporting Documents

Citations

Non-affiliated (85) | Affiliated (12)


Non-affiliated authors

Ferney Chaves; David Jiménez; Jordi Suñé (2010), "Explicit quantum potential and charge model for double-gate MOSFETs," *Solid-State Electronics*, **54**, 5: pg. 530-535, 02. (DOI: 10.1016/j.sse.2010.01.015).

[BibTex](#) [EndNote](#)

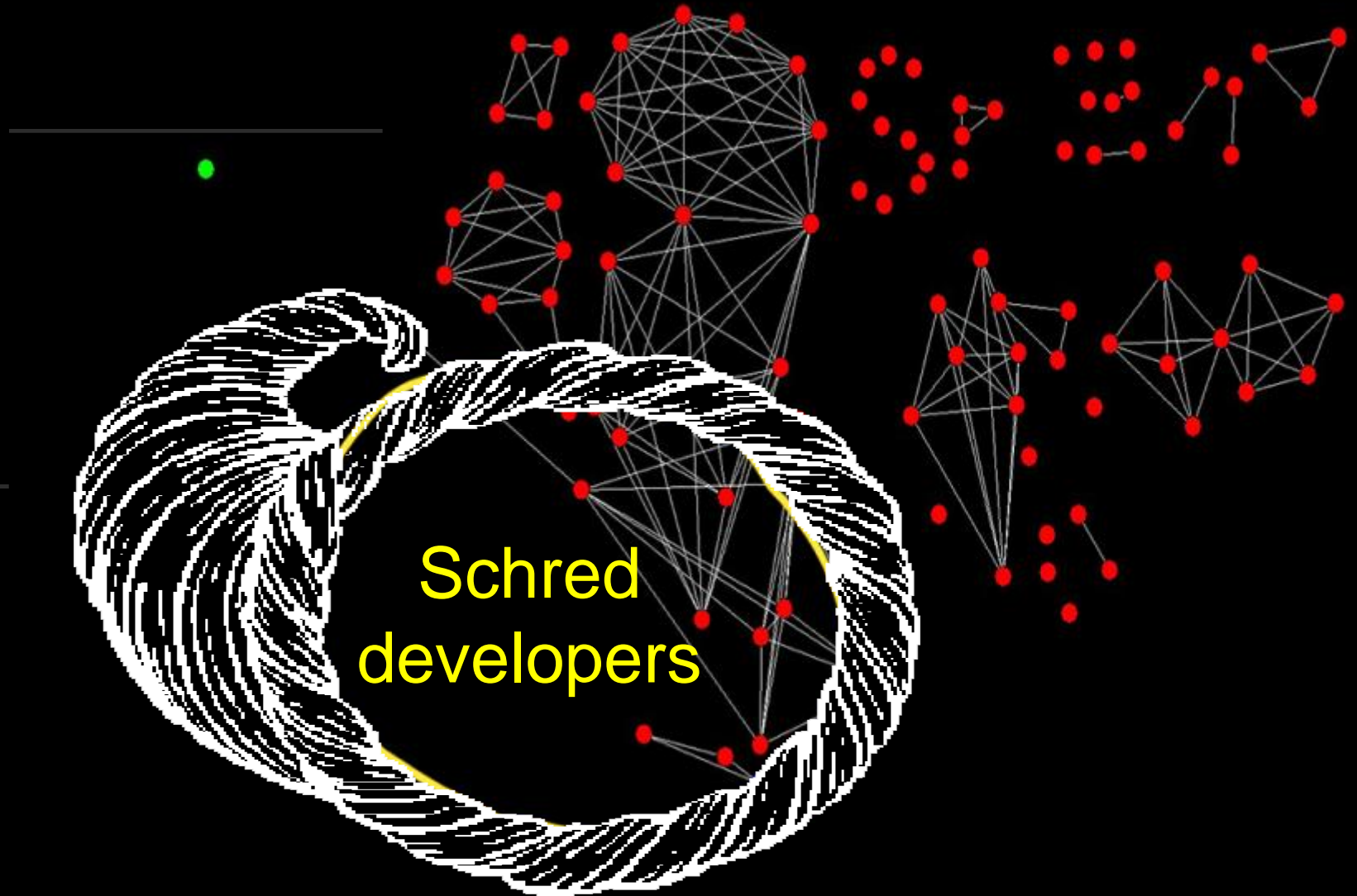
Ferney Chaves; David Jiménez; Jordi Suñé (2010), "Explicit quantum potential and charge model for double-gate MOSFETs," *Solid-State Electronics*, **54**, 5: pg. 530-535, 02. 0038-1101. (DOI: 10.1016/j.sse.2010.01.015).

[BibTex](#) [EndNote](#)


Navid Paydavosi; M. Meysam Zargham; Kyle D. Holland; Curtis M. Dublanko; Mani Vaidyanathan (2009), "Non-Quasi-Static Effects and the Role of Kinetic Inductance in Ballistic Carbon-, " *IEEE Transactions on Nanotechnology*, **99**: pg. 001-001, 09. 1536-125X. (DOI: 10.1109/TNANO.2009.2032918).

[BibTex](#) [EndNote](#)

Schred citation network



A course on nanophotonics



an ncn project

ONLINE SIMULATION AND MORE
FOR NANOTECHNOLOGY

LoginRegister

HomeMy HUBResourcesMembersExploreAboutSupport

Help!


You are here: Members › Vladimir M. Shalaev › Usage

Vladimir M. Shalaev

ProfileContributionsUsageFavorites

Table 1: Overview

Item	Value
Contributions:	24
Total "and more" Users Served:	20,631
Rank by Contributions:	18 / 731
First Contribution:	04 Oct 2005



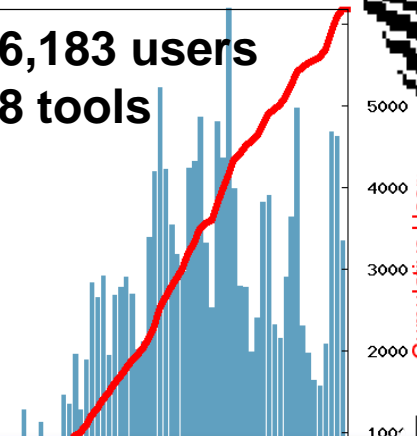
Next Generation Faculty:

Shaikh Ahmed

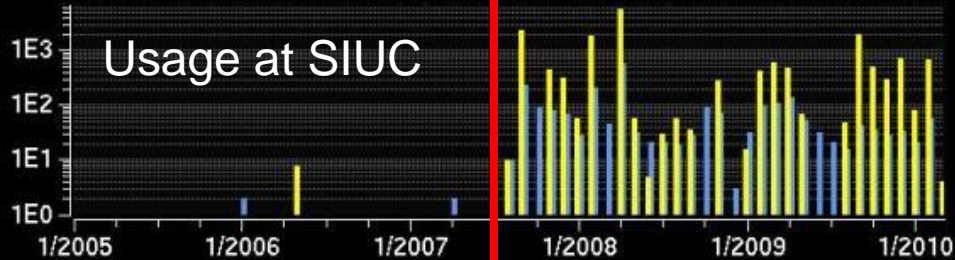
Simulation Tools Authored by Shaikh S. Ahmed (6,183 Users)



6,183 users
8 tools



Usage at SIUC



Post Doc
at Purdue

Faculty at
SIUC

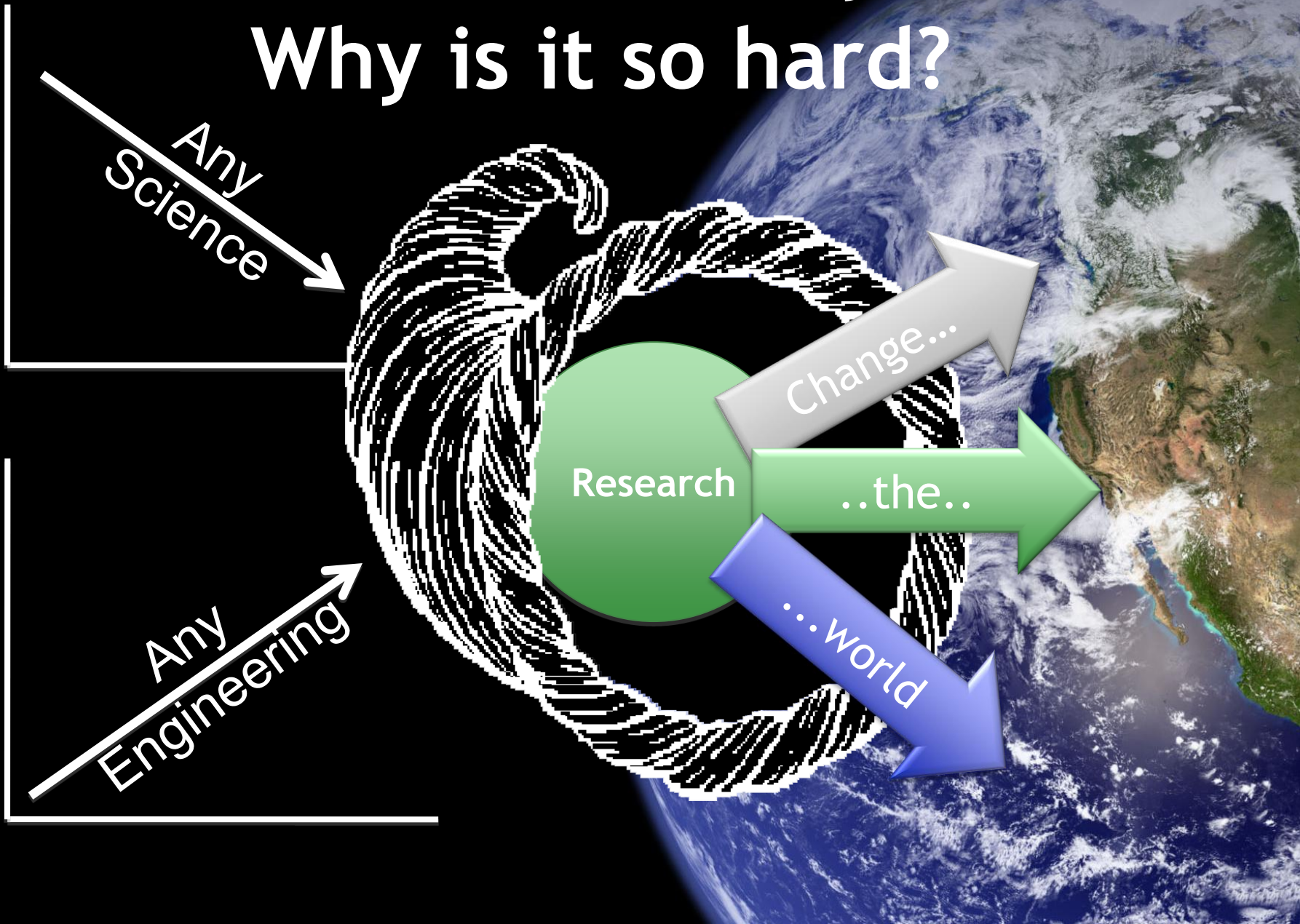
- Infused nanoHUB into existing classes
- Built nanoelectronics curriculum
- Used nanoHUB for research

Recently Dr. Ahmed was promoted to tenured Associate Professor. I would like to emphasize that Dr. Ahmed's use of nanoHUB in education and research, which earned him national and international visibility, did play a significant positive role in his early promotion case

Glaftos Galanos
Chair, Dept. of Electrical and Computer Engineering, SIUC

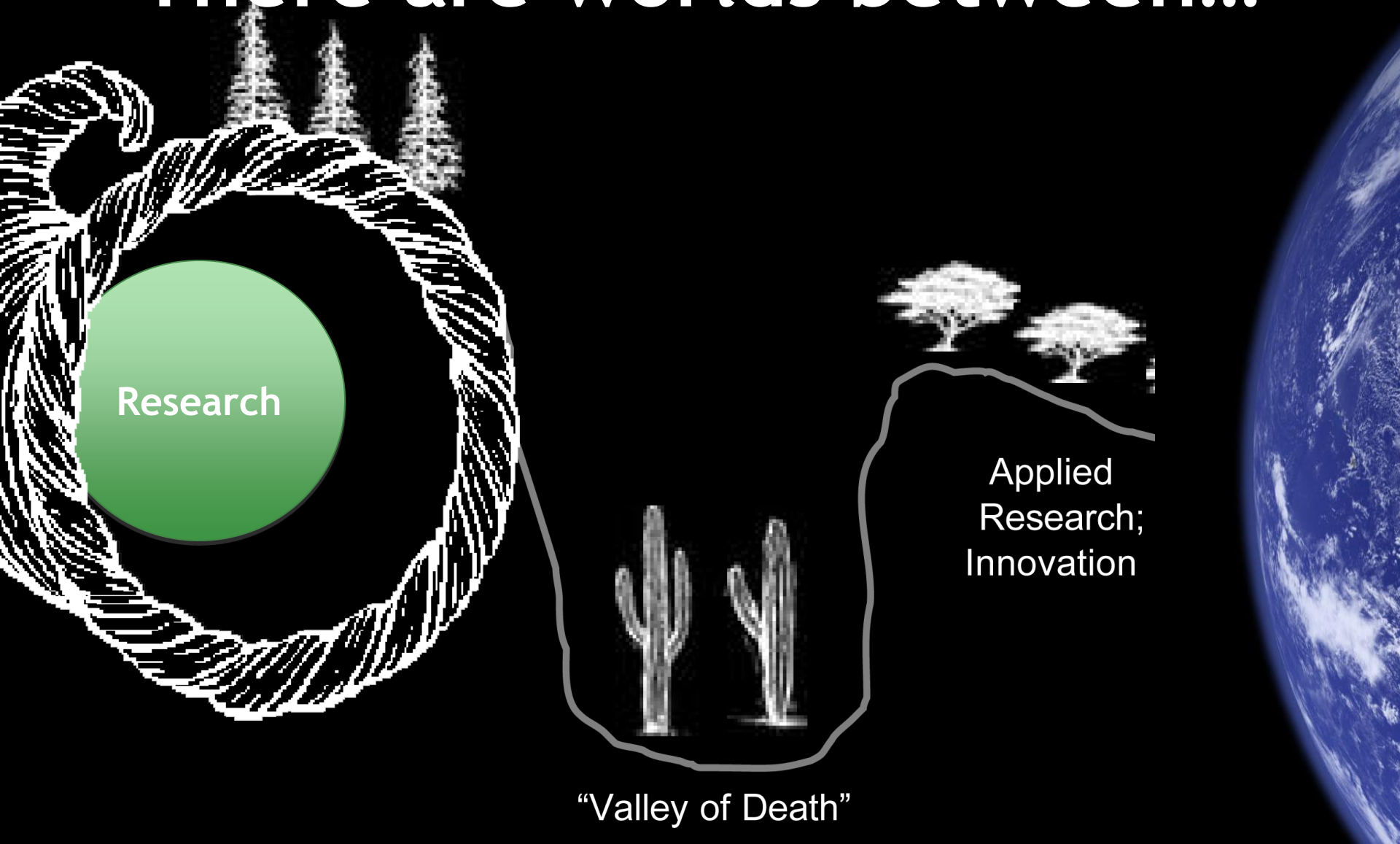
The Science Gateway Dream

Why is it so hard?



The Science Gateway Dream

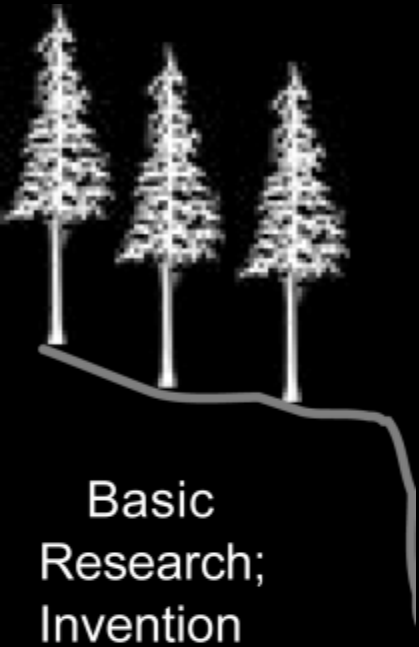
There are worlds between...



6 Criteria

for Successful
Science Gateways

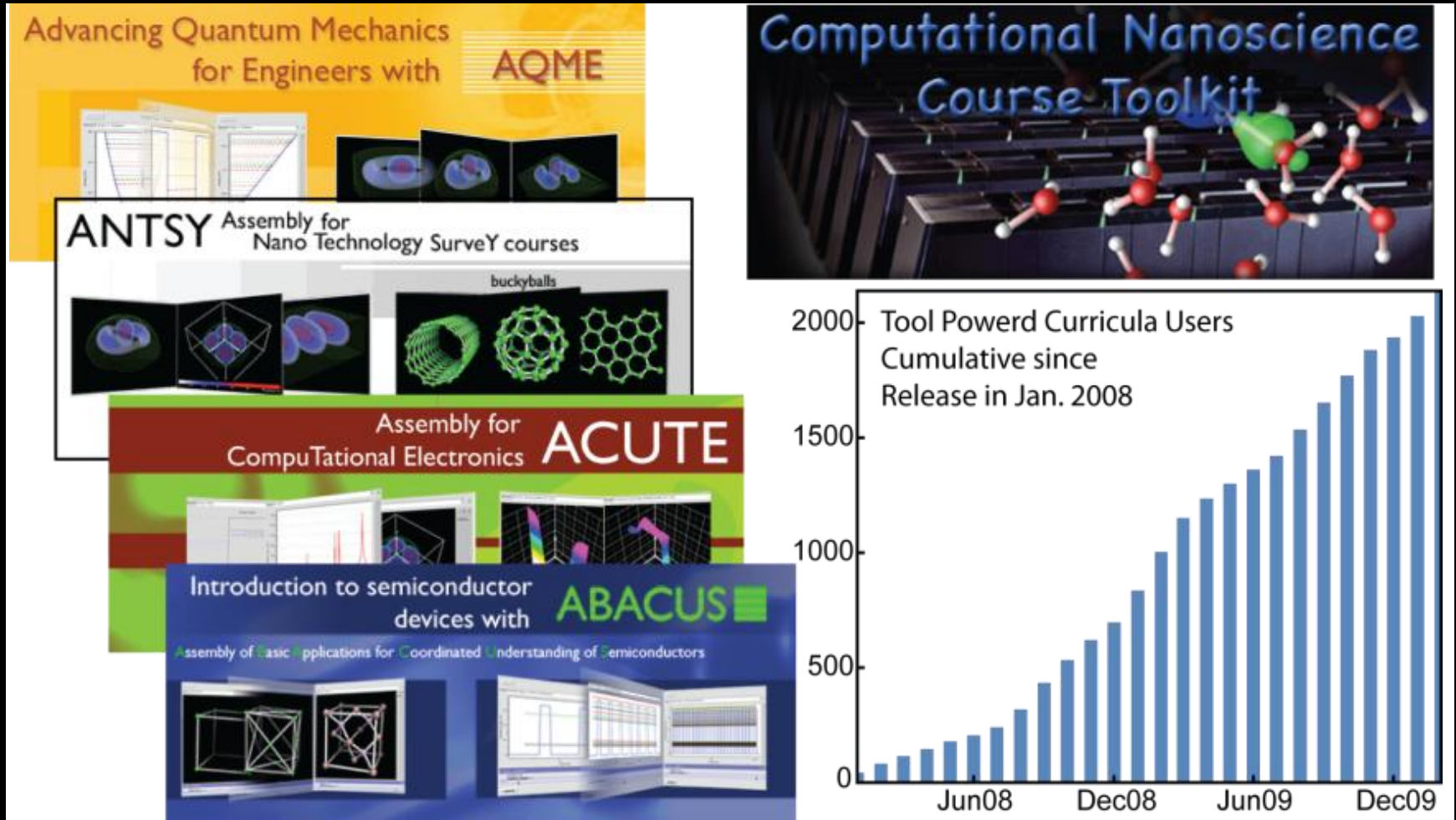
1: Outstanding content



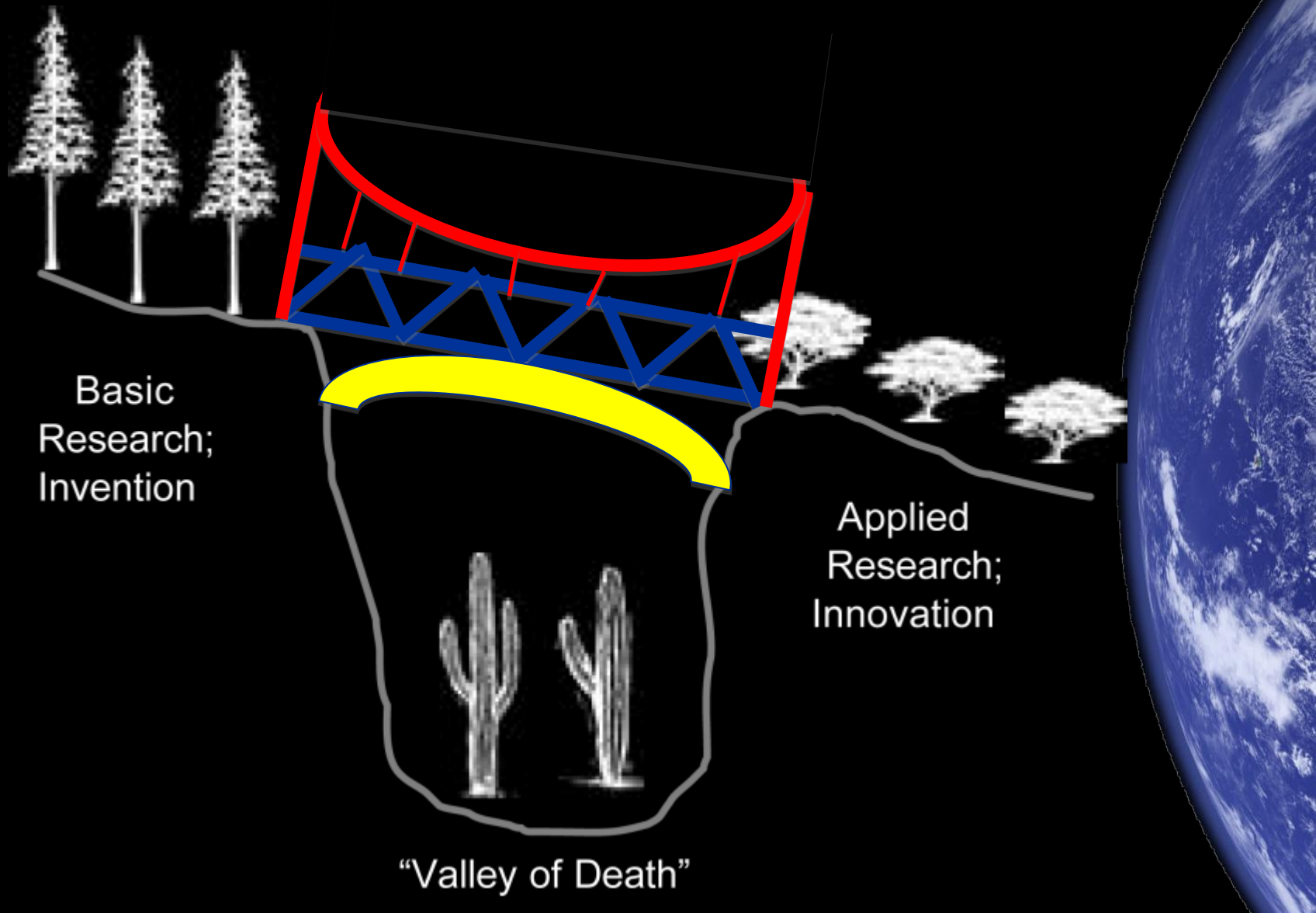
- 723 nanoHUB authors to date
- NCN-supported tools
- Reviews
- Ratings
- Questions & Answers
- Exposed usage data
- Citations list



2: Commitment to usefulness



3: Utterly dependable technology



3: Utterly dependable technology

Less than 20 hours
downtime last year!



Basic
Research;
Invention



Applied
Research;
Innovation



"Valley of Death"



4: Rapid content deployment

Content adaptation support team



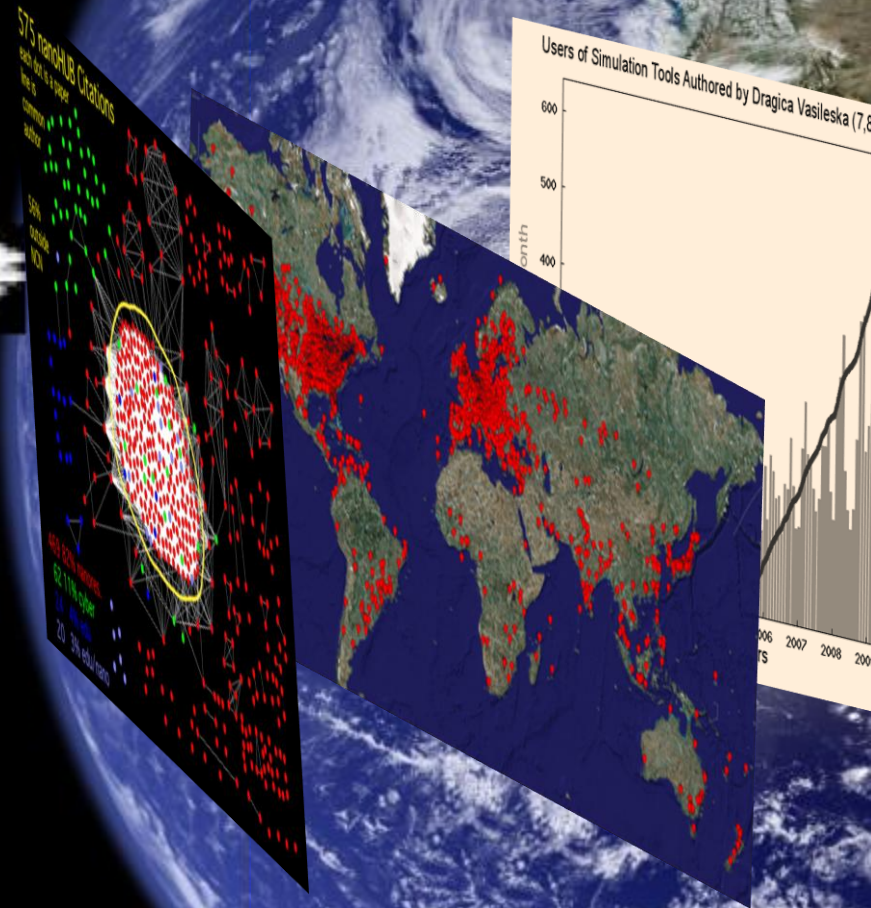
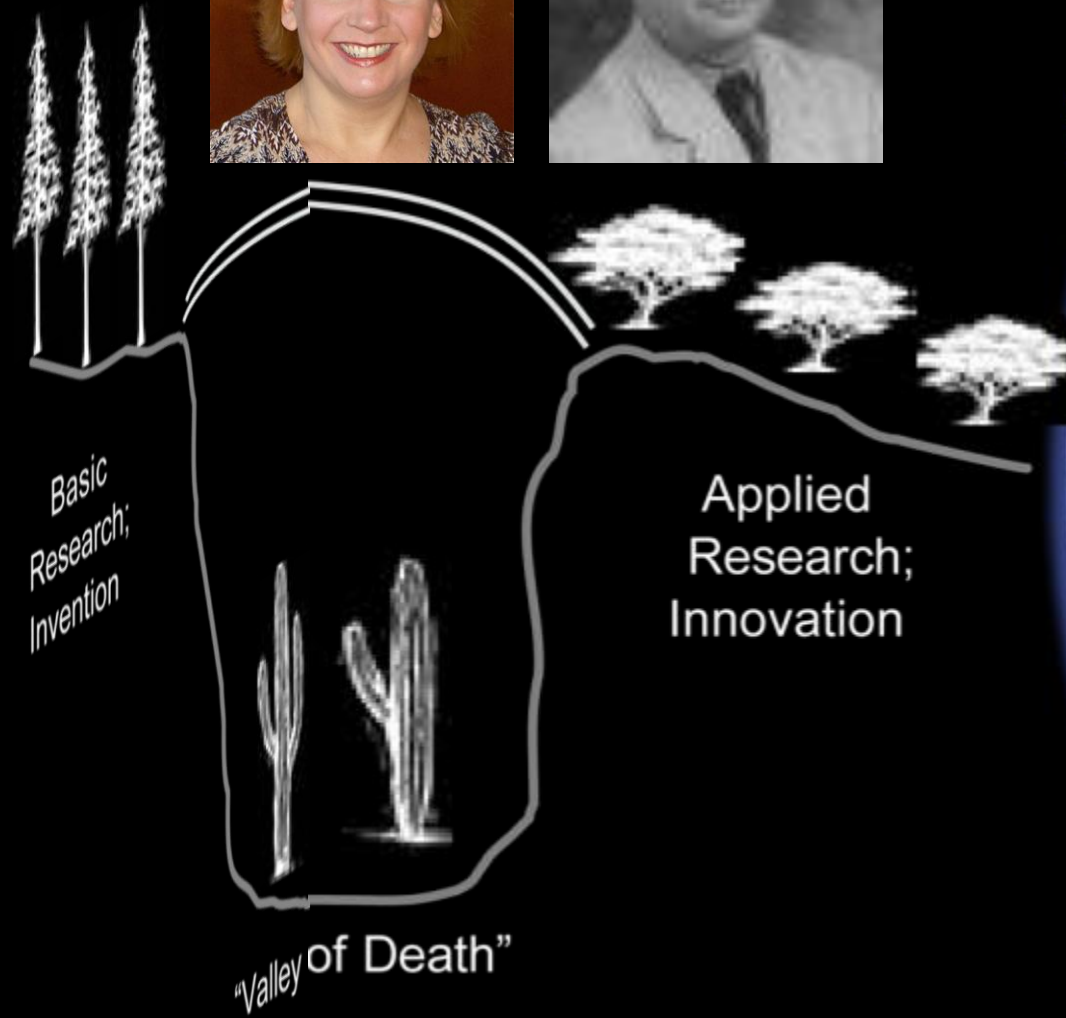
Basic
Research;
Invention

Rappture Toolkit

Applied
Research;
Innovation

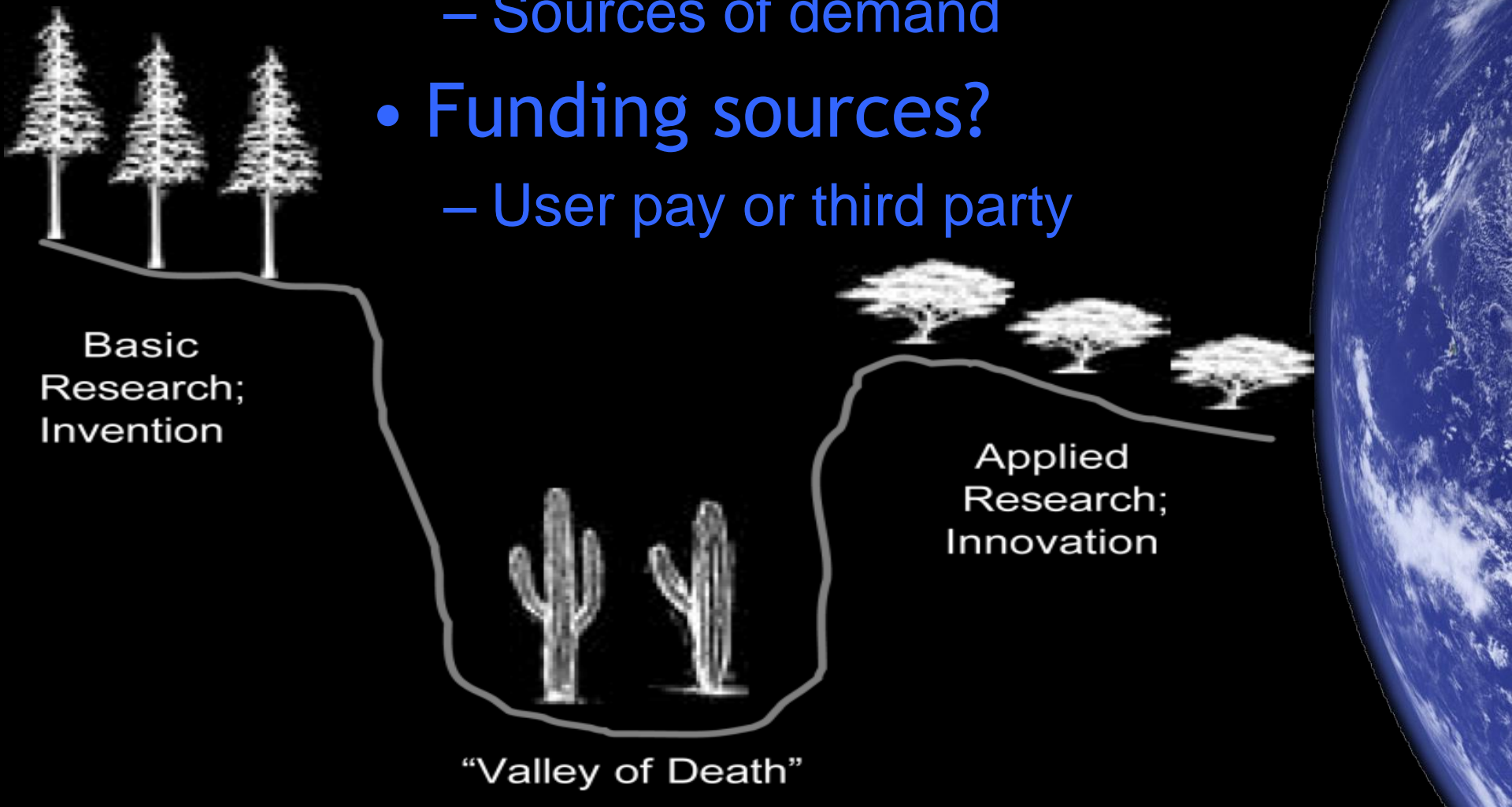
“Valley of Death”

5: Open usage and assessment



6: Sustaining business model

- Who benefits?
 - Sources of demand
- Funding sources?
 - User pay or third party



HUBzero™ Roadmap

George Adams and Michael McLennan
HUBzero Consortium

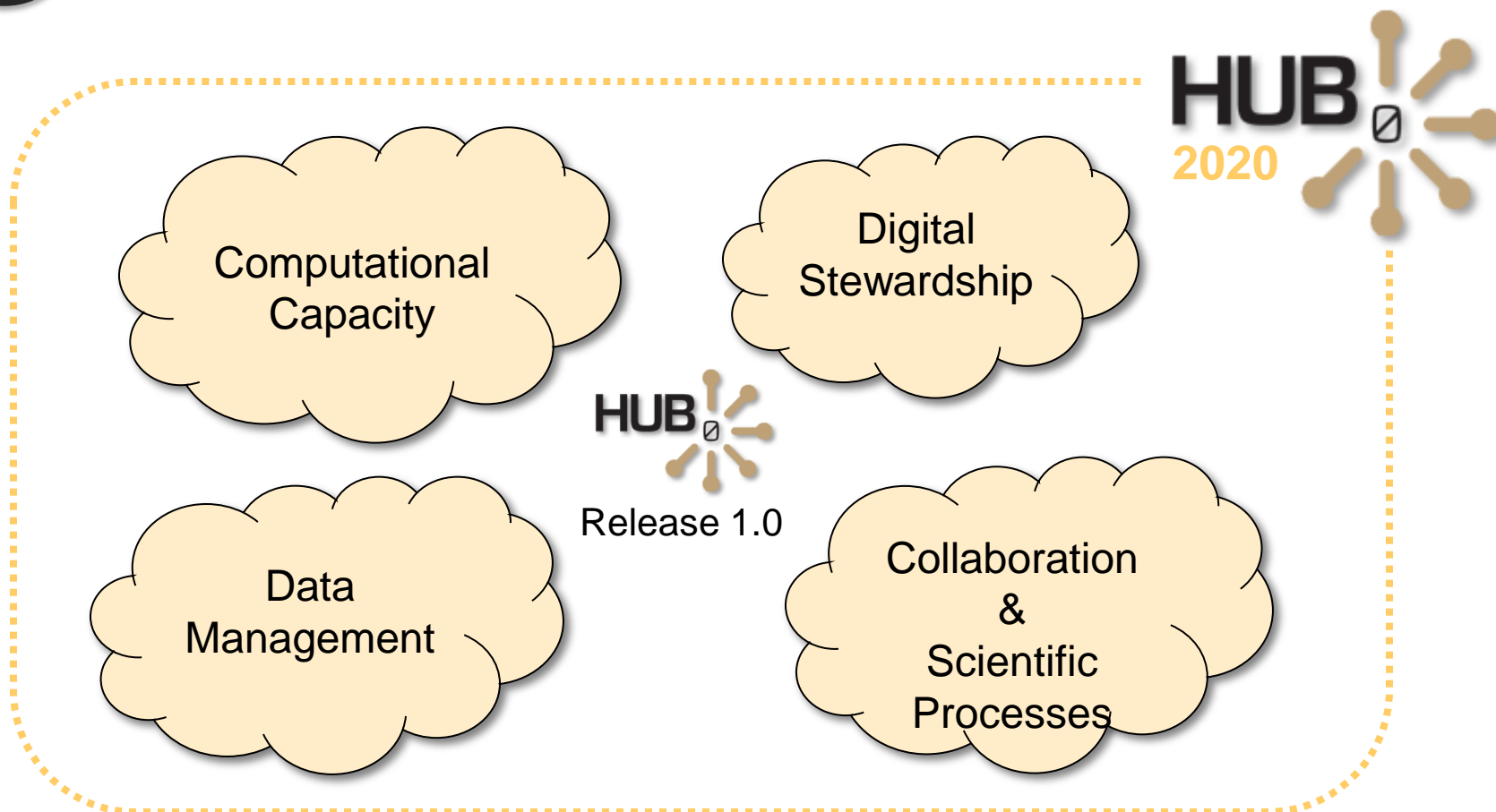
Challenges: Dealing with large data sets, usability, visualization

*Feedback from
our survey*

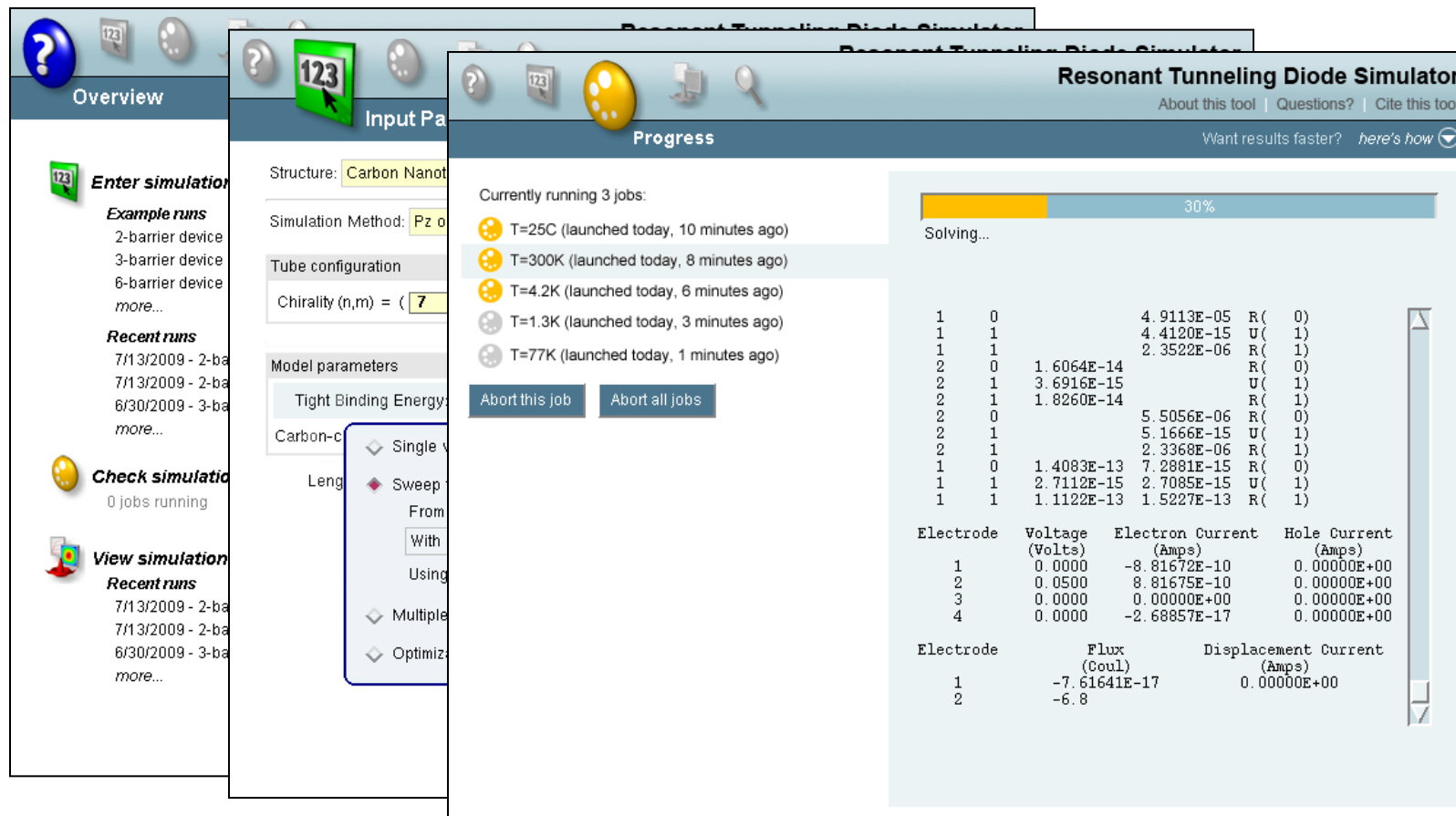
Federated access to the hub so I can integrate a variety of web resources and so my users can seamlessly access resources in multiple security domains.

Creating the tools to enable community authoring of content to share between teachers, as well as enabling and enforcing the proper relationships and data privacy for teacher/student and teacher/class relationships.

Elevate computing and software development to the same level of reproducibility and peer review as traditional publishing.



The best way to predict the future is to invent it.
Alan Kay



Overview

Enter simulation

Example runs

- 2-barrier device
- 3-barrier device
- 6-barrier device
- more...

Recent runs

- 7/13/2009 - 2-barrier device
- 7/13/2009 - 2-barrier device
- 6/30/2009 - 3-barrier device
- more...

Check simulation

0 jobs running

View simulation

Recent runs

- 7/13/2009 - 2-barrier device
- 7/13/2009 - 2-barrier device
- 6/30/2009 - 3-barrier device
- more...

Input Parameters

Structure: Carbon Nanotube

Simulation Method: Pz o

Tube configuration

Chirality (n,m) = (7

Model parameters

Tight Binding Energy

Carbon-c

Length

Single v

Sweep

From

With

Using

Multiple

Optimize

Progress

Currently running 3 jobs:

- T=25C (launched today, 10 minutes ago)
- T=300K (launched today, 8 minutes ago)
- T=4.2K (launched today, 6 minutes ago)
- T=1.3K (launched today, 3 minutes ago)
- T=77K (launched today, 1 minutes ago)

Abort this job Abort all jobs

Resonant Tunneling Diode Simulator

About this tool | Questions? | Cite this tool

Want results faster? [here's how](#)

Solving... 30%

Electrode	Voltage (Volts)	Electron Current (Amps)	Hole Current (Amps)
1	0.0000	-8.81672E-10	0.00000E+00
2	0.0500	8.81675E-10	0.00000E+00
3	0.0000	0.00000E+00	0.00000E+00
4	0.0000	-2.68857E-17	0.00000E+00

Electrode	Flux (Coul)	Displacement Current (Amps)
1	-7.61641E-17	0.00000E+00
2	-6.8	

nanoHUB.org Middleware

- \$1.35M NSF SDCI award, Michael McLennan (PI)
- Redesign Rappture for sweeps/optimizations
- Release HUBzero as Open Source

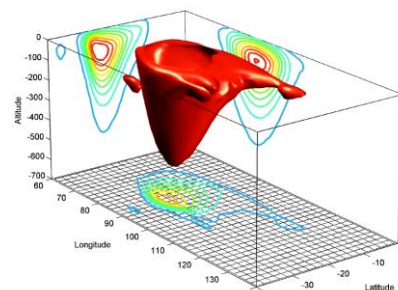


Instant-On Computing for nanoHUB.org

- \$1.4M NSF ARRA award, Gerhard Klimeck (PI)
- Execute jobs without waiting in a queue
- Make TeraGrid “wide” and “open”
- Partner: UT / Oak Ridge National Lab

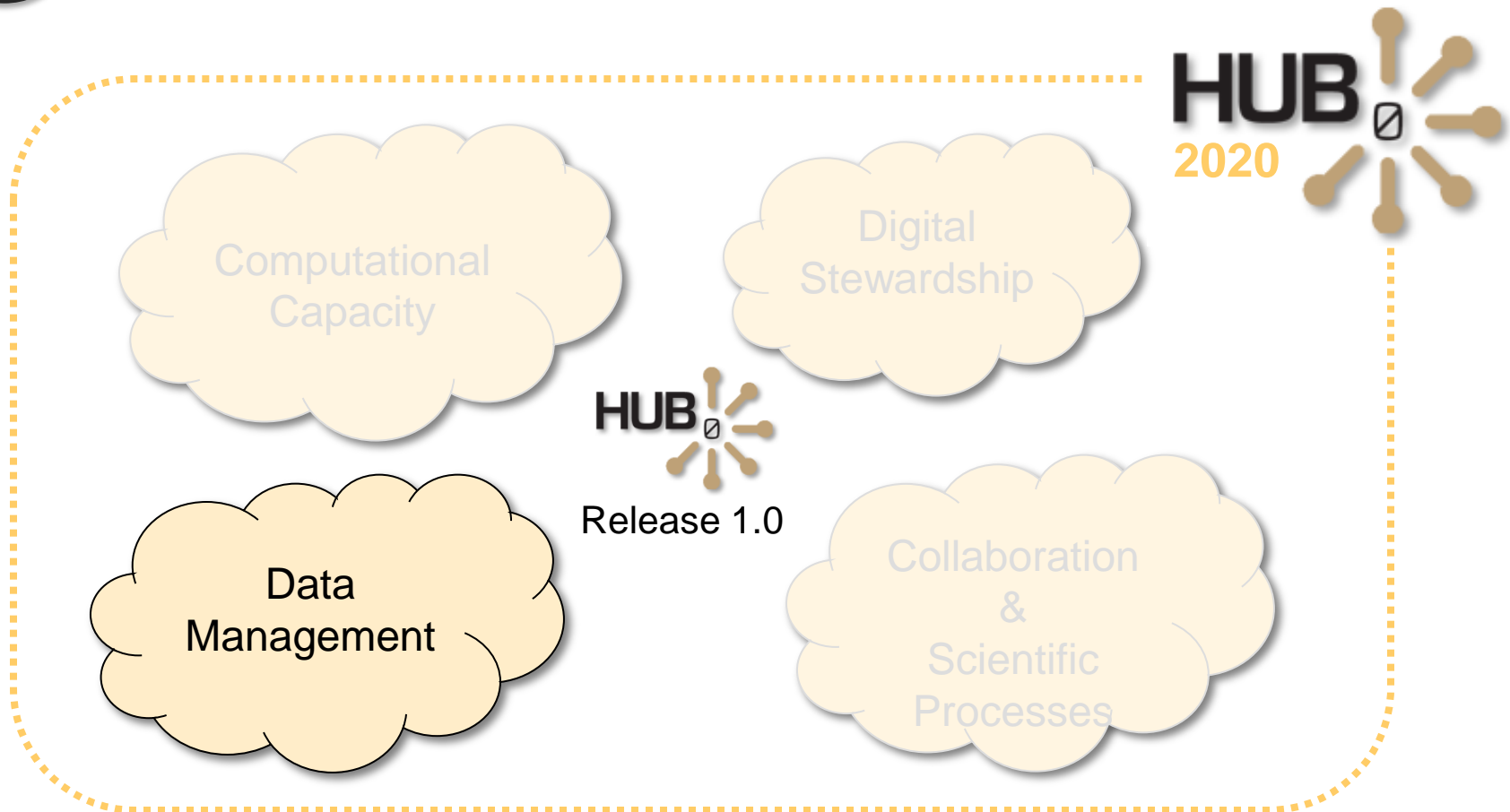
Cornell MATLAB Cluster

- \$660K NSF ARRA award, David Lifka (PI)
- Send nanoHUB.org MATLAB jobs to Cornell cluster



Pharmaceutical Engineering Pipeline

- \$1.9M NSF CDI award, Rex Reklaitis (PI)
- Build a workflow system for Rapture-based models
- Study pharmaceutical performance in diverse patient populations



The best way to predict the future is to invent it.
Alan Kay

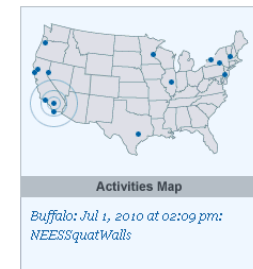


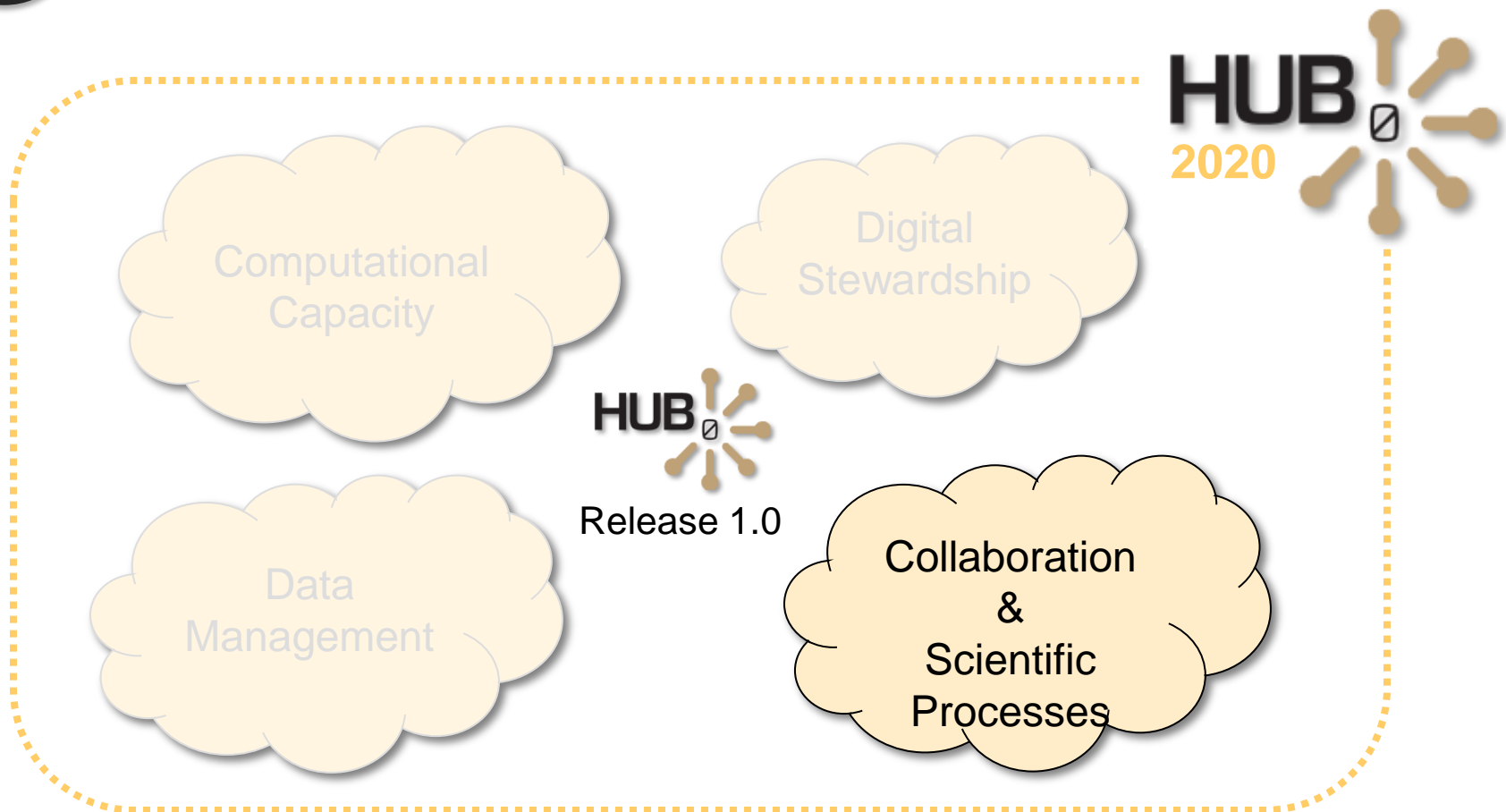
Cancer Care Engineering - cceHUB.org

- Led by Ann Christine Catlin
- Built a Rappture-like spec for databases
- Support analysis of blood samples

Network for Earthquake Engineering Simulation (NEES)

- \$105M NSF project across 14 institutions
- Share/analyze experimental data

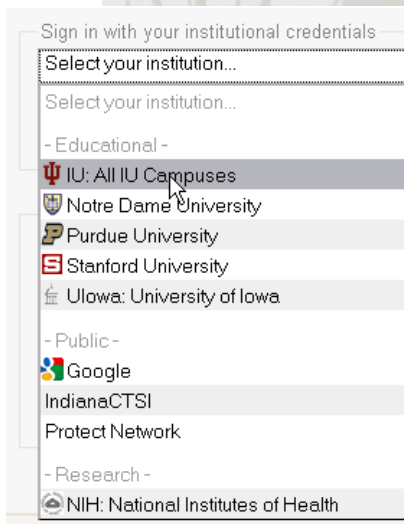




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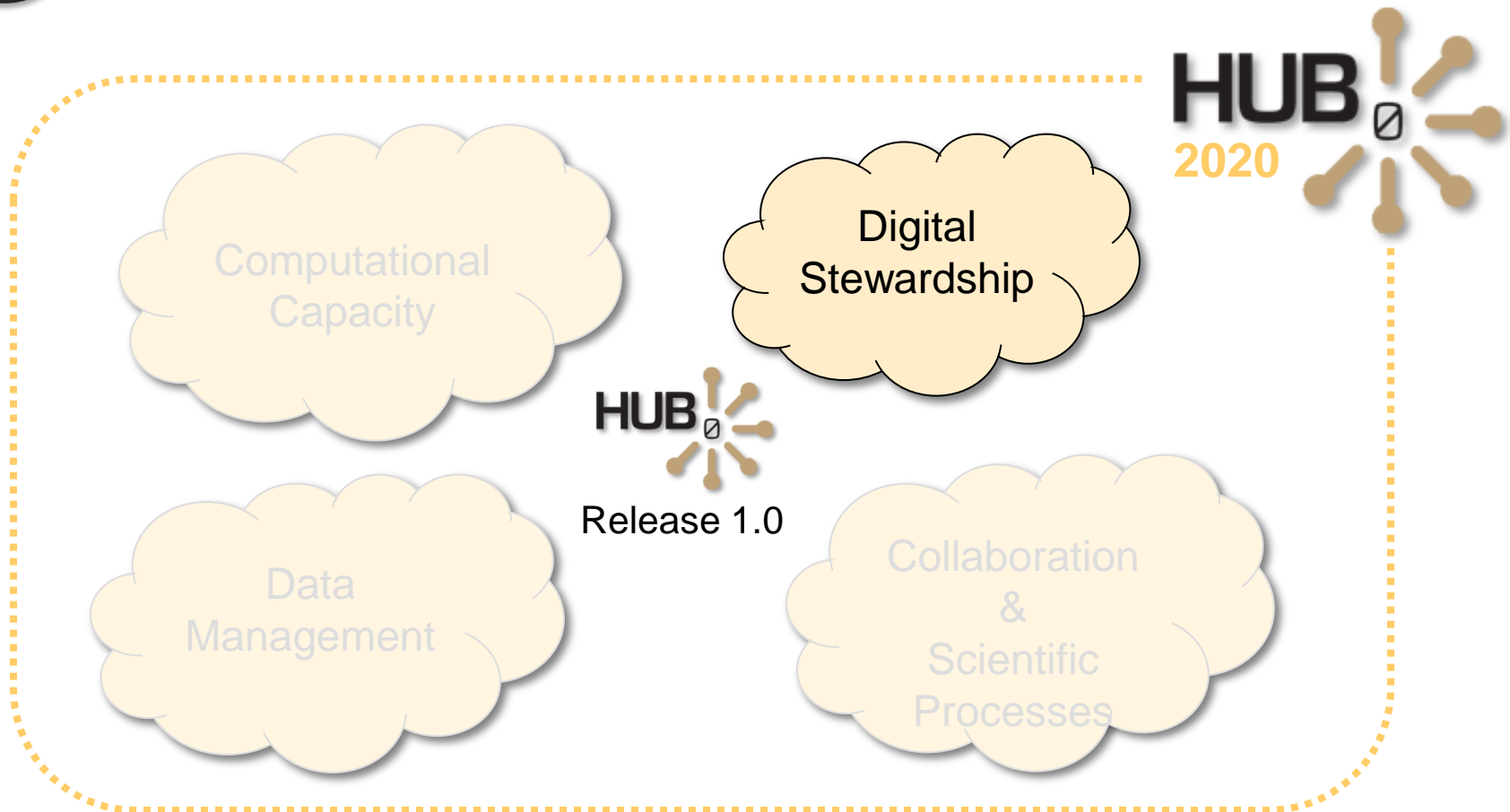
Single Sign-on for researchers from multiple institutions

- Use institutional credentials
- Login is transparent with little additional overhead
- Logins managed institutionally so there is confidence in the real identities
- Authentication credentials can be carried to multiple resources with one login
- As new staff/faculty come on board, they are automatically authenticated

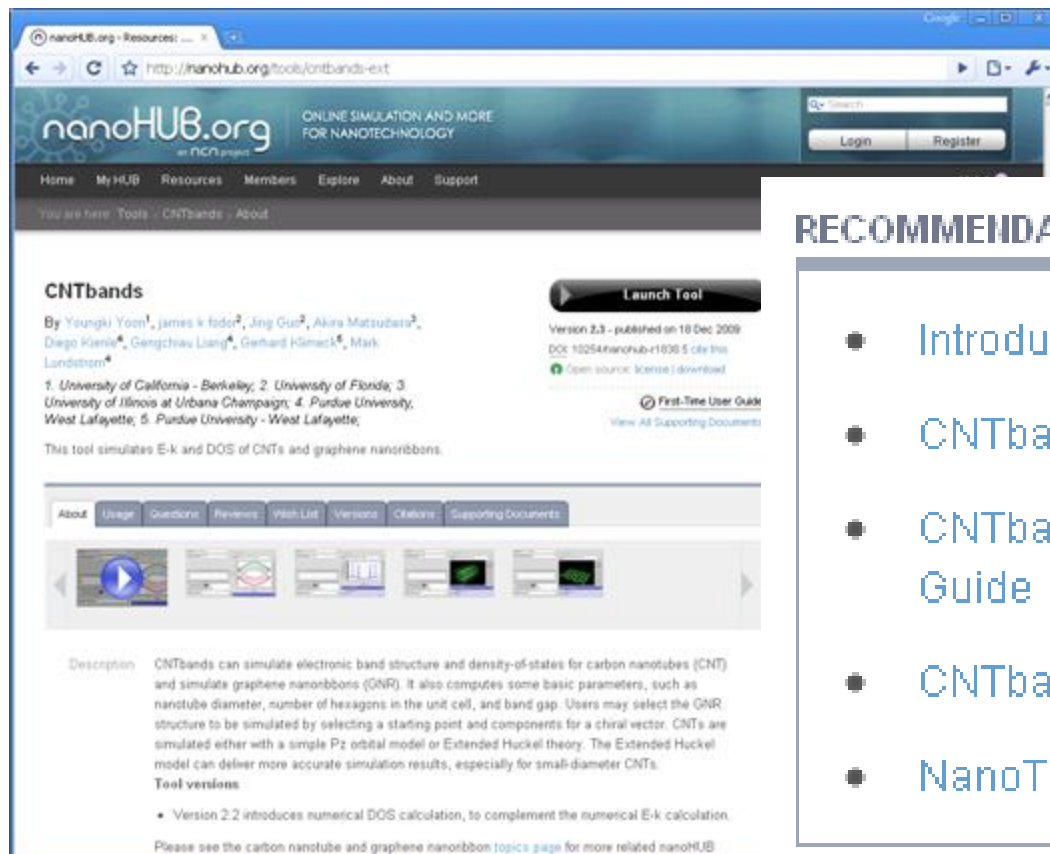


Indiana University - IndianaCTSI.org

- Bill Barnett, Director of Advanced IT Core, IUSM
- Indiana is the first CTSA org to accept InCommon
- NIH pushing InCommon
 - Uses it on their sites (eg., CTSASWeb.org)
- NSF moving toward InCommon



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The screenshot shows the nanoHUB.org website. The main header features the nanoHUB.org logo and the tagline "ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY". Below the header is a navigation bar with links: Home, MyHUB, Resources, Members, Explore, About, Support. A search bar is located on the right side of the header. The main content area displays the "CNTbands" tool page. It includes a "Launch Tool" button, the version number "Version 2.3 - published on 18 Dec 2009", and a list of authors: By Youngki Yoon¹, James K. Fodor², Jing Guo³, Akira Matsubara³, Diego Klenke⁴, Gengchao Liang⁴, Gerhard Klimek⁵, Mark Lundstrom⁴. The page also features a "First-Time User Guide" link and a "View All Supporting Documents" link. A description of the tool is provided, along with a list of tool versions and a link to the carbon nanotube and graphene nanoribbon topics page.

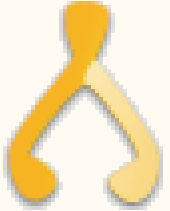
RECOMMENDATIONS

- [Introduction to CNTbands](#)
- [CNTbands](#)
- [CNTbands: First Time User Guide](#)
- [CNTbands Download](#)
- [NanoTCAD VIDES](#)

Powered by ...

Seed Project: Recommendation engine for nanoHUB.org

- Luo Si, Assistant Prof in Computer Science, Statistics
- Suggest resources based on similarity and access patterns



Make a “wish”

<http://hubzero.org/wishlist>

Digital objects archive

New visualization modalities: Paraview, VISIT, GIS

Integration with Facebook, LinkedIn, Skype

...

What do you want?

Data Collection and Curation

Tools for Innovation, Analysis, and Simulation

Data Accessibility and Information Sharing

Acknowledgements

- This work was supported by the U.S. National Science Foundation through awards EEC-0956819 and EEC-0634750 and by Purdue University
- HUBzero™ is a trademark of Purdue University
- Thanks to the entire nanoHUB.org and HUBzero team

Why publish a simulation tool?

nanoHUB.org
an ncn project

ONLINE SIMULATION AND MORE
FOR NANOTECHNOLOGY

[Home](#) [My HUB](#) [Resources](#) [Members](#) [Explore](#) [About](#) [Support](#)

You are here: [Resources](#) > [Tools](#) > [Schred](#) > [About](#)

Schred

By Dragica Vasileska¹, Shaikh S. Ahmed², Matteo Mannino³, Akira Matsudaira⁴, Gerhard Klimeck⁵, Mark Lundstrom³

1. Arizona State University; 2. Southern Illinois University at Carbondale; 3. Purdue University, West Lafayette; 4. University of Illinois at Urbana Champaign; 5. Purdue University - West Lafayette;

Calculates the envelope wavefunctions and the corresponding bound-state energies in a typical MOS (Metal-Oxide-Semiconductor) or SOS (Semiconductor-Oxide-Semiconductor) structure and a typical SOI structure

Version 2.2
DOI: 10254/
Open so

9.0 RANKING

Advanced

1667 user(s), detailed usage

4 questions (Ask a question)

5 review(s) (Review this)

2 wish(es) (Add a new wish)

97 Citation(s)

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Description **Schred** calculates the envelope wavefunctions and the corresponding bound-state energies in a typical MOS (Metal-Oxide-Semiconductor) or SOS (Semiconductor-Oxide-Semiconductor) structure

SEE ALSO

ABACUS—Introduction to Semiconductor Devices

Part of: NCN Nanoelectronics: Simulation Tools for Research

a TCAD Lab

ACUTE—Assembly for Computational Electronics

AOME Advancing Quantum