Uso de simulaciones en investigación y educación en ciencia e ingeniería

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Seminario Internacional EAFIT, Medellin, Colombia

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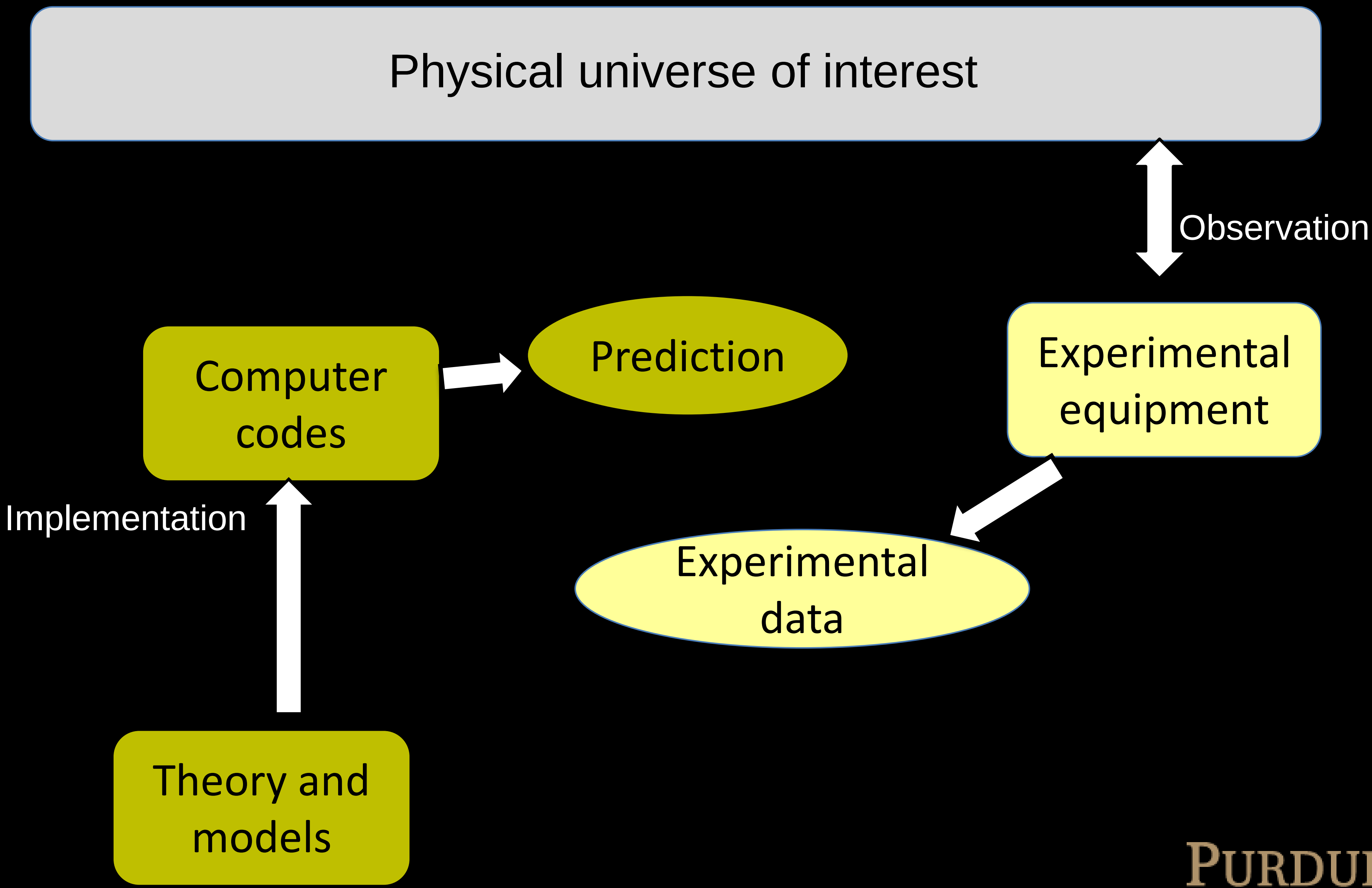
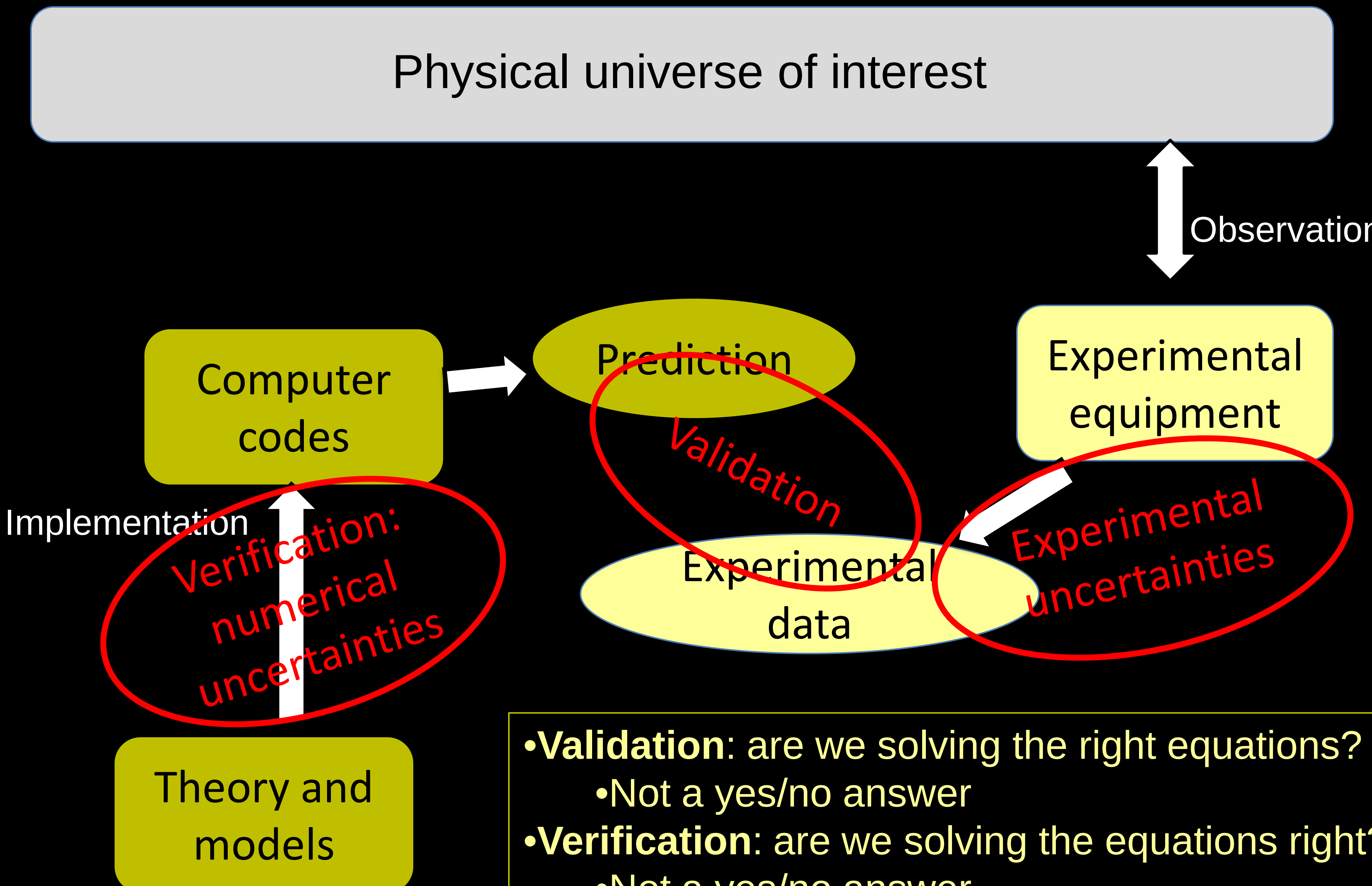
What is a simulation?



Verification and validation



- **Validation**: are we solving the right equations?
  - Not a yes/no answer
- **Verification**: are we solving the equations right?
  - Not a yes/no answer

Simulations in science and engineering

Aircraft and aerospace

- 1980’s 70+ wind tunnel tests for wing design
- Boeing 777: only 11 experiments due to CDF
- 2013 revenues: $86 B

Electronics industry

- SPICE (Simulation Program with Integrated Circuit Emphasis)
  - Circuit simulator from UC Berkeley
- SUPREME (Stanford University Process Modeling)
  - Fabrication of semiconductor devices
- $300B in sales in 2013

What is next?

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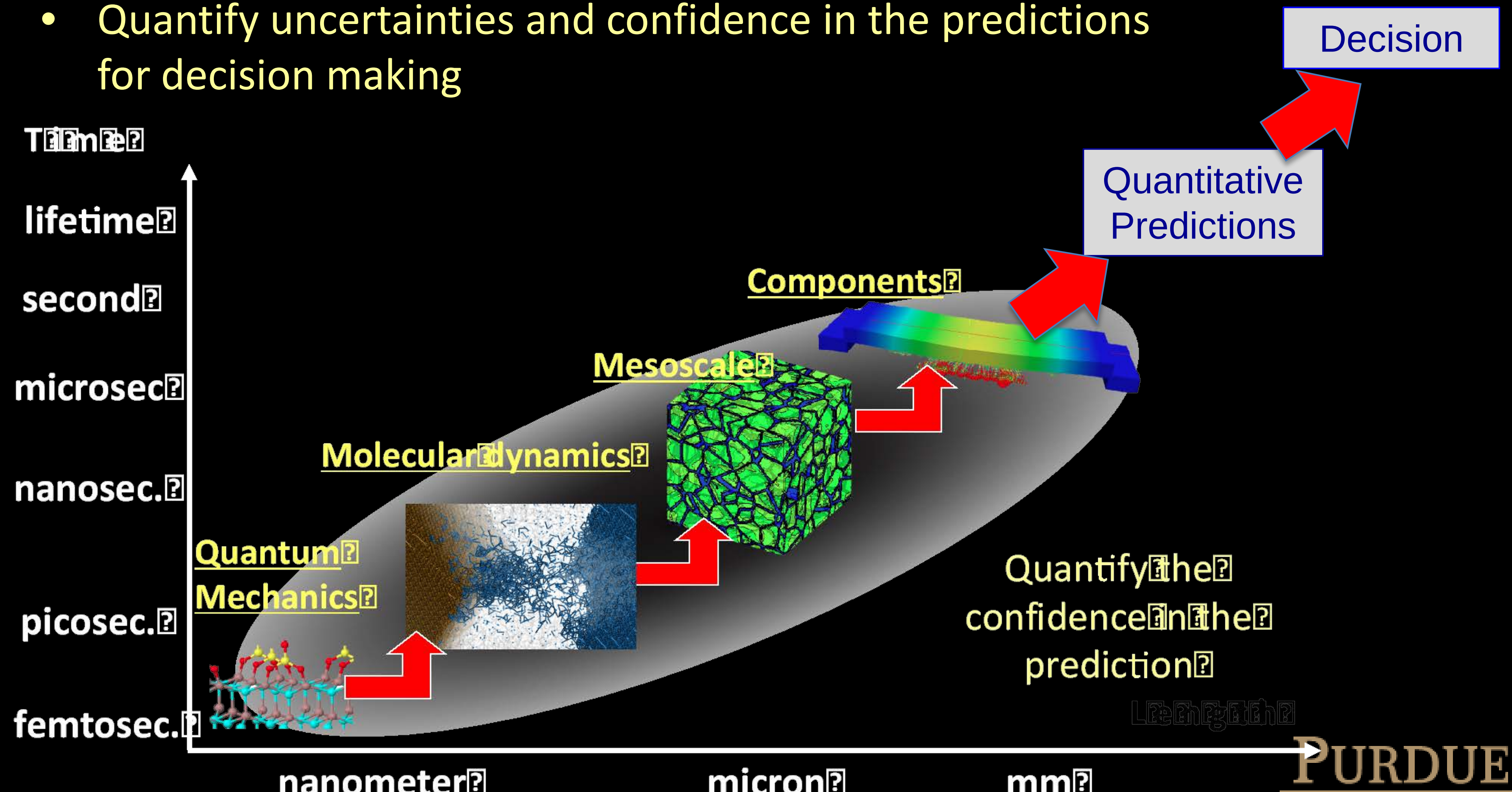
Materials modeling and simulations

- Uncover and characterize the molecular-level mechanisms that govern materials
- Contribute to the design and certification of materials
- Quantify uncertainties and confidence in the predictions for decision making



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Key technologies & infrastructure

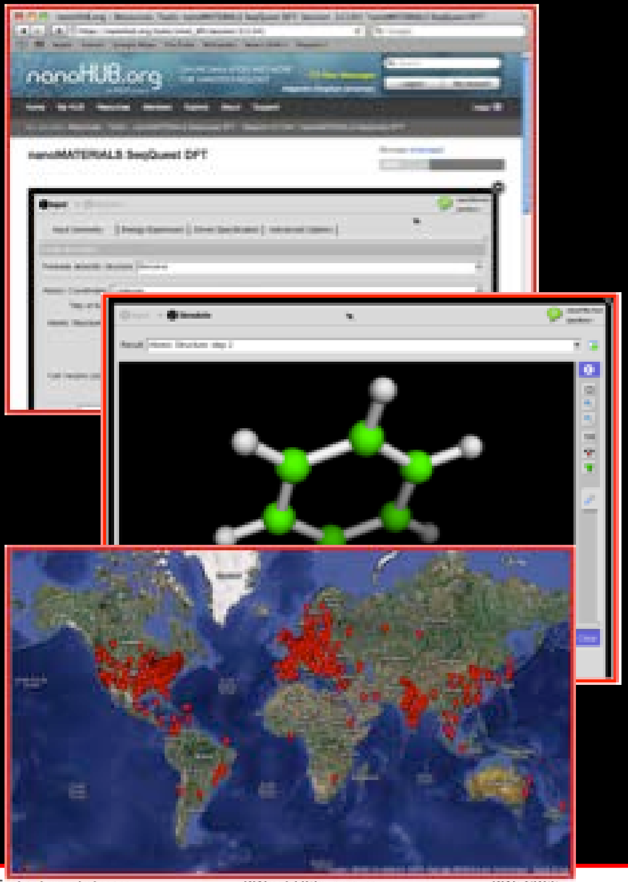
New material/device design

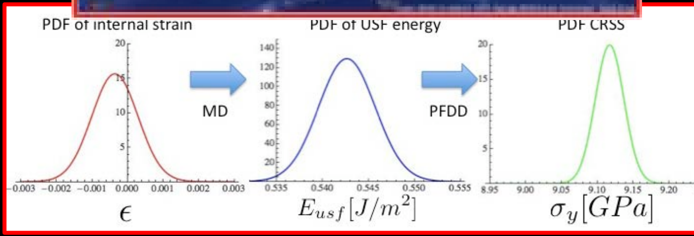
- Apply/develop state of the art science and engineering to real-world problems
- Efficient technology transfer between collaborators

Uncertainty quantification for decision making

Certification

- Rapid adoption/testing of new technology by the scientific community





- Next-generation engineers and scientists familiar with predictive modeling

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Simulations universally accessible & useful


```
xterm
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-rw-r--r-- sjplimp/sjplimp   5761 2010-01-14 18:33:28 lammps-20Feb10/examples/peptide/log.peptide.15Jan10.linux.1
[strachan@coates-fe02 LAMMPS]$
```
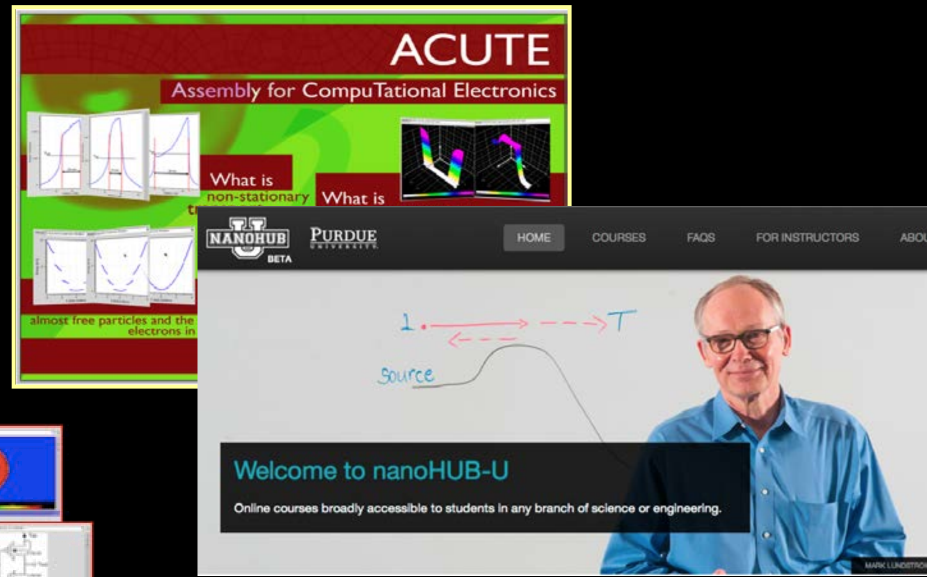
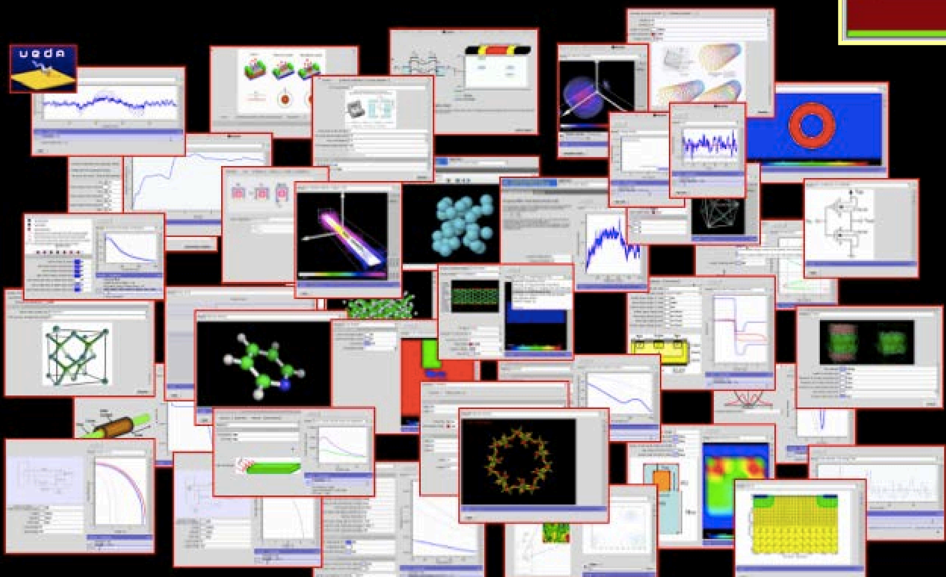

- How do I compile it?
- What libraries do I need?
- Where do I run the simulations?
- What queuing system does the supercomputer use?

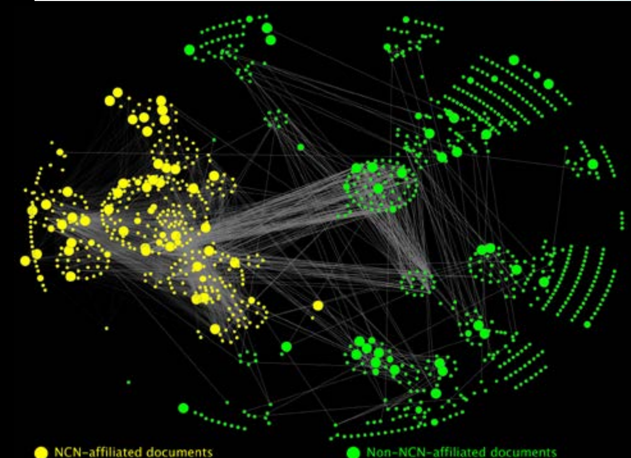
nanoHUB

Education
- nanoHUB-U
- 500+ teaching materials

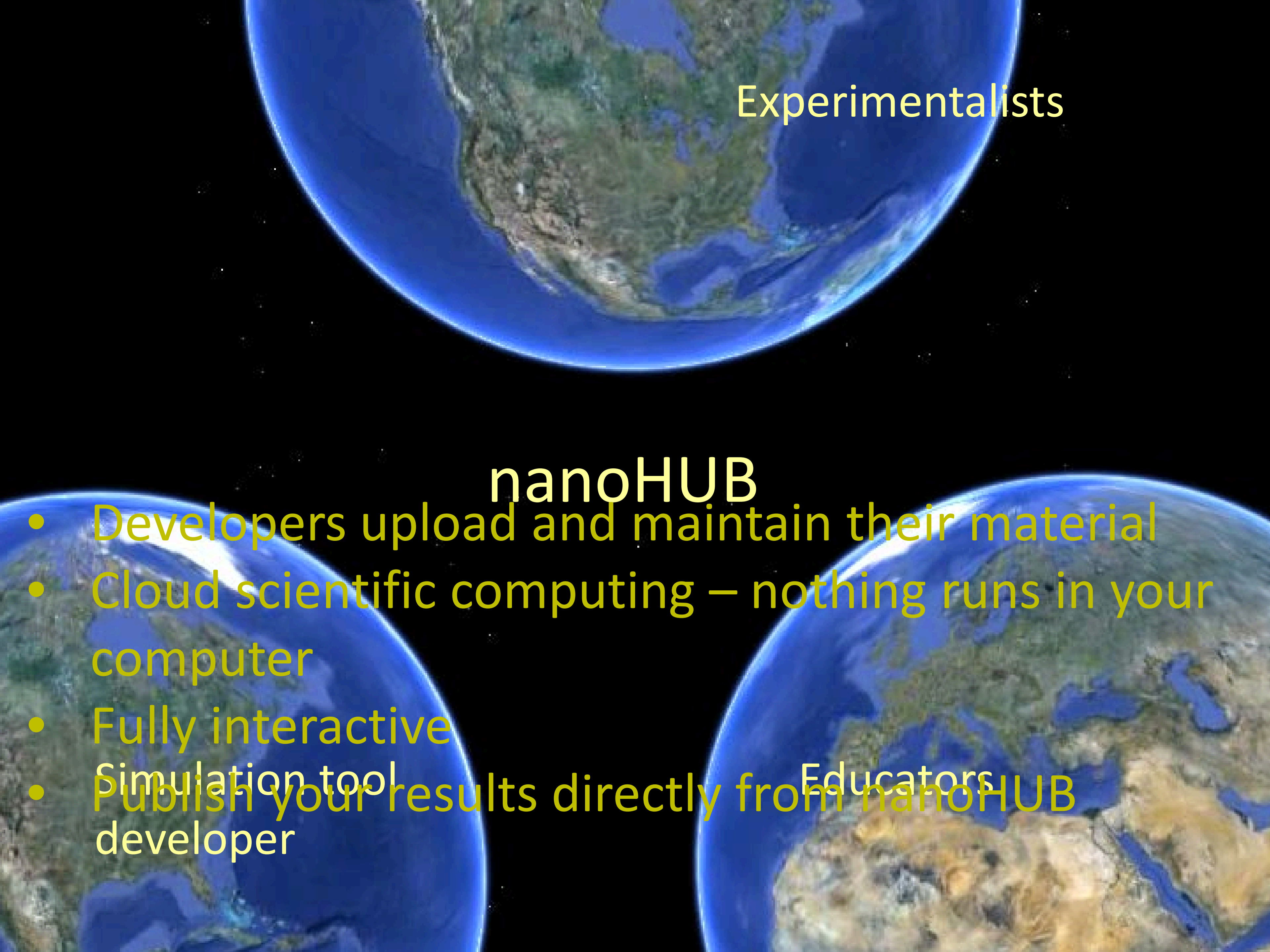


Research in the cloud
- 350+ simulation tools
- 2,500 online seminars





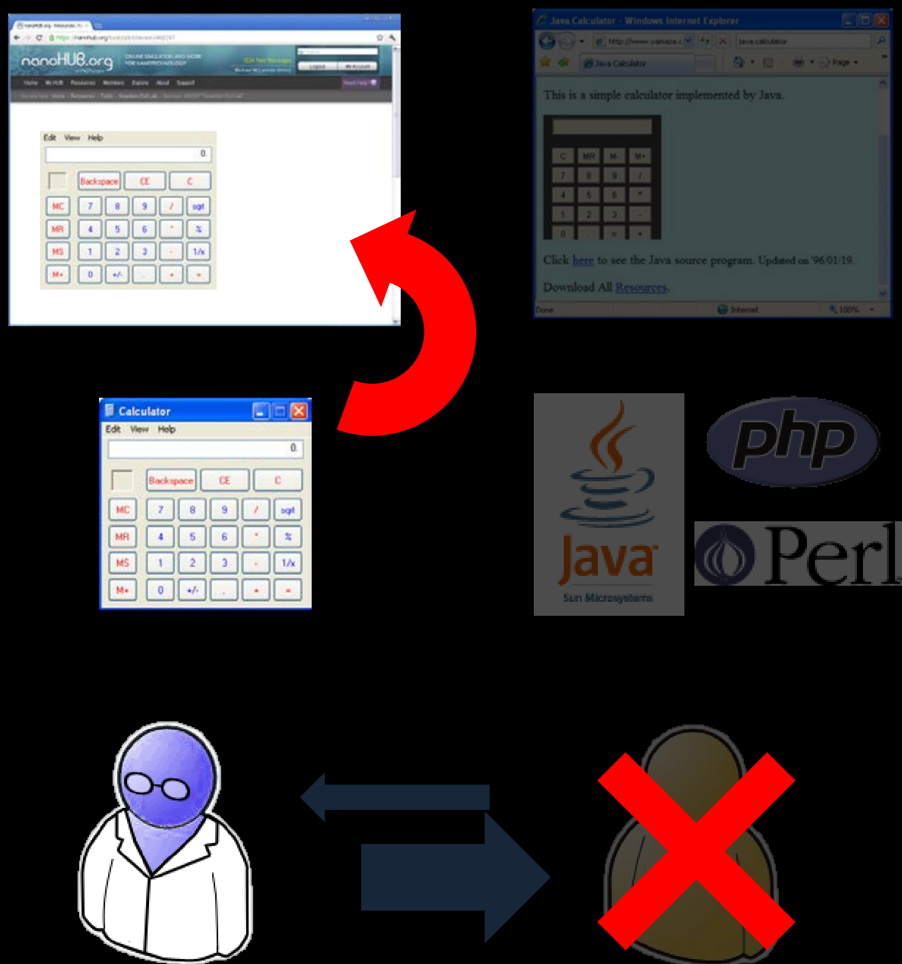
Global collaboration & community



nanoHUB

- Developers upload and maintain their material
- Cloud scientific computing – nothing runs in your computer
- Fully interactive
- Publish your results directly from nanoHUB

Empowering User Contributions



- Faster turn-around: 2-3 years ➔ 1-2 weeks
- Eliminate bottlenecks
- Researcher retains ownership of code
- Rappture toolkit simplifies development

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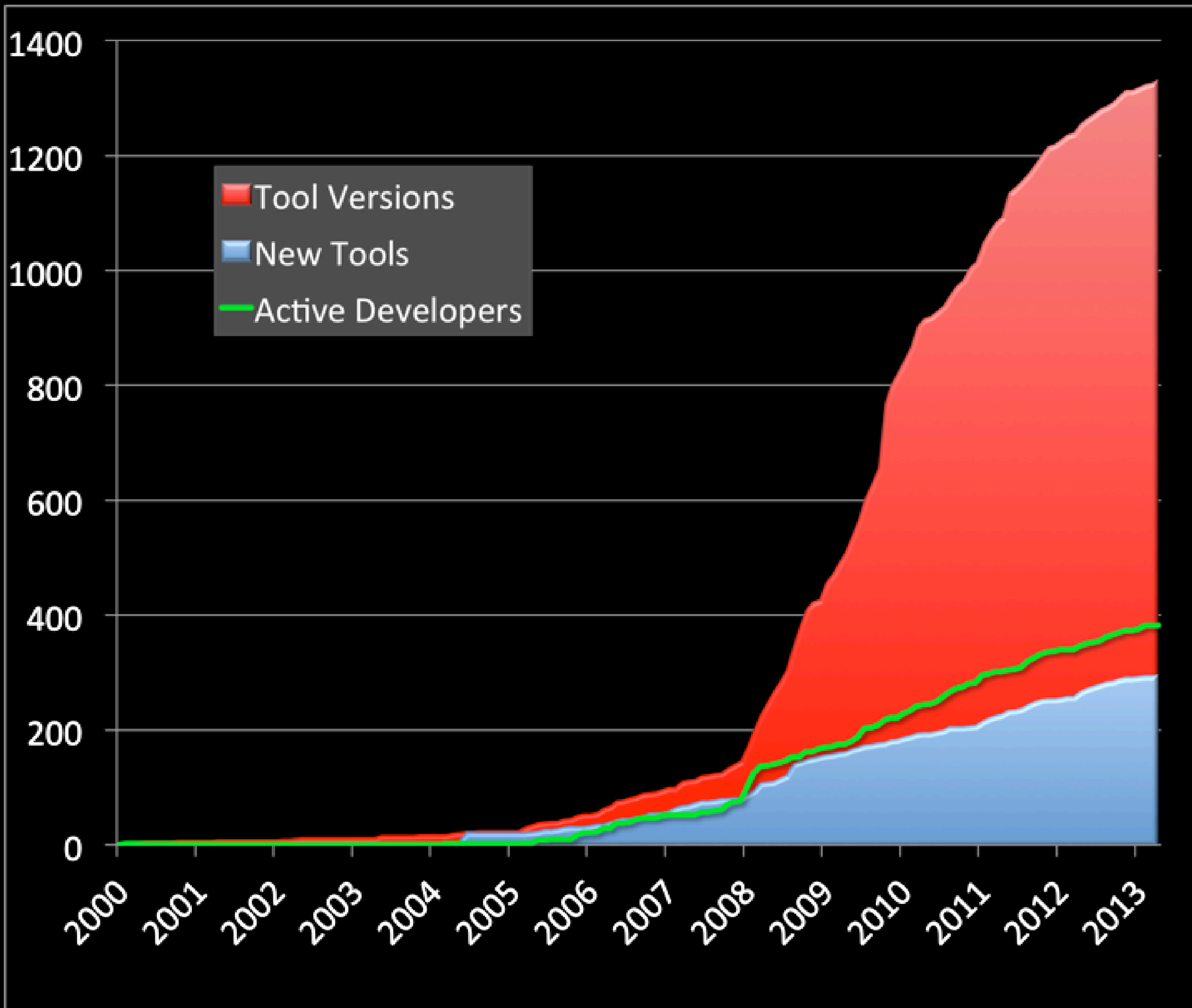
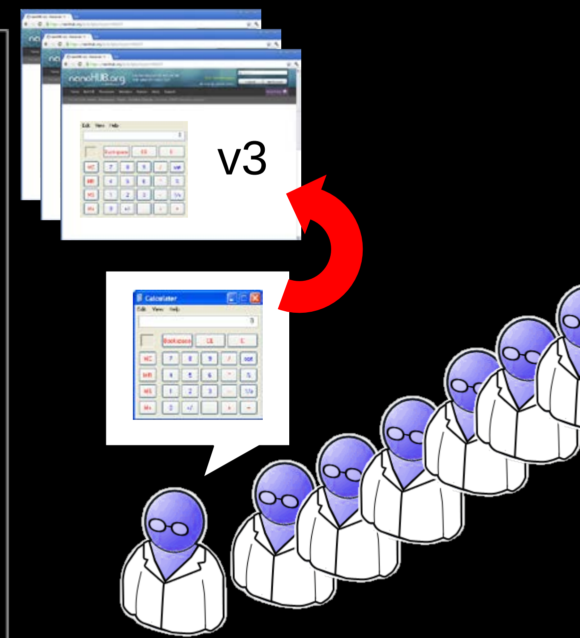
Up to date tools, a community of developers



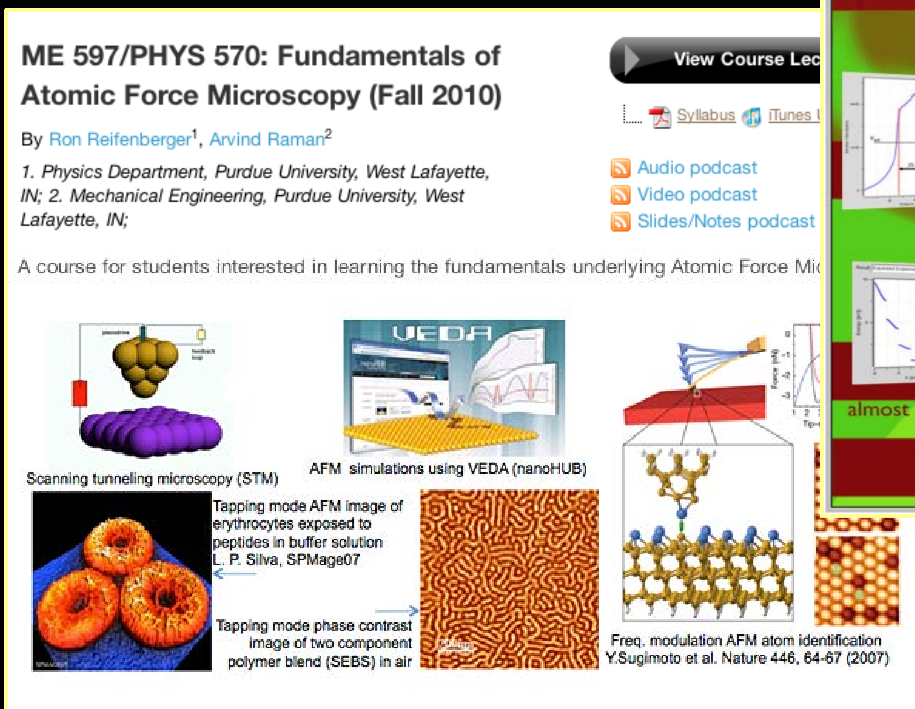


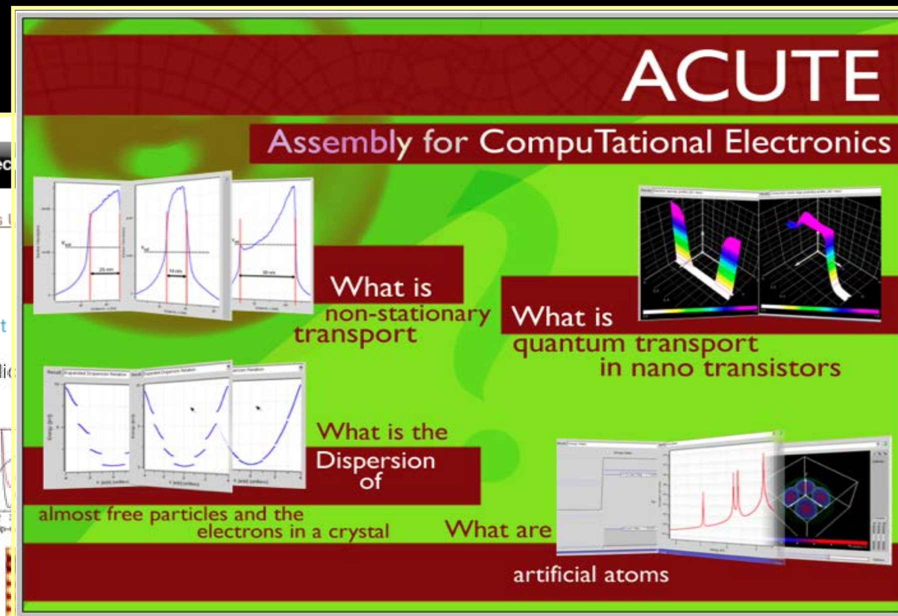
Continual Engagement

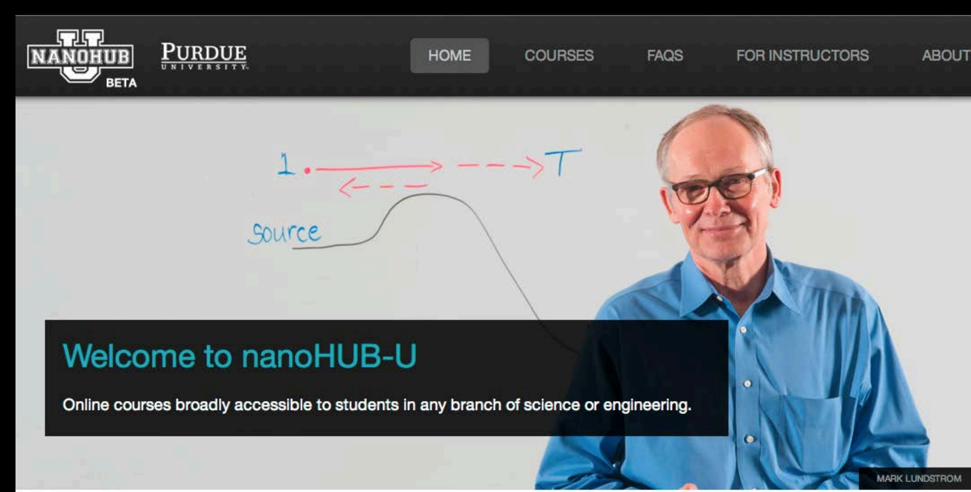
380+ Developers NOT PAID by NCN

nanoHUB simulations in education

Educational material tightly coupled to simulation tools







ABACUS: 3,900+ users

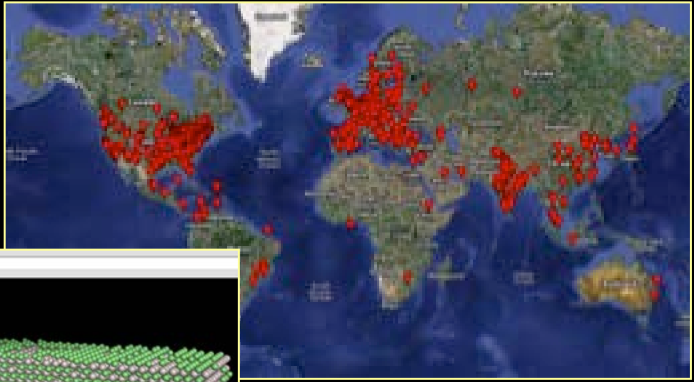
VEDA: 1,300 users

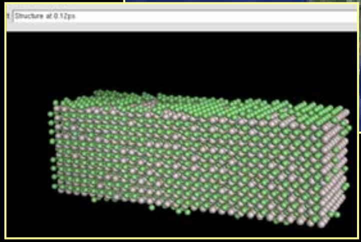
nanoMATERIALS MD: 2,000+ users

Impact at Purdue

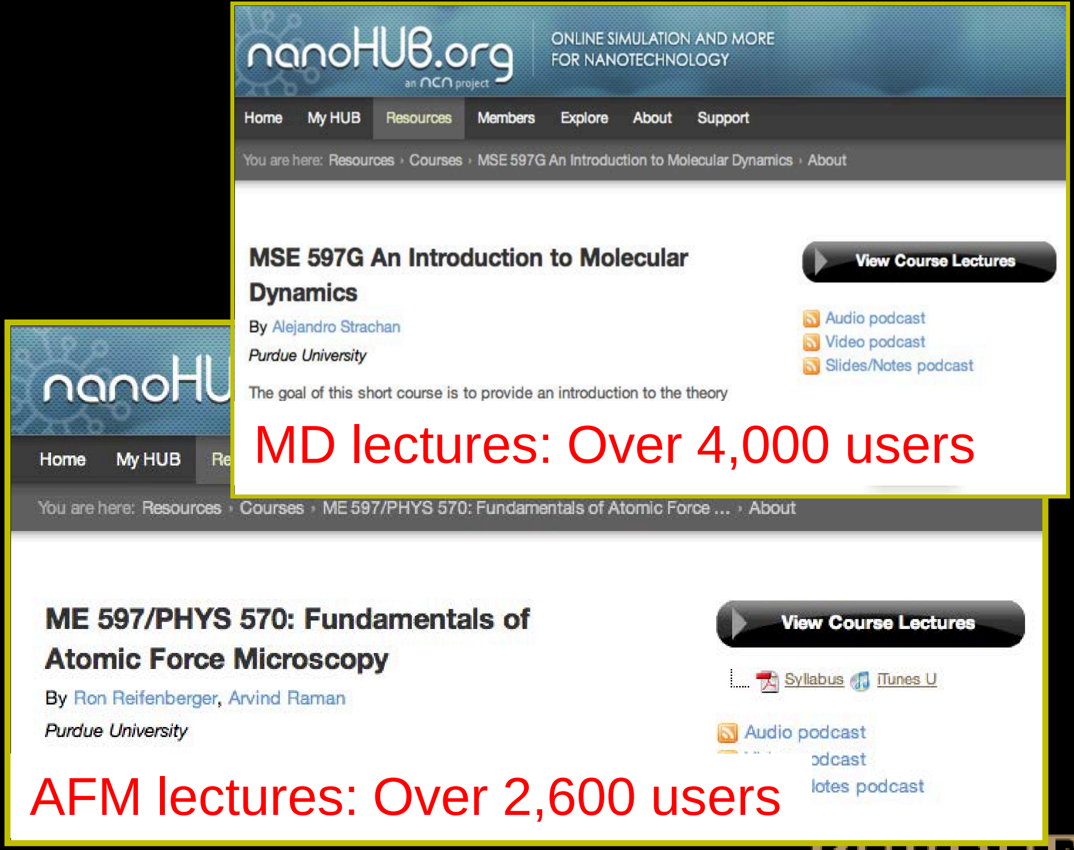
ALL Purdue MSE UG students are exposed to:

- Molecular dynamics simulations (MSE235)
- *Ab initio* electronic structure calculations (MSE270)
- Computational thermodynamics (MSE 260)





nanoMATERIALS simulation tool
Over 2,000+ users



MD lectures: Over 4,000 users

AFM lectures: Over 2,600 users

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Simulation-enhanced Materials learning

Goal

- Enhance learning or explore new topics via online simulations

https://nanohub.org/topics/LearningModulePlasticityMD

nanoHUB.org – Wiki: Learning Module: Atomic Picture of Plastic Deformation in Metals

https nanohub.org/topics/LearningModulePlasticityMD

FacultyCluster Blackboard Learn ClusterQueues Web of Kno...ience Home Apple Disney ESPN Yahoo!

nanoHUB.org an ncn project — ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

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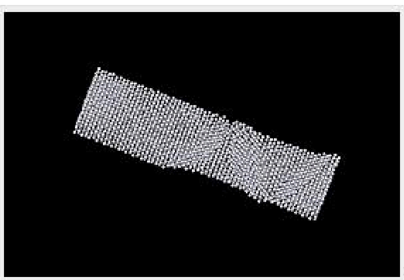
Home › Topics › Learning Module: Atomic Picture of Plastic Deformation in Metals

Learning Module: Atomic Picture of Plastic Deformation in Metals

by Joseph M. Cychosz, Alejandro Strachan

Article | Edit | Comments | History



The main goal of this learning module is to introduce students to the atomic-level processes responsible for plastic deformation in crystalline metals and help them develop a more intuitive understanding of how materials work at molecular scales. *Image to the right shows plastic deformation of a metallic nanowire.*

The module consists of:

- Two introductory lectures (50 minutes each) available online as audiovisual presentations
  - Overview Lecture
  - Prelab Lecture

Format

- Introductory/Background Lecture
- Pre-lab lecture:
  - Tutorial to run a meaningful simulation and analyze the results
- Hands-on lab activity

Additional material

- Learning objectives
- Audience

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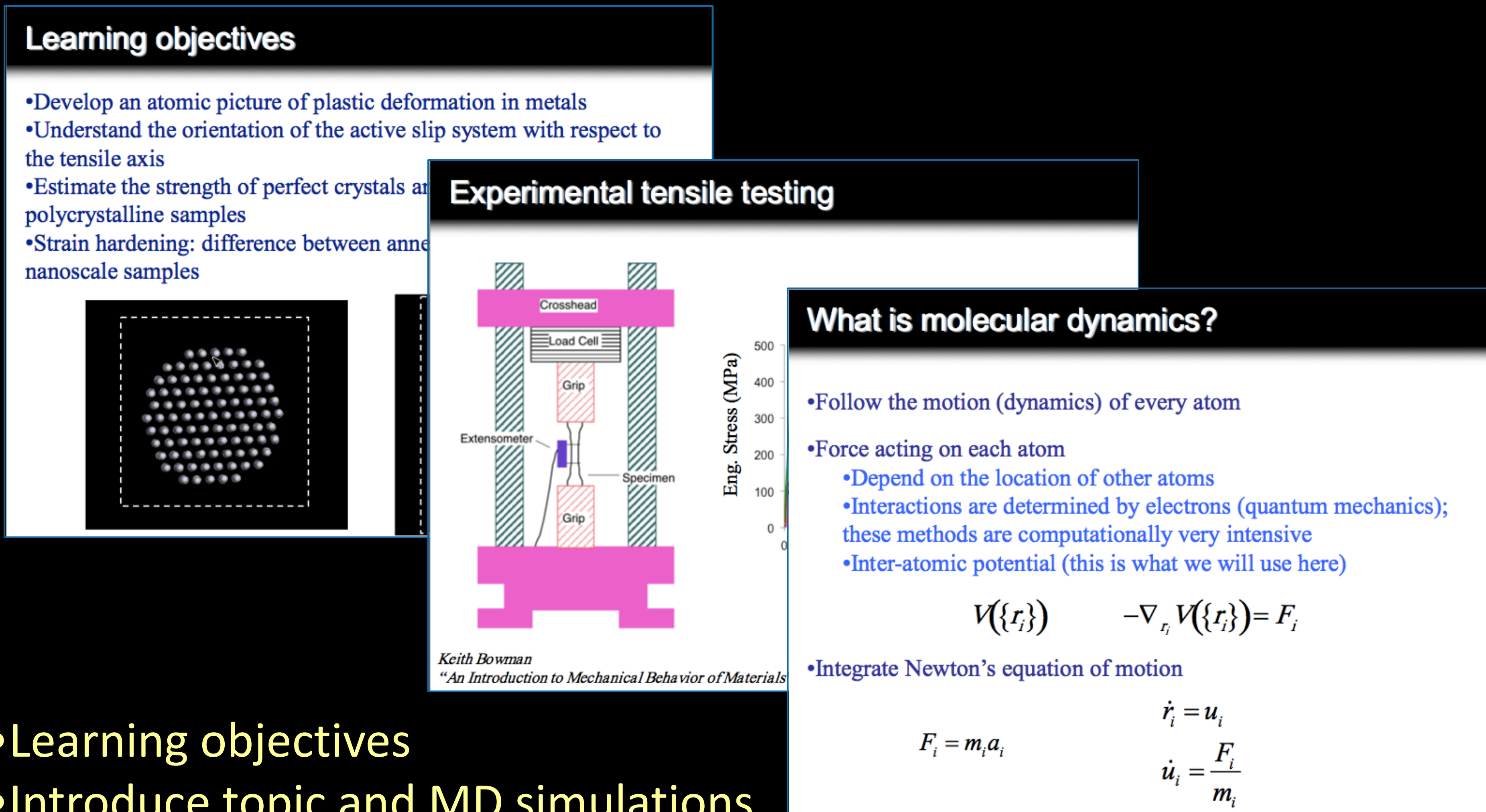
Atomic View of Plasticity: background lecture

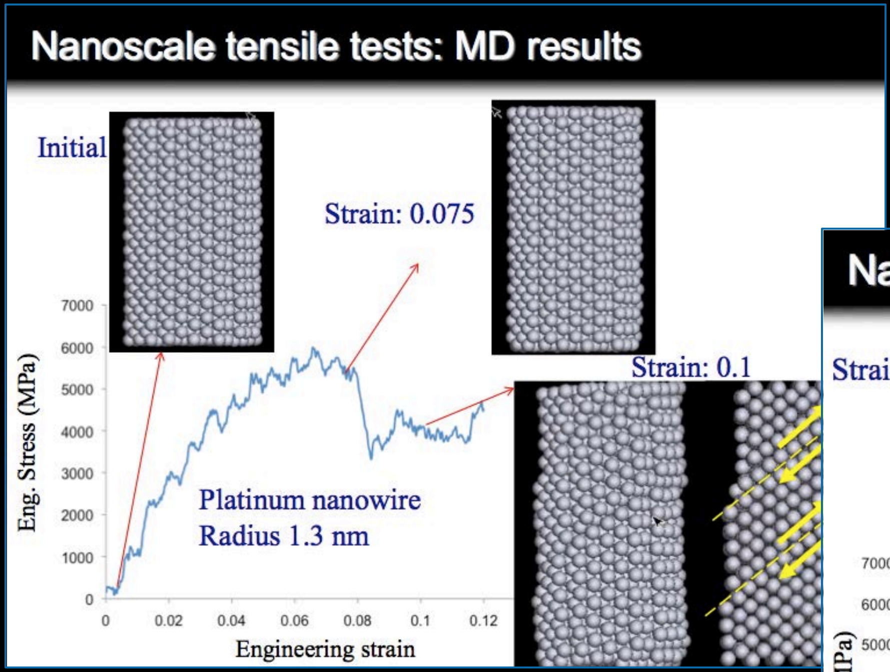
Introductory and background lecture

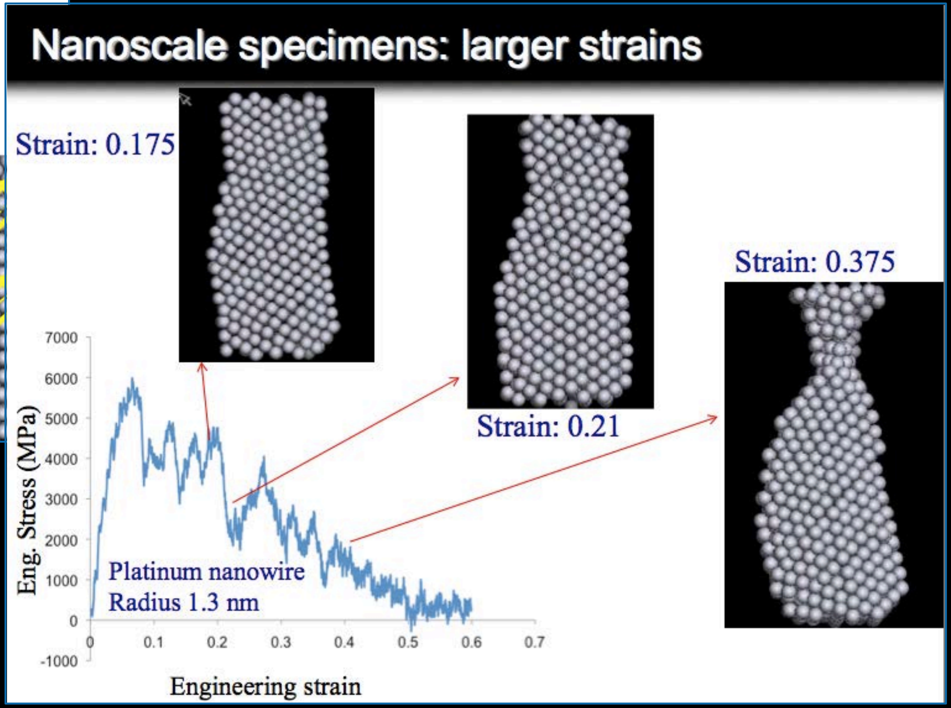


- Learning objectives
- Introduce topic and MD simulations

Atomic View of Plasticity: background lecture

Introductory and background lecture

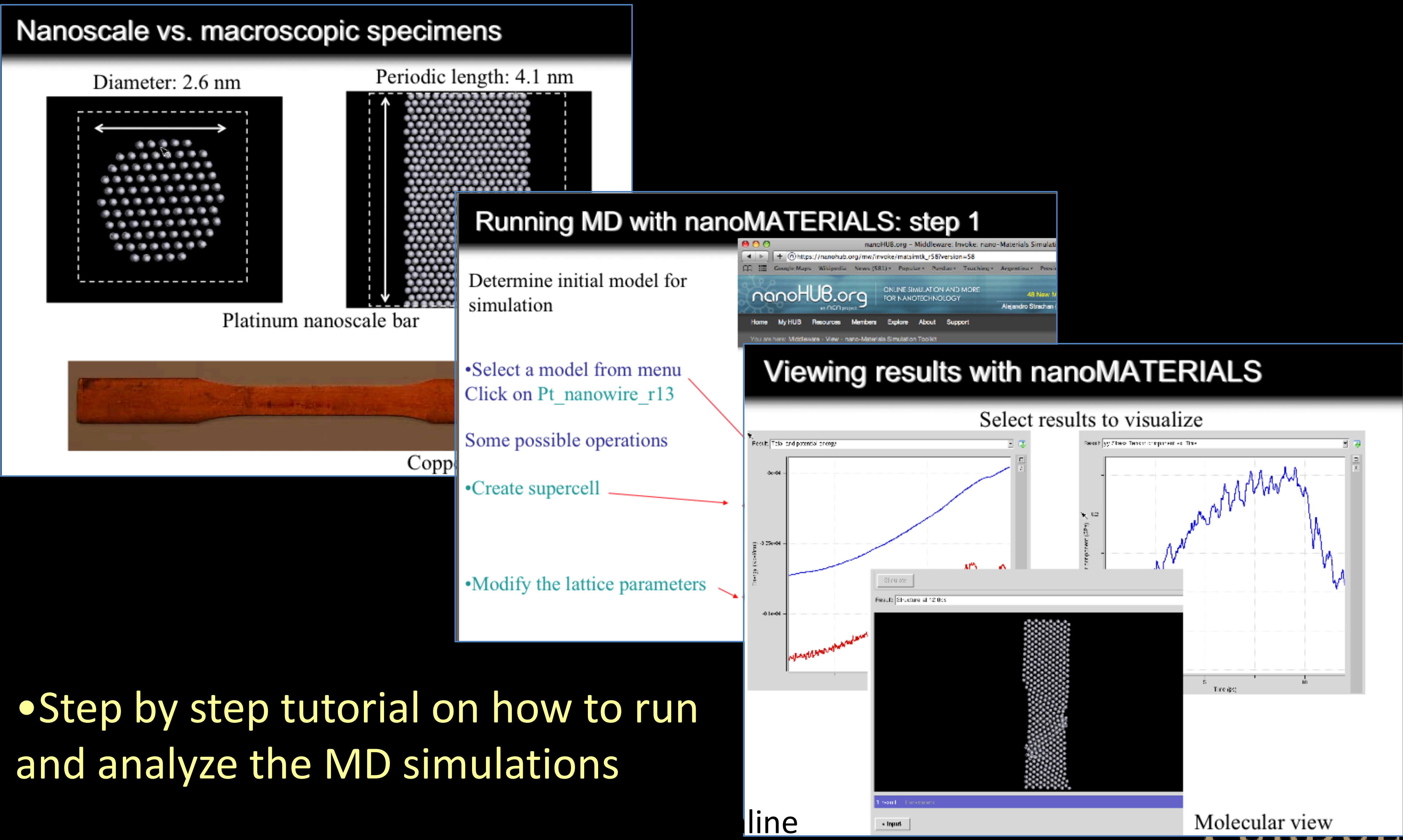




- Show some key results

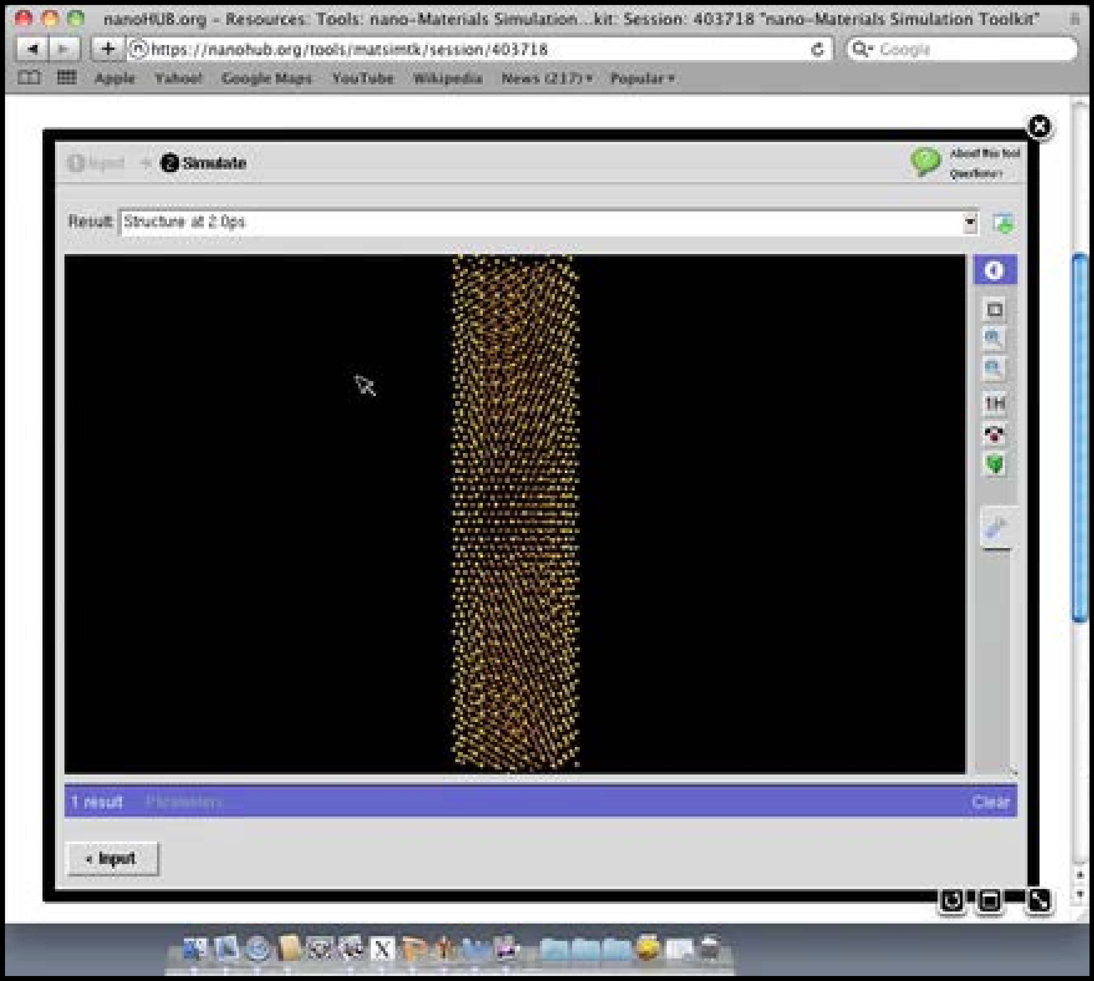
Atomic View of Plasticity: tutorial

Pre-lab lecture

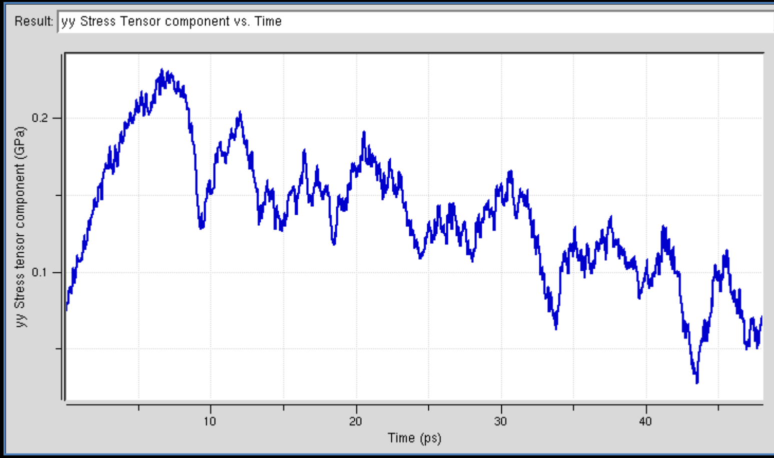


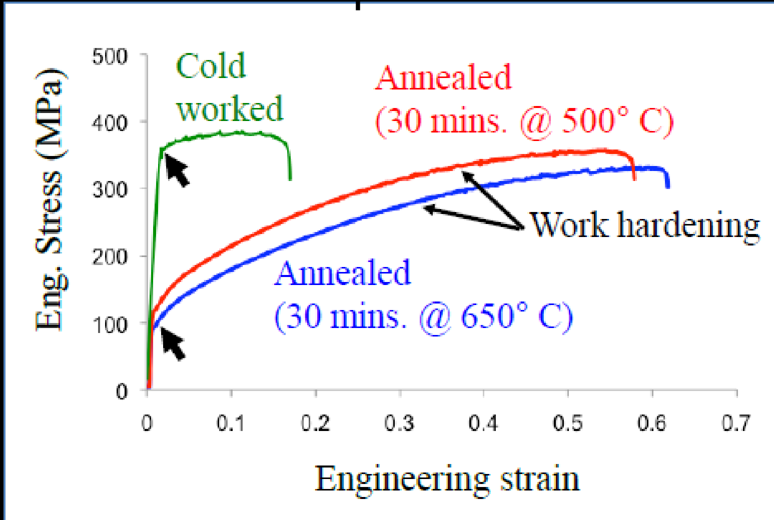
- Step by step tutorial on how to run and analyze the MD simulations

Hands-on activities



Stress vs strain from MD





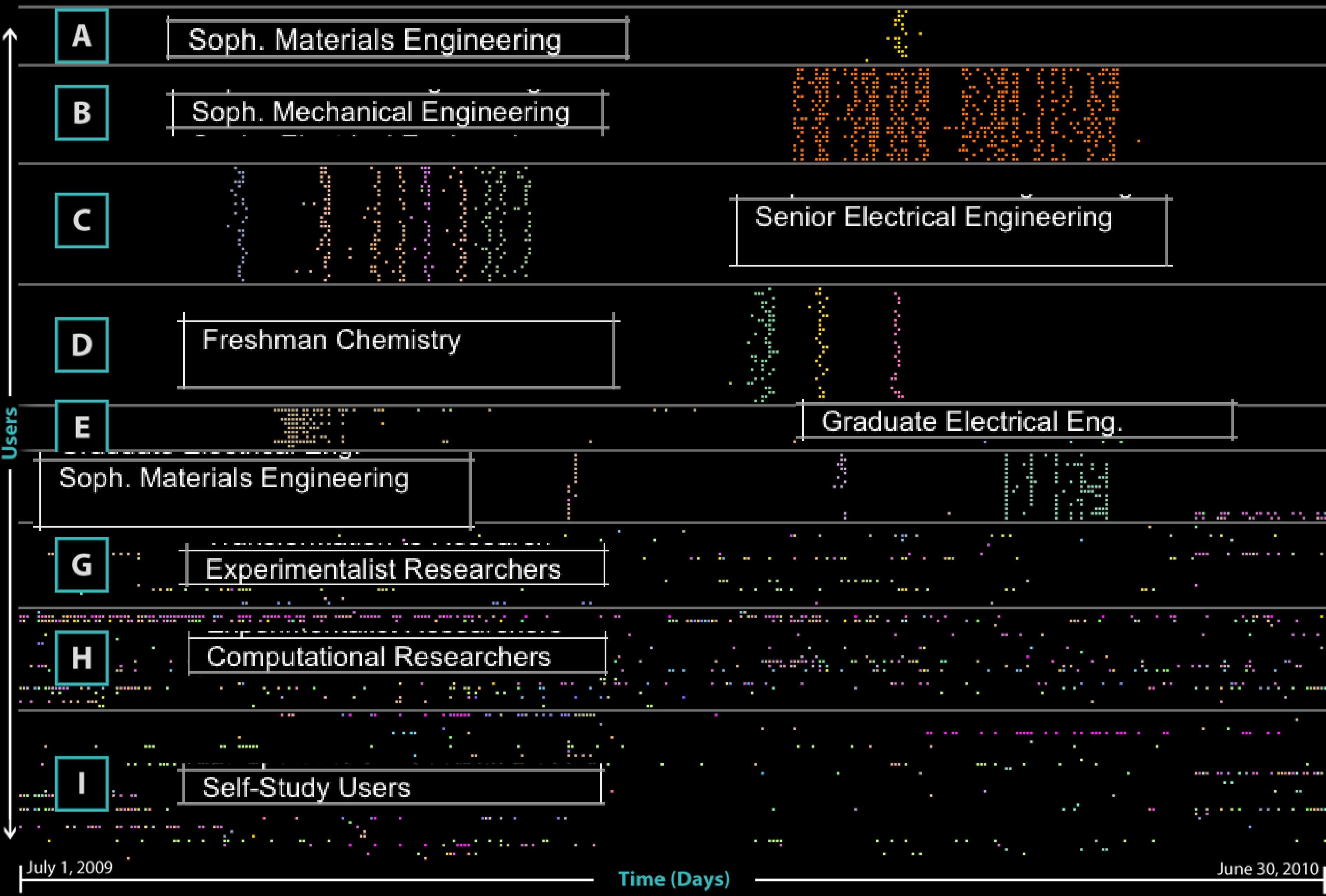
nanoHub User Behavior

Users

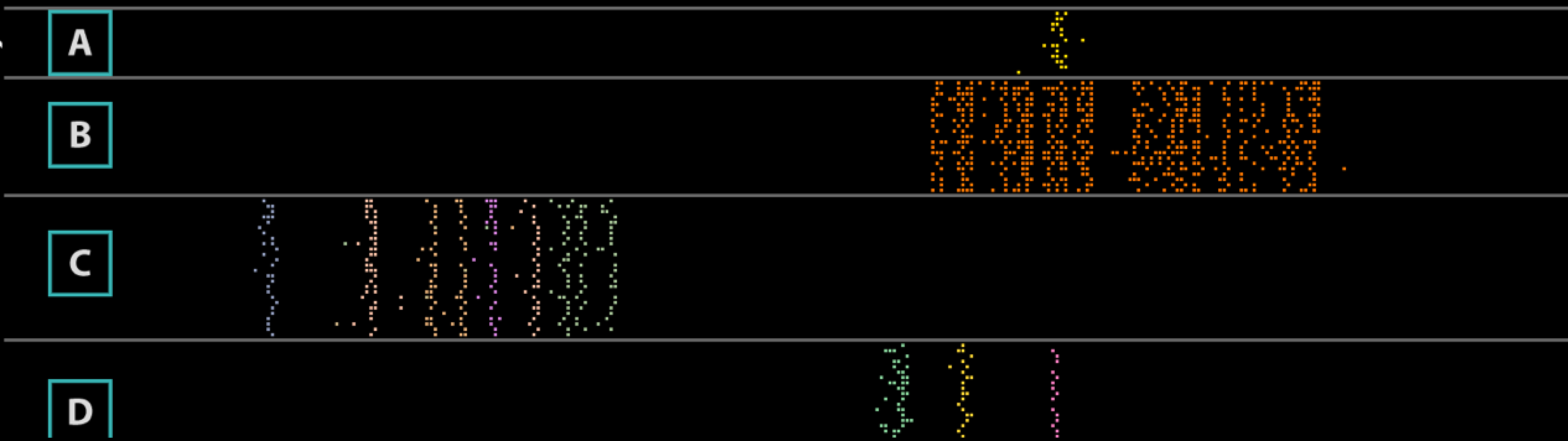
Time (days)

2010-06-30 6 users 1 days of history

Formal Education vs. Research



Formal Education vs. Research



	Tools and Usage Pattern	Validated Subset Shown	Classes Like This	Total Users
A	Single Tool, Single Use	Soph. Materials Engineering	96	1392
B	Single Tool, Semester Use	Soph. Mechanical Engineering	5	253
C	Multiple Tools, Periodic and Repeated Use	Senior Electrical Engineering	1	84
D	Multiple Tools, Periodic Single Use	Freshman Chemistry	41	803
E	Single Tool, Intensive Use	Graduate Electrical Eng.	6	142
F	Multiple Use in 3 Classes, Transformation to Research	Soph. Materials Engineering	1	35
G	Experimentalist Researchers	18 users		31
H	Computational Researchers	22		94
I	Self-Study Users	33 (not validated)		5,685

Assessing students learning

Advances in Engineering Education

WINTER 2013

Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding

SEAN P. BROPHY
Engineering Education

ALEJANDRA J. MAGANA
Computer and Information Technology

AND

ALEJANDRO STRACHAN
Materials Engineering
Purdue University
West Lafayette, IN

Study details

Lectures		Assessment 1 (A1)	MD Simulation Lab	Assessment 2 (A2)
Lecture (50 minutes)	Prelab (50 minutes)	Pretest (Posttest of lectures) (10 minutes)	Simulation (3 hours)	Posttest of entire sequence (10 minutes)

Table 1. Sequence of treatments and measures of student learning during the learning process

Group	Learning Activity		
	Lecture	Prelab	Simulation
1 (N=6)	No	No	Yes
2 (N=16)	Yes (or No)	No (or Yes)	Yes
3 (N=24)	Yes	Yes	Yes

Table 2. Definition of groups

Assessment

Yield stress (Q1): Asked students to compare the yield stress of a defect-free nanowire with that of a polycrystalline metal.

Plastic deformation in compression (Q2a) and plastic deformation in tension (Q2b): Asked students to sketch the atomic displacement involved during compressive (part a) and tensile (part b) plastic deformation of a nanowire.

Strain hardening (Q3): Asked students to compare the amount of strain hardening expected in the nanowire and the macroscopic samples (a cold-worked specimen and one that has been annealed)

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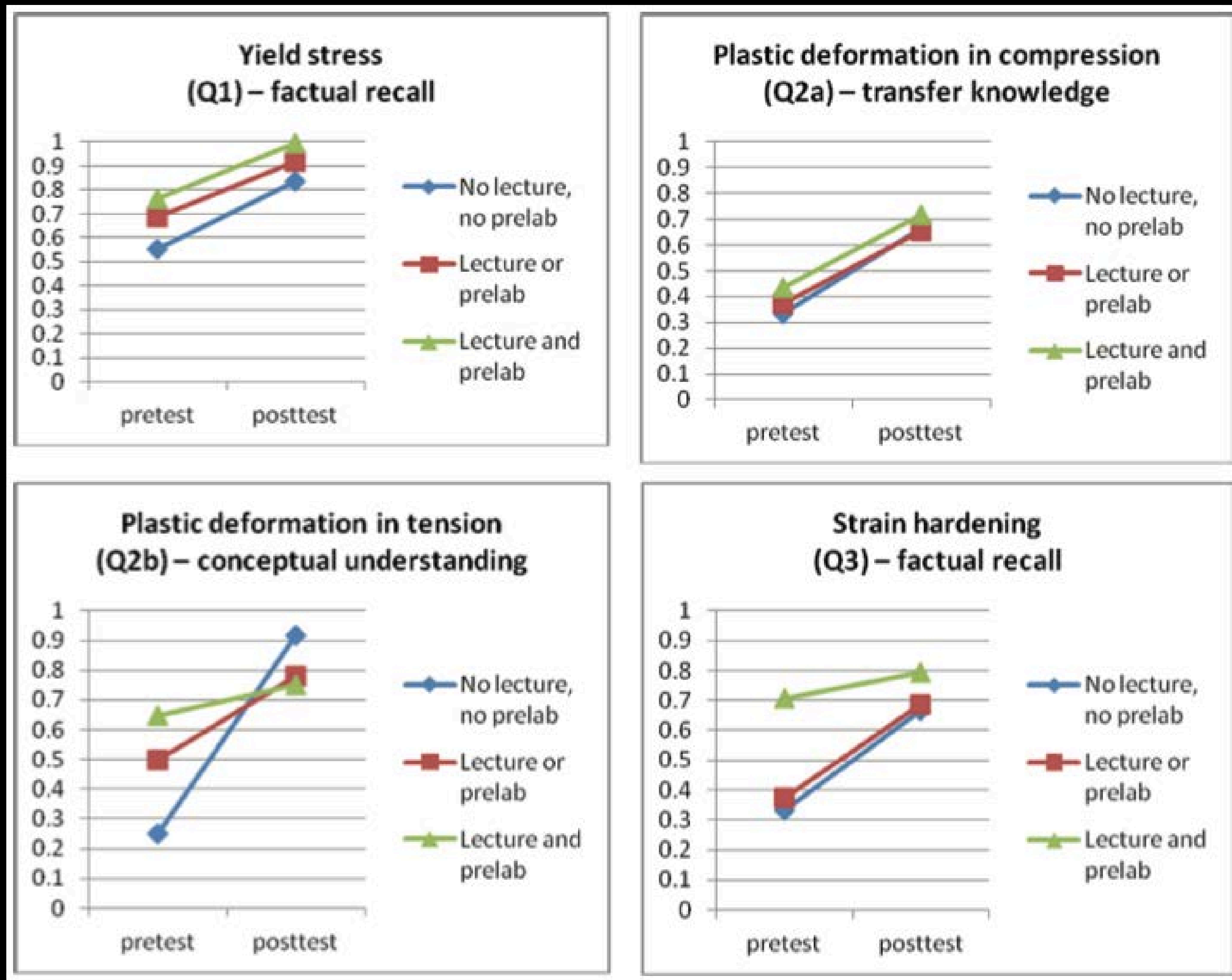
Results



Yield stress
(Q1) – factual recall
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
pretest
posttest
No lecture, no prelab
Lecture or prelab
Lecture and prelab
Plastic deformation in compression
(Q2a) – transfer knowledge
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
pretest
posttest
No lecture, no prelab
Lecture or prelab
Lecture and prelab
Plastic deformation in tension
(Q2b) – conceptual understanding
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
pretest
posttest
No lecture, no prelab
Lecture or prelab
Lecture and prelab
Strain hardening
(Q3) – factual recall
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
pretest
posttest
No lecture, no prelab
Lecture or prelab
Lecture and prelab

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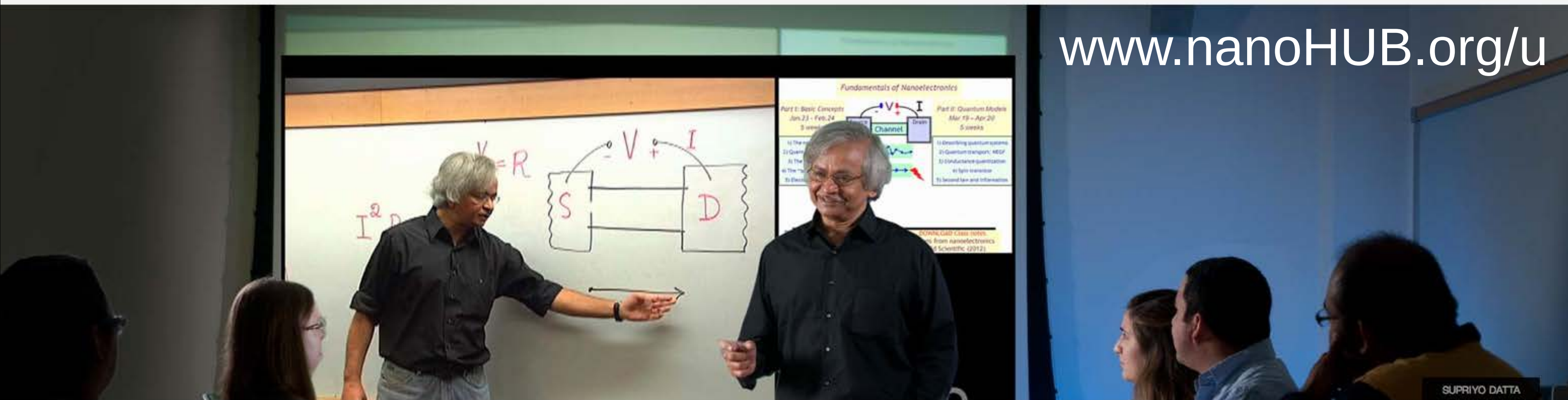
HOME | COURSES | FAQS | FOR INSTRUCTORS | ABOUT

Truly a fabulous learning experience." — *past nanoHUB-U student*



Welcome to nanoHUB-U

Transcending disciplines with short courses accessible to students in any branch of science or engineering.

Cutting-edge topics distilled into short lectures with quizzes, homework, practice exams.

SELF-PACED COURSES FOR FREE

Learn at your own pace.

LIVE SHORT COURSES FOR $30

Interact with nanoHUB-U profs

Coming Fall 2013: "Thermoelectric Science and Technology" and "Electronic Biosensors"

EDUCATORS

Use nanoHUB-U on your campus

CERTIFICATES, BADGES, CREDIT

Learn more about receiving credit and/or recognition

Nano-tuts

Short tutorials taught succinctly by our award-winning professors.

Topics based on your suggestions!

Lessons from Nanoscience

Low-cost lecture notes from World Scientific Publishing Co.

World Scientific
Connecting Great Minds

WEEK 5 A quick look at: ultimate limits, other transistors, and circuits Posted

LECTURES

L5.1: The Ultimate MOSFET and Beyond - Fundamental Limits
› Play video › YouTube › Download › L5.1 Slides › Quiz

L5.2: The Ultimate MOSFET and Beyond - Heterostructure FETs
› Play video › YouTube › Download › L5.2 Slides › Quiz

L5.3: The Ultimate MOSFET and Beyond - Heterostructure BJTs
› Play video › YouTube › Download › L5.3 Slides › Quiz

L5.4: The Ultimate MOSFET and Beyond - The CMOS Inverter
› Play video › YouTube › Download › L5.4 Slides › Quiz

L5.5: The Ultimate MOSFET and Beyond - CMOS Logic Performance
› Play video › YouTube › Download › L5.5 Slides › Quiz

L5.6: The Ultimate MOSFET and Beyond - Analog/RF CMOS
› Play video › YouTube › Download › L5.6 Slides › Quiz

DISCUSSION FORUM

› Week 5 discussion

HOMEWORK

› Week 5 homework
› Submit Week 5 homework here

› Load VSspice › VS Model 45nm CMOS.txt

**Special Thanks to Professors Dimitri Antoniadis and Jacob White of MIT for the HW exercises and and the SPICE like circuit simulation tool.

› Extended Homework Problem Set

› Solutions
› Extended Homework Problem Set Solutions

Tutorial: The Ultimate MOSFET and Beyond - Homework Solution
› Play video › YouTube › Download

EXAM

› Week 5 exam › Retake (optional)

For more details, see the Course Exam Policies on the FAQ Page

REFERENCES AND SUPPLEMENTAL MATERIALS

› Comments about Digital Circuits

nanoHUB-U curriculum

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INSTRUCTOR-LED SH

Interact with nanoH

Bioelectricity (open for re

Coming soon:

"Fundamentals of Batteri

EDUCATORS

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Learn more about r

101: Fundamentals of Nanoelectronics, Part I
Supriyo Datta
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102: Fundamentals of Nanoelectronics, Part II
Supriyo Datta
Tell me more about the course and instructor
Join for Free!/Access Course

103: Fundamentals of Atomic Force Microscopy, Part I
Ronald Reifenberger
Tell me more about the course and instructor
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104: Fundamentals of Atomic Force Microscopy, Part II
Arvind Raman
Tell me more about the course and instructor
Join for Free!/Access Course

105: Nanoscale Transistors
Mark Lundstrom
Tell me more about the course and instructor
Join for Free!/Access Course

106: Thermal Energy at the Nanoscale
Timothy Fisher
Tell me more about the course and instructor
Join for Free!/Access Course

107: From Atoms to Materials: Predictive Theory and Simulations
Alejandro Strachan

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nanoHUB-U for Educators

NANOHUB U PURDUE UNIVERSITY nanoHUB.org

HOME COURSES FAQS FOR INSTRUCTORS ABOUT

For Educators

For instructors preparing nanoHUB-U courses:

A set of resources including best practices and examples is available.

For instructors wishing to use nanoHUB-U materials in their own classes:

The instructional materials used in nanoHUB-U self-paced courses are available as open content under a Creative Commons license, and instructors are encouraged to incorporate these materials in their own courses, in accordance with the Creative Commons license terms.

For universities wishing to offer nanoHUB-U courses on their own campus:

Contact us to explore how nanoHUB-U can be used to support a unique nano-curriculum on your own campus.

Contact
For questions about nanoHUB-U, contact the support team at nanohub-u@nanohub.org.

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about nanoHUB-U

- A forum for evolving, original viewpoints that should become mainstream.
- Short but not too short (5 weeks) and not superficial.
- Designed to "transcend disciplines" and be broadly accessible (no long list of prerequisites).
- Focus on seniors, beginning grad students, working engineers.

nanoHUB-U numbers

- Launched in Spring 2012
- 9 courses offered by 8 different instructors
- More than 4000 registrations:

  503 universities represented
  76 countries represented
  93 companies represented

- Increasing use on the Purdue campus in “blended courses”

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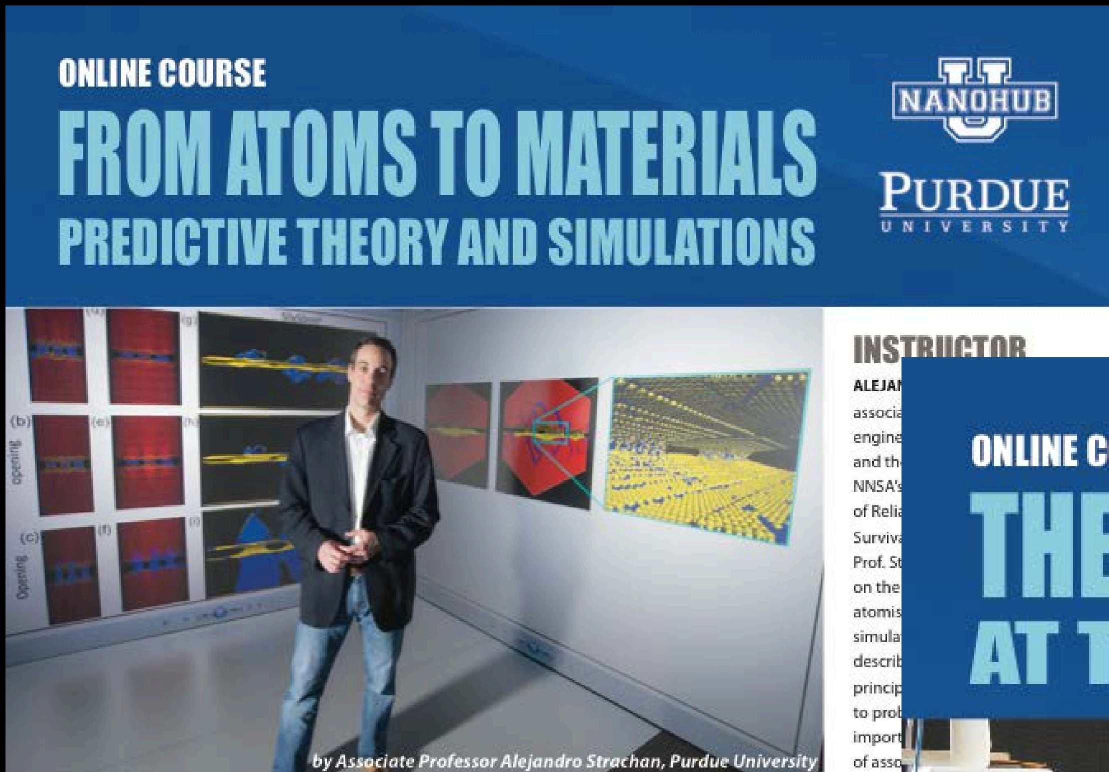
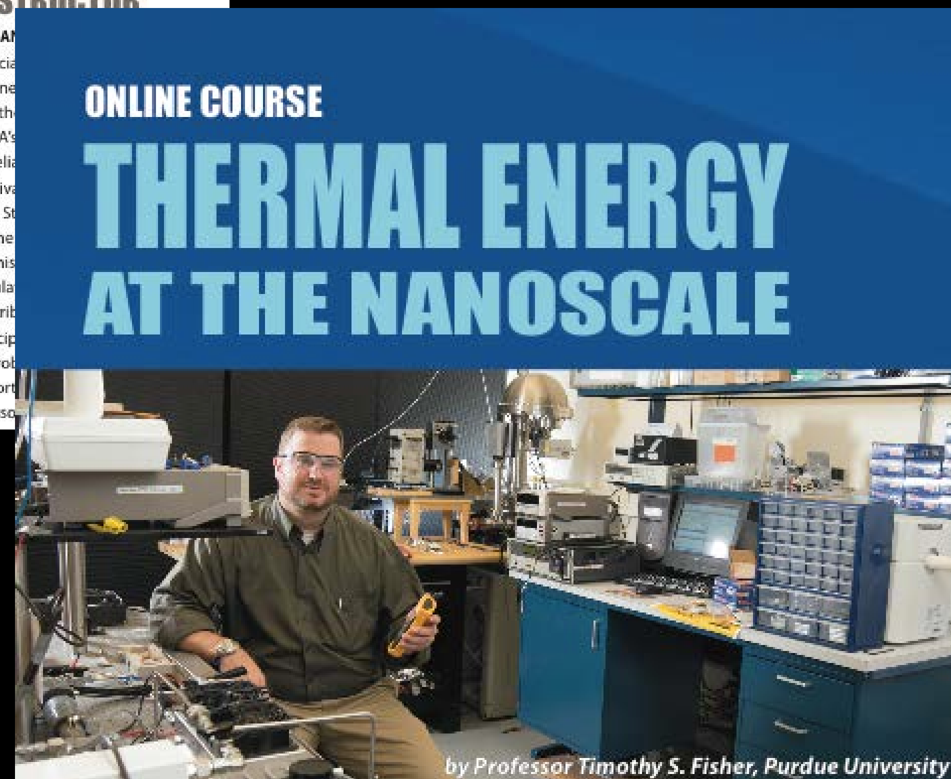
nanoHUB-U



230 students
20+ from industry



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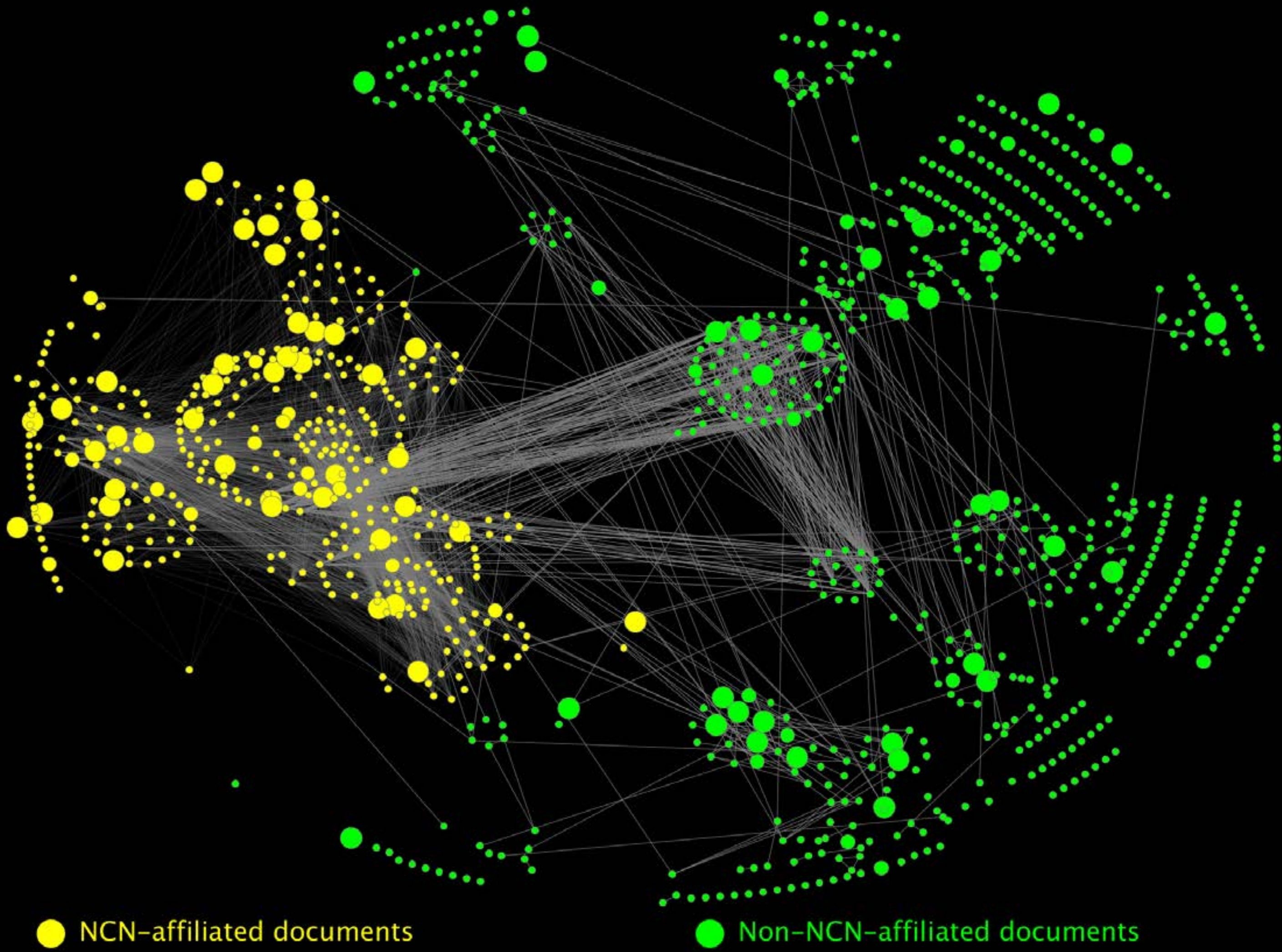
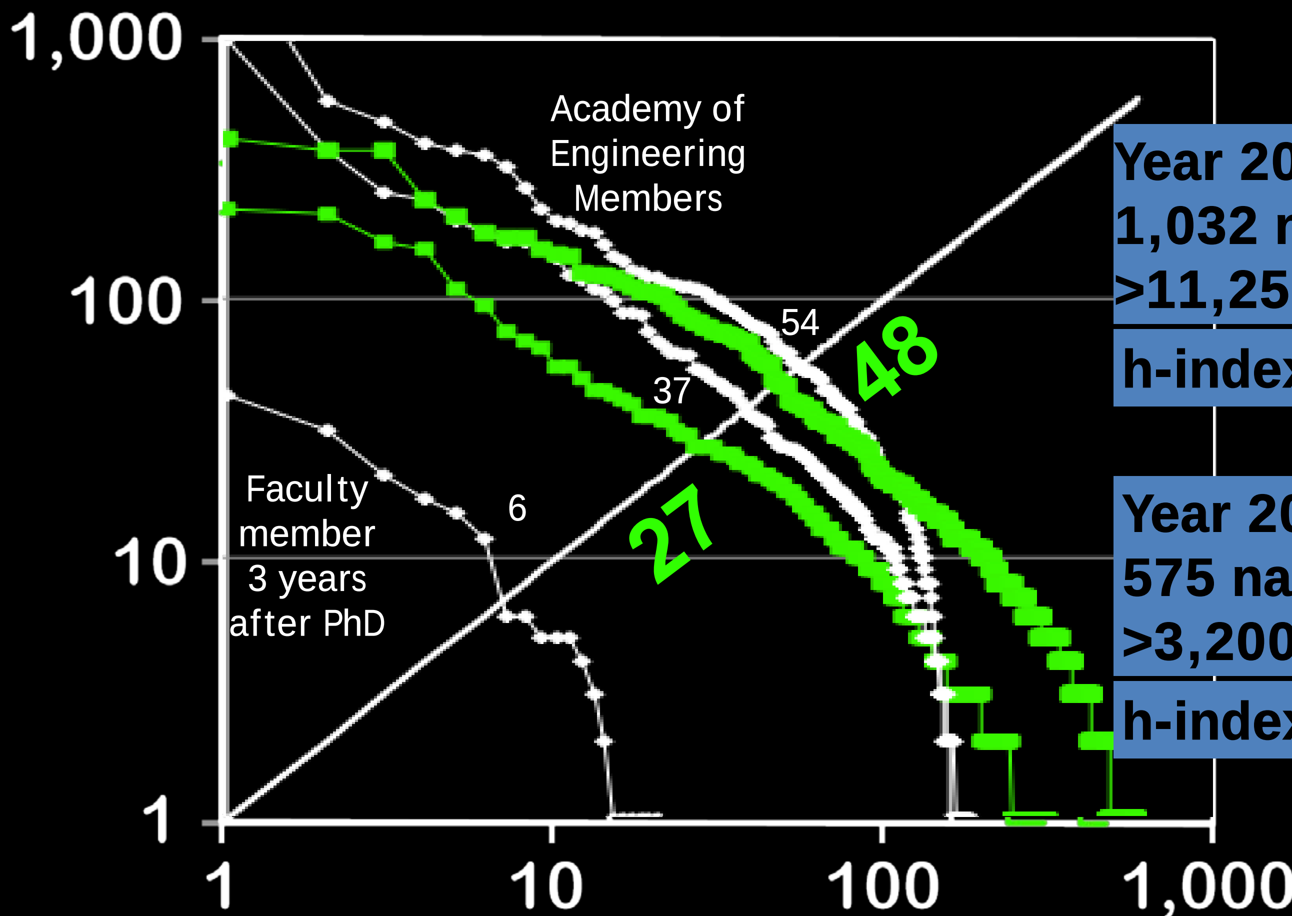
nanoHUB – use in research



* Small dots represent papers with relatively low secondary citations, medium dots indicate papers with potential to influence h-index, large dots represent papers affecting the h-index

h-index: Research Quality Indicator



Year 2013
1,032 nanoHUB citations
>11,250 secondary citations

h-index: 48

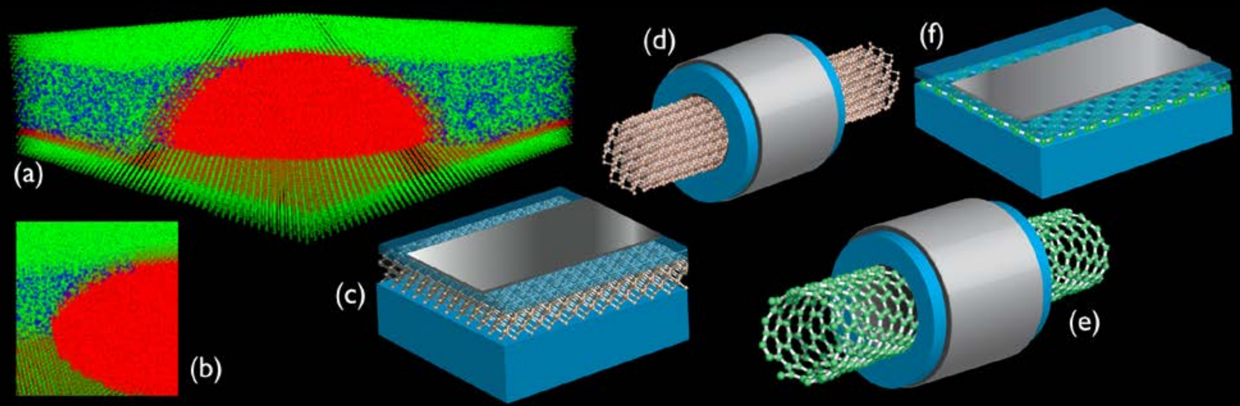
Year 2009
575 nanoHUB citations
>3,200 secondary citations

h-index: 27

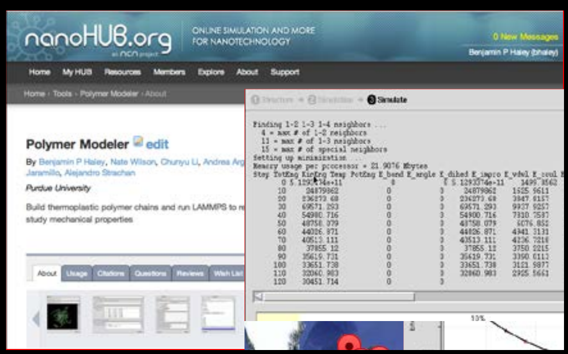
Is it good research?

“deep learning CPUs”

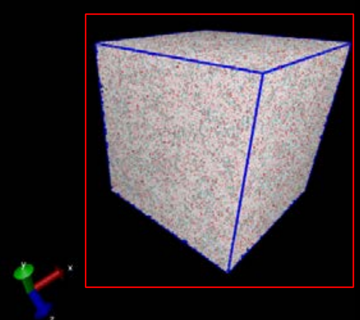
Compute intensive tools



NEMO/OMEN
nanoelectronics



PolymerModeler
Build structures & run MD



siesta

LAMMPS

Meep

WANNIER90

SeqQuest

QUANTUMESPRESSO

abinit.org

qwalk

QWalk: Continuum electronic structure quantum Monte Carlo

GAMESS

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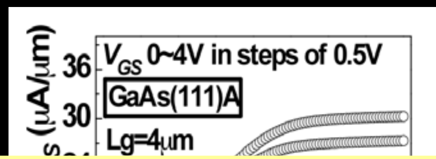
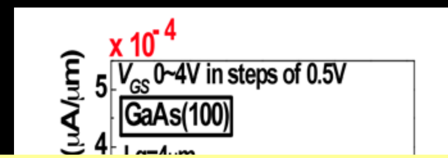
nanoHUB.org enhancing research

Peide Ye: NMOSFET performance of Al_2O_3 ALD oxide on GaAs depends strongly on surface type

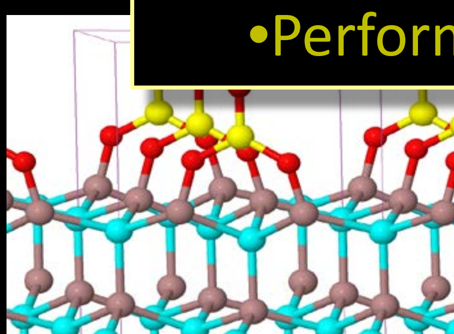


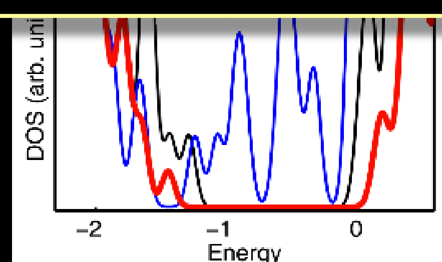


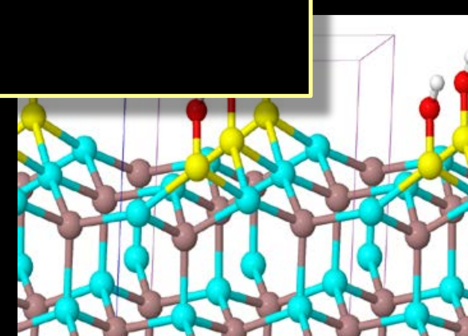
- Deploy research codes
- Store and disseminate research data
- Make research data available and useful
  - Reproduce results
  - Perform further exploration

t al. IEDM, 2009

- DFT calculati
- Structures a







G. Hegde, G. Klimeck, A. Strachan, APL (2011)

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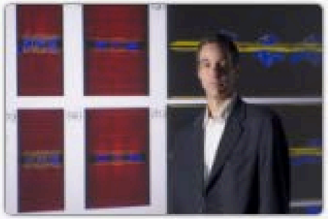
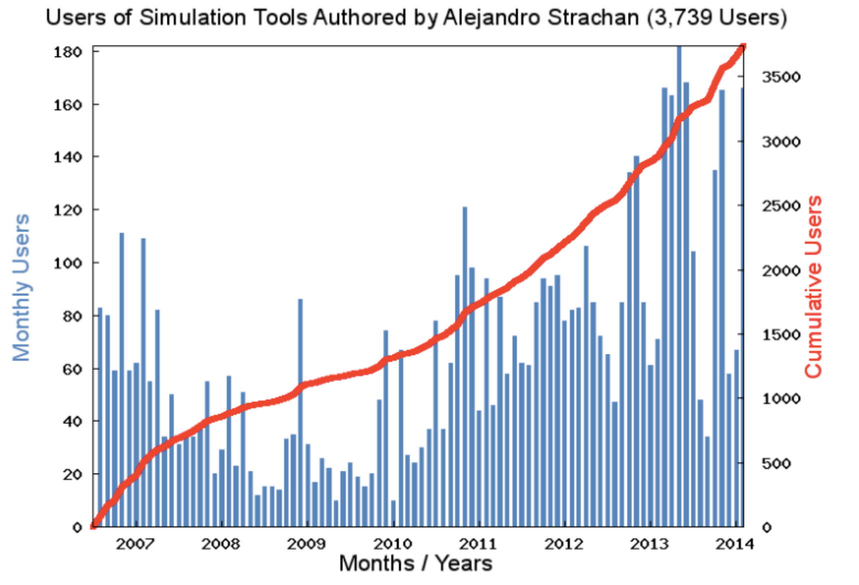
Measuring impact of contributors





Alejandro Strachan ▸ Usa

- Dashboard
- Profile
- Account
- Contributions 43
- Groups 26
- Points 10106
- **Usage**
- Favorites
- Messages 1096

Table 1: Overview

Item	
Contributions:	36
Total Simulation Users Served:	3,739
Total "and more" Users Served:	18,226
Rank by Contributions:	33 / 1379
First Contribution:	16 Nov 2005
Last Contribution:	06 Feb 2014
Citations on Contributions:	5
Usage in Courses/Classrooms:	694 users served in 61 courses from 7 institutions

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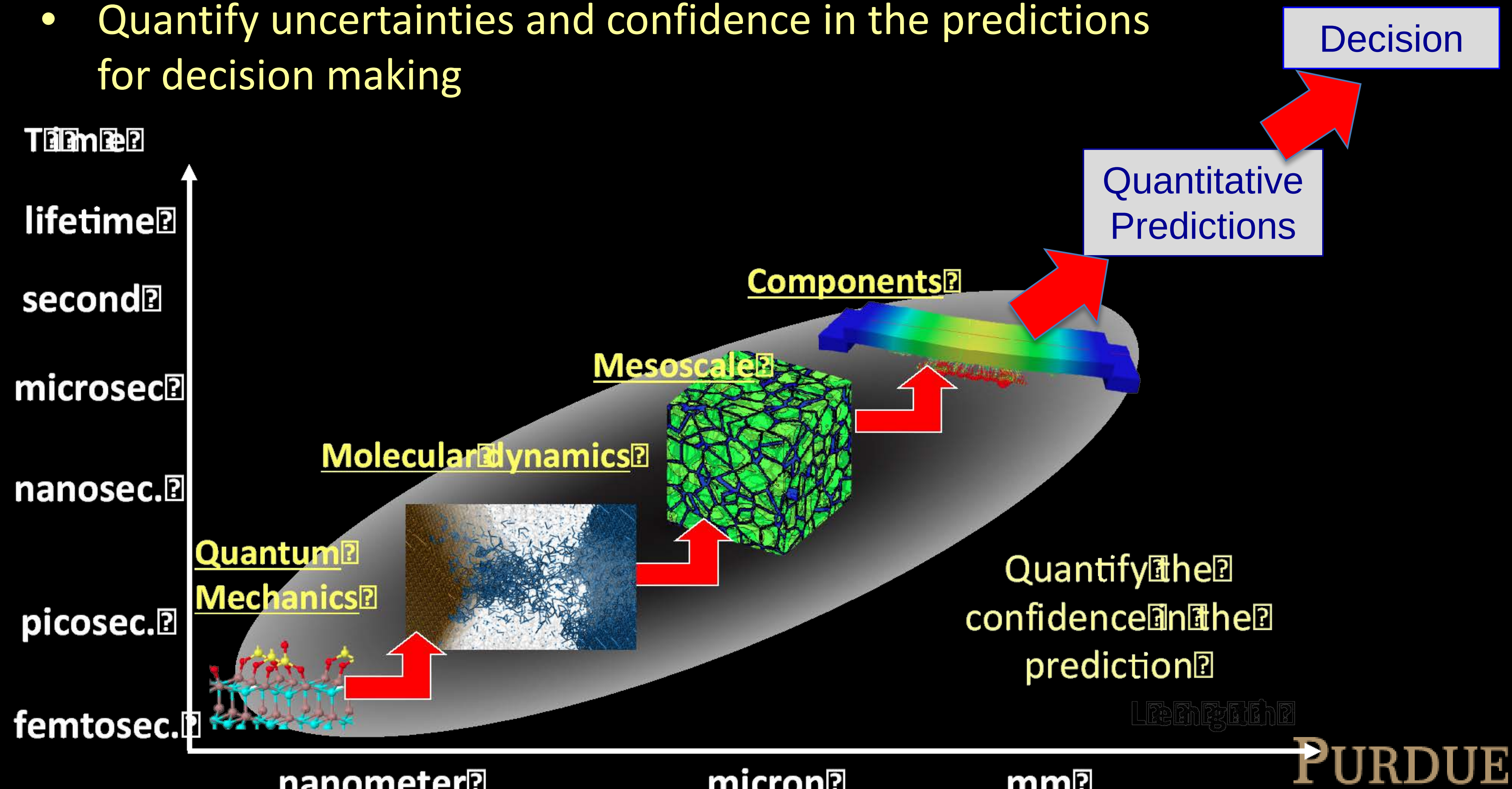
Materials modeling and simulations

- Uncover and characterize the molecular-level mechanisms that govern materials
- Contribute to the design and certification of materials
- Quantify uncertainties and confidence in the predictions for decision making



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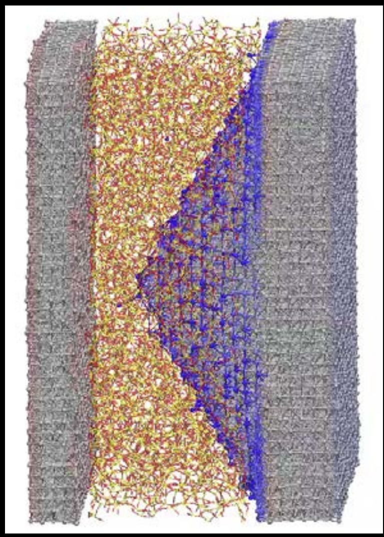
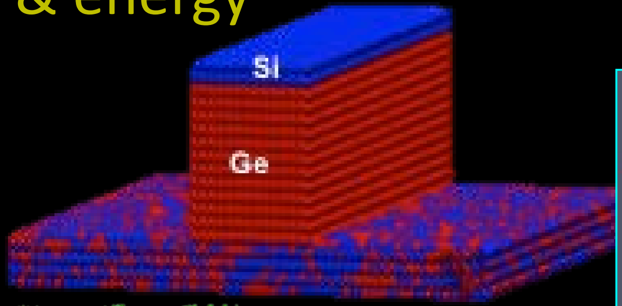
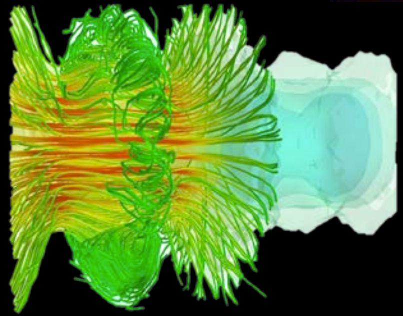
Application areas of interest

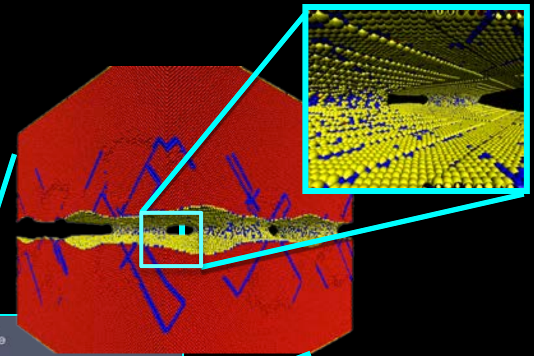
Nanoelectronics & energy

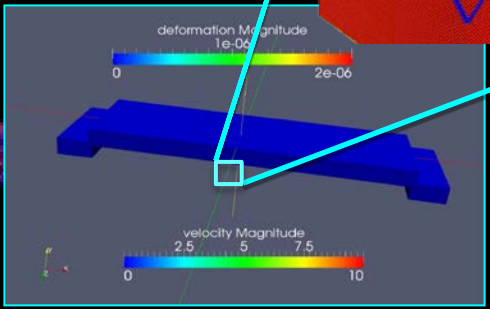




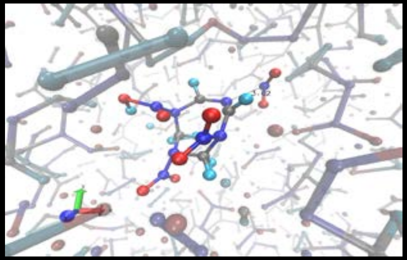


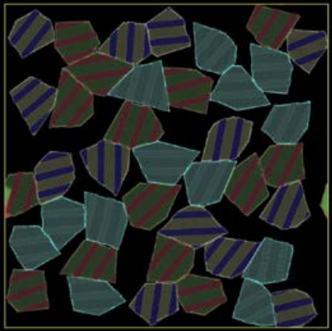
MEMS



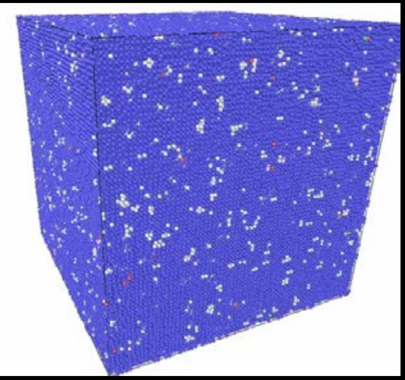


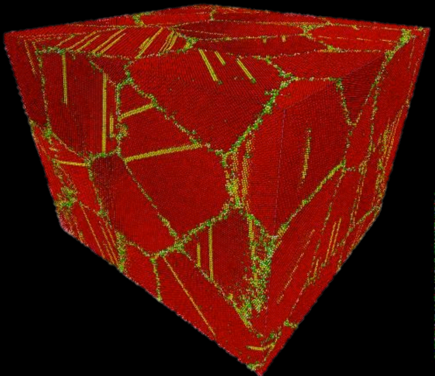
High-energy density materials



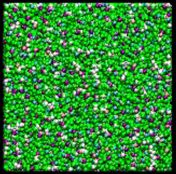


Thermo-mechanical response



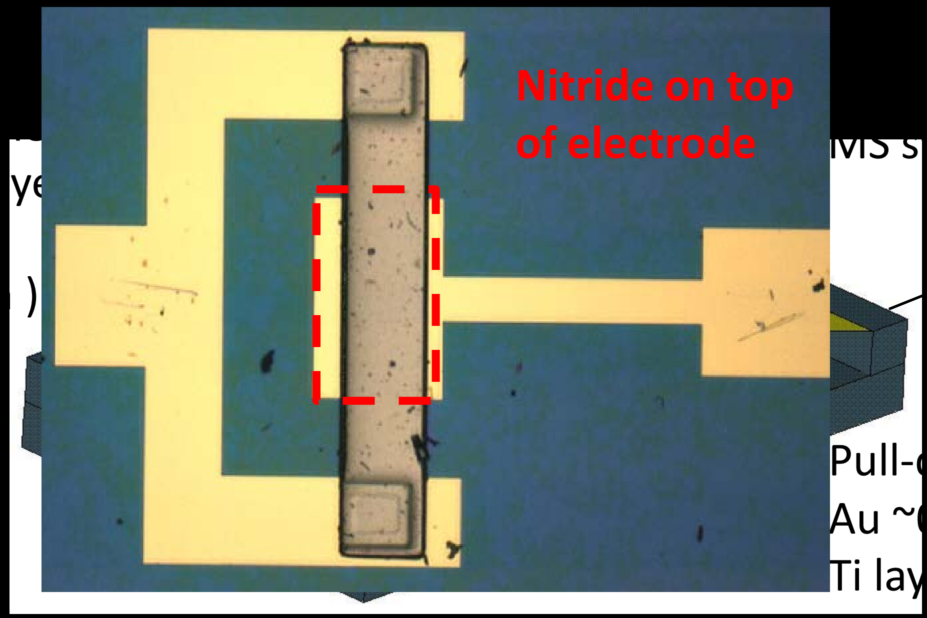


Polymers and composites



NNSA PSAAP Center: PRISM

Center for the prediction of reliability, integrity and survivability of microsystems



Goal: Predict performance and reliability of RF-MEMS device

- Multi-physics modeling from electrons to device
- Fabrication and experimental testing for validation
- Uncertainty quantification at all scales in models and experiments

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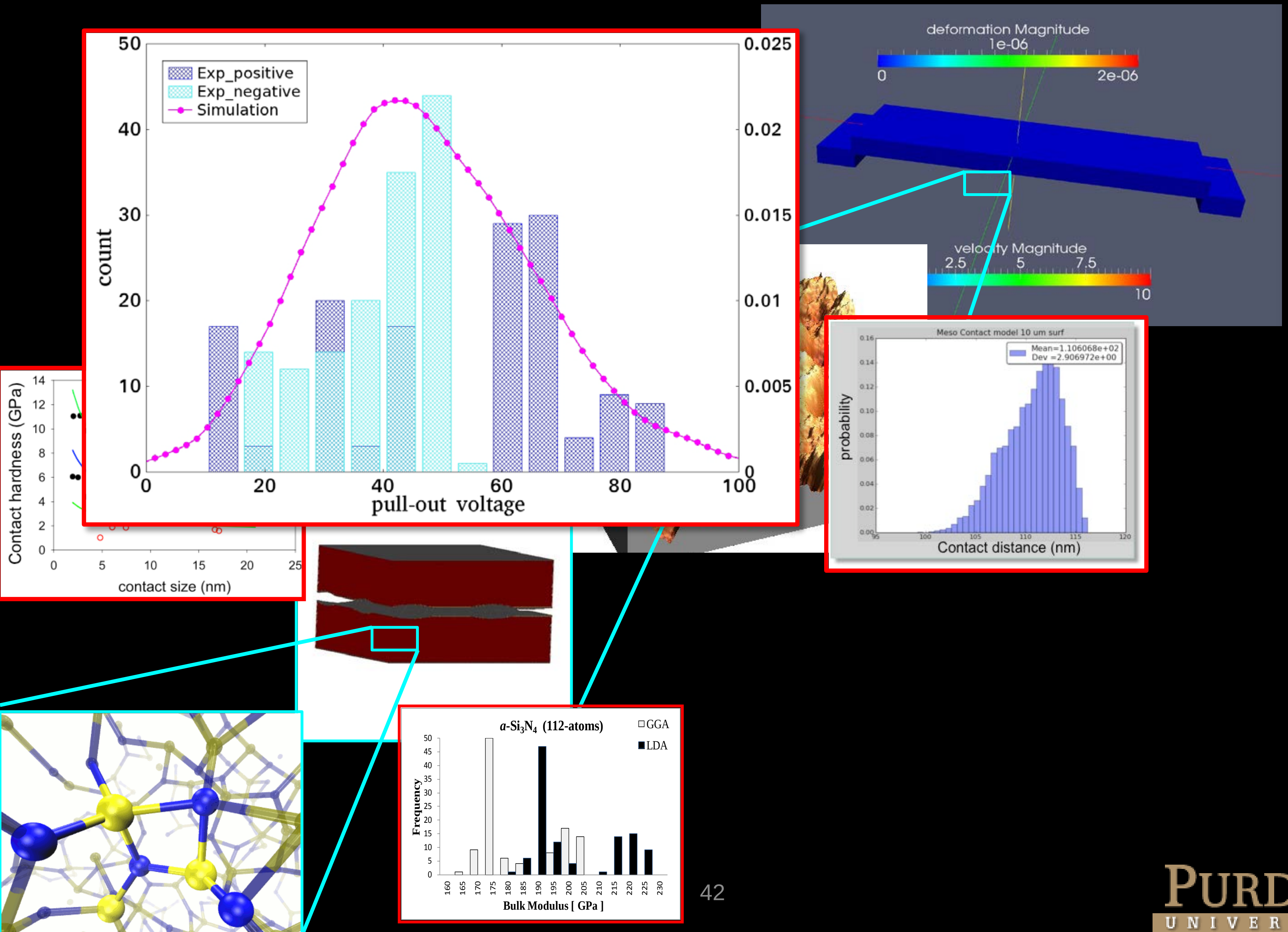
Multiscale, multiphysics w/ quantified uncertainties



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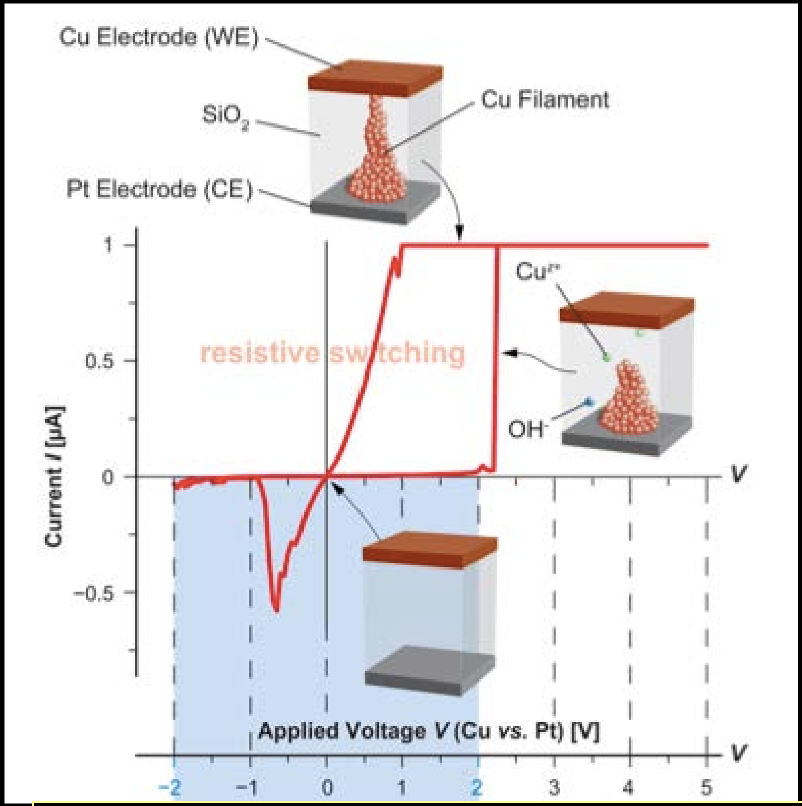
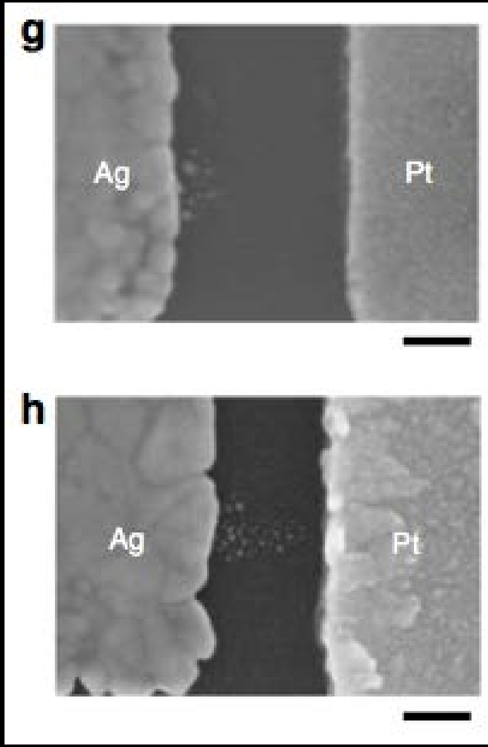
Nanoelectronics: electrometallization cells

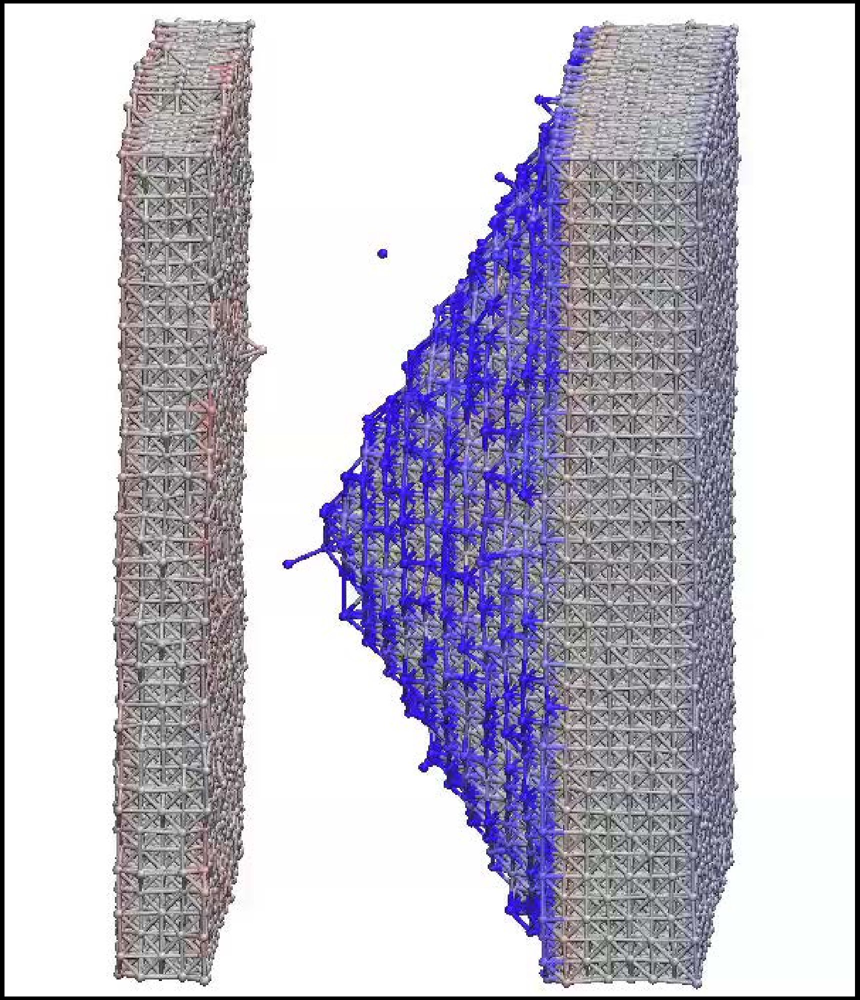
- Resistance switching devices
  - Creation and dissolution of conductive metallic bridges



Tappertzhofen et al. ACS Nano (2013)



Atomic processes of switching



Forming

- Aggregation into small clusters
- Stabilization via reduction as they become connected to inactive electrode

Reset

- Dissolution starts near inactive electrode
- Nanofilaments connected to active electrode remains

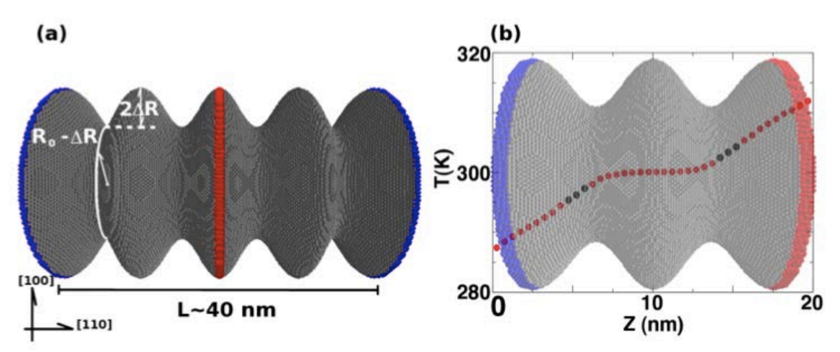
Set

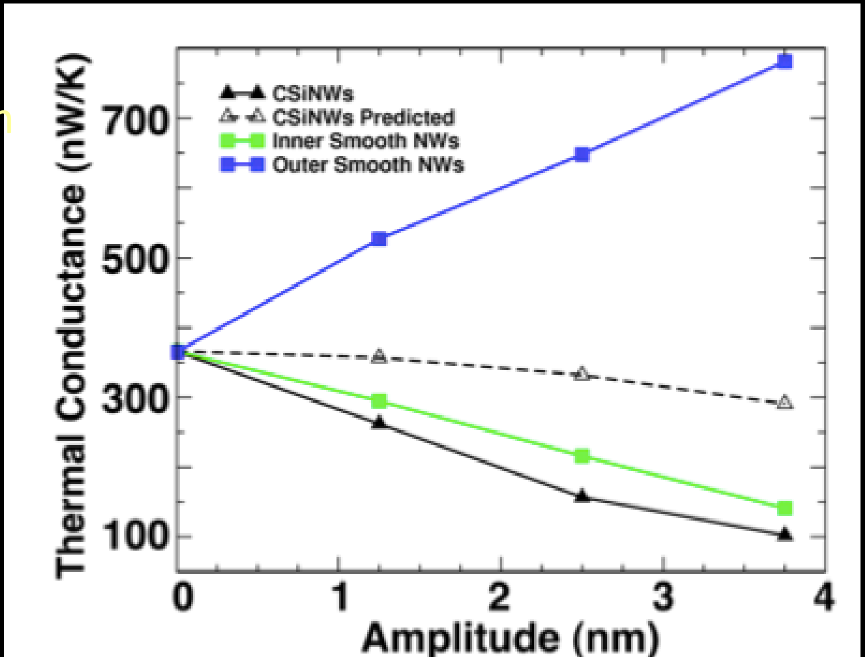
- Nanofilament dissolves
- Aggregation and reduction

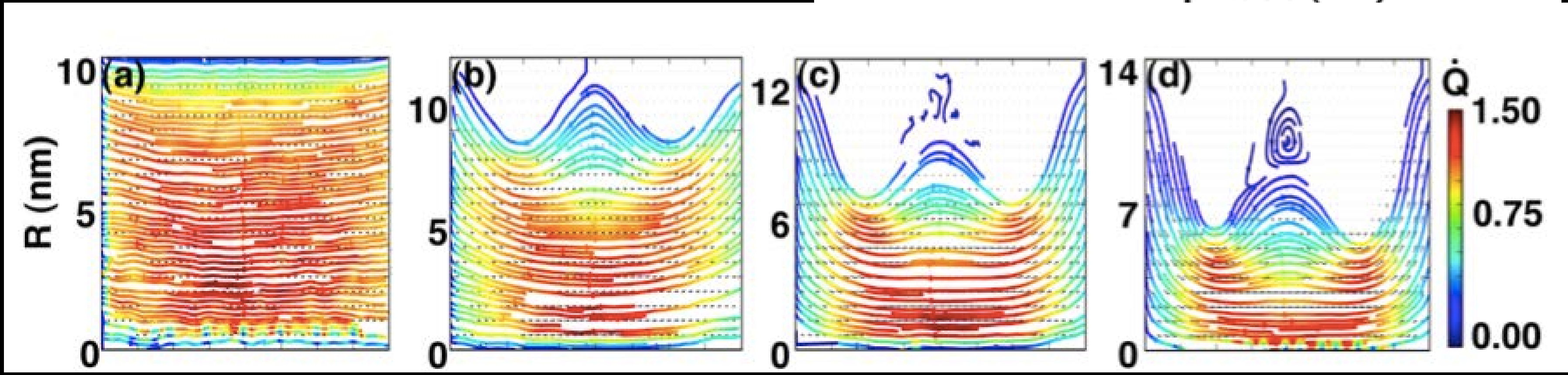
Thermal transport at the nanoscale

Corrugated Si nanowires

- Conductance smaller than straight wires with inner core diameter

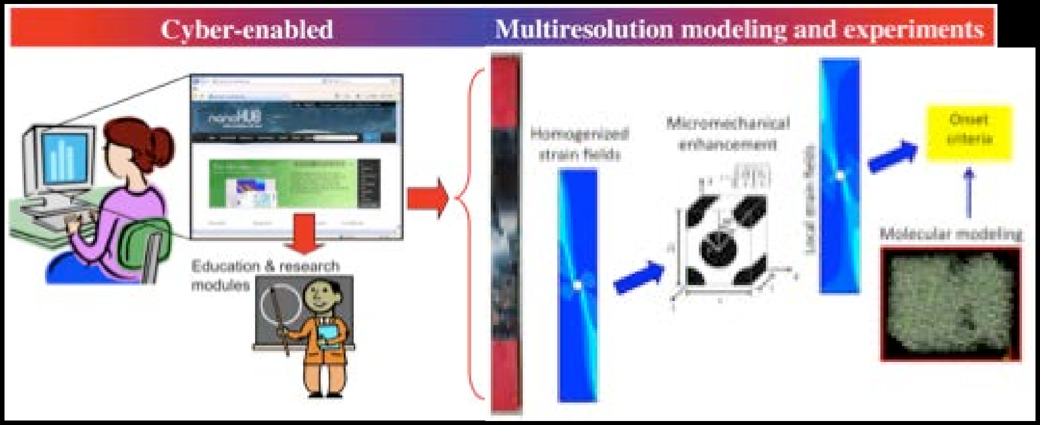






Polymer composite projects

NSF: cyber-enabled predictive models for polymer nanocomposites: multiresolution simulations and experiments



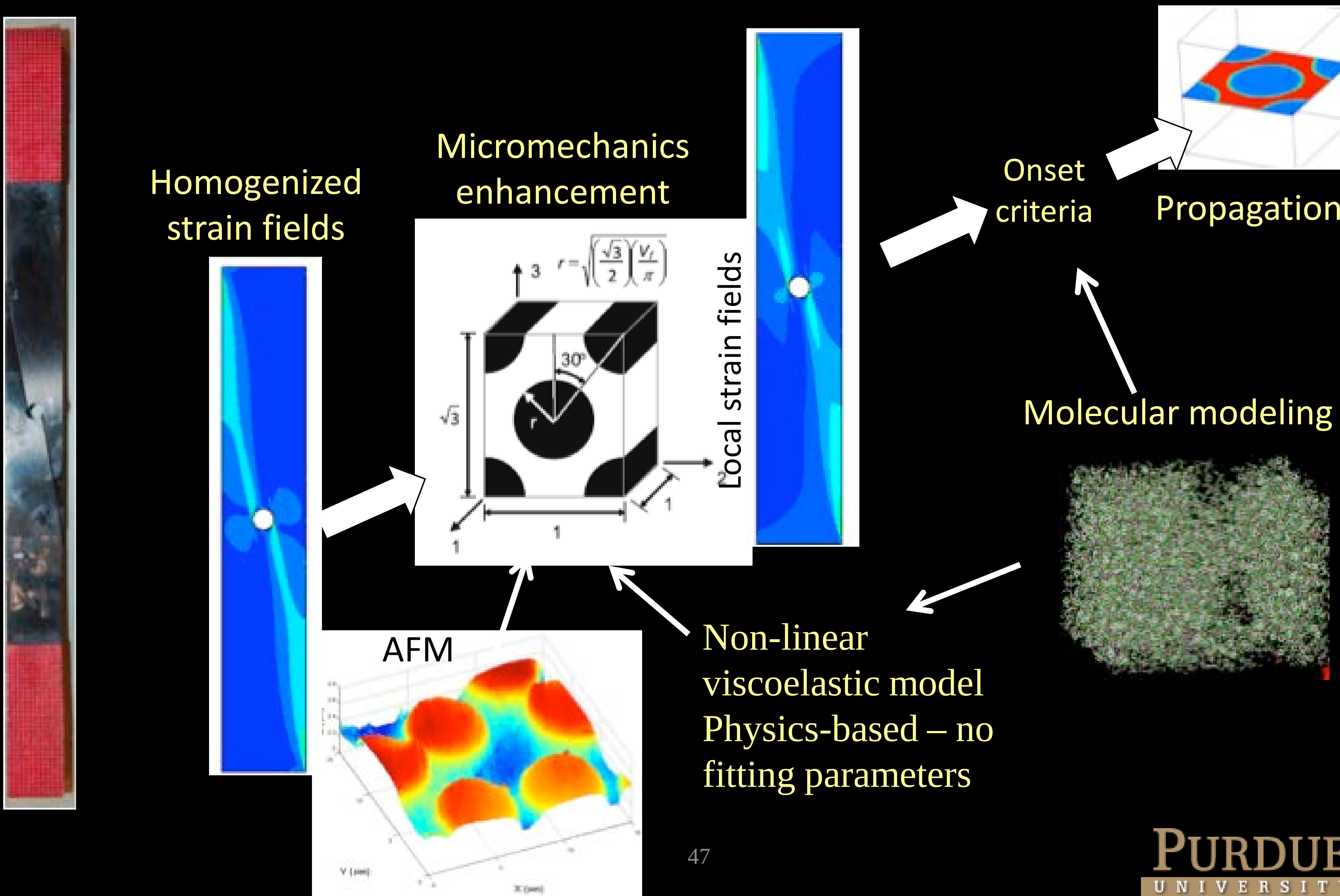
- Ultimate mechanical properties of nanocomposites
- Poly-imides and PMMA with CNTs and graphne

Boeing – Purdue: atoms to aircraft

- Prediction of onset of irreversible deformation and damage propagation in epoxy formulations
- Continuous carbon fiber reinforced composites

Co-PIs: Pipes, Koslowski, Raman, Caruthers

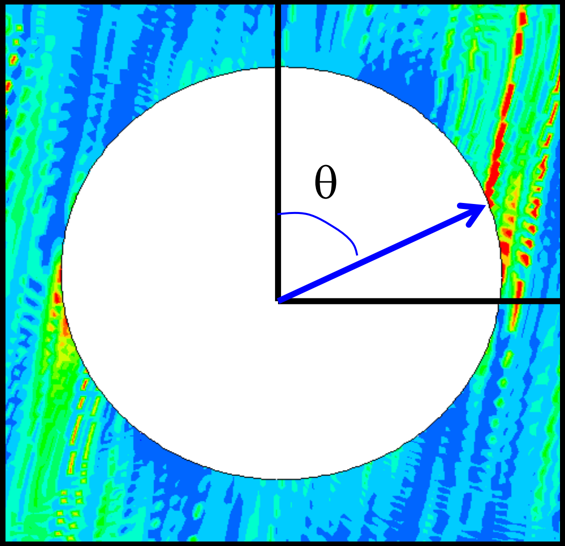
Prediction of onset of permanent damage



Predicting failure under tension

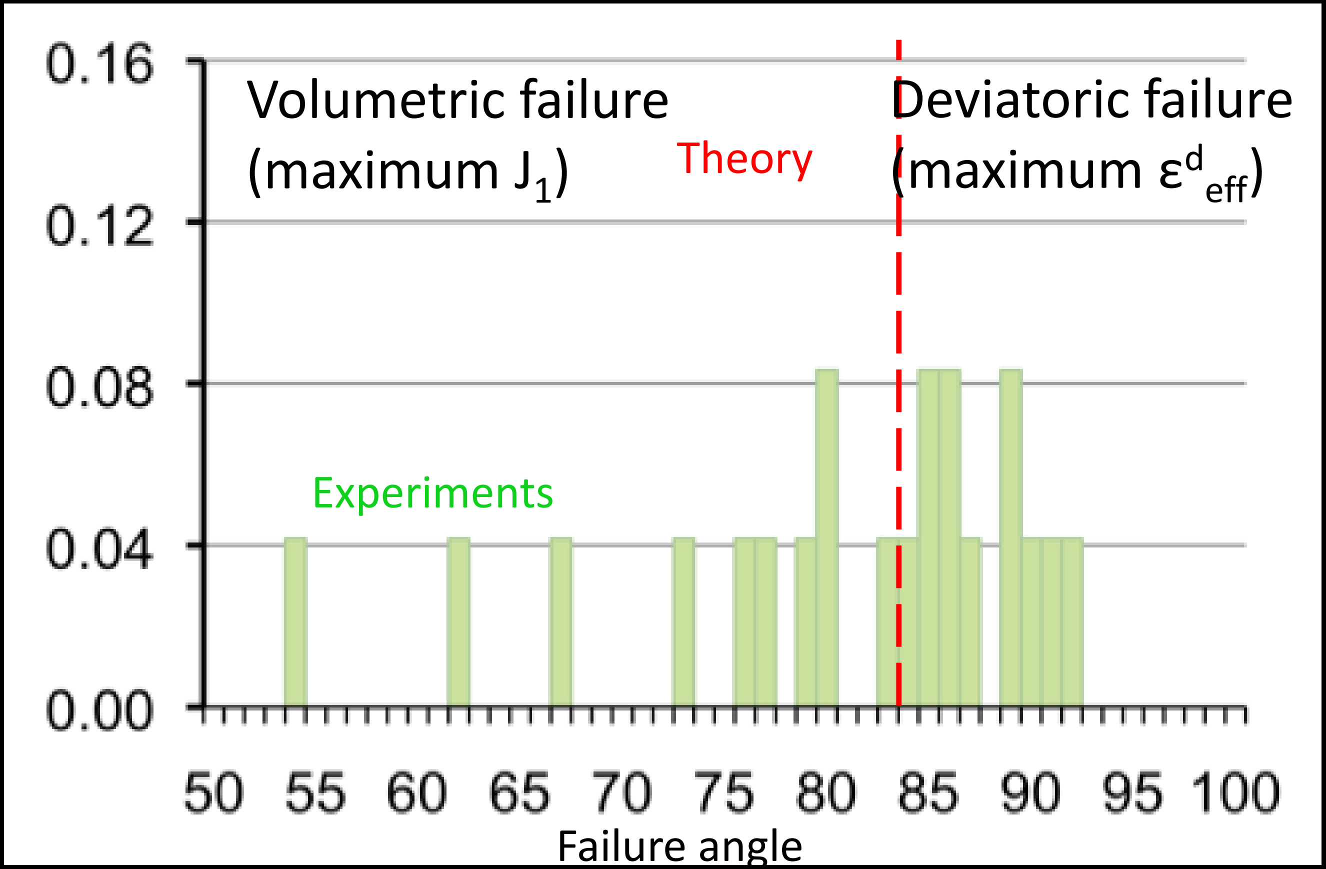
Open hole tensile test

Quantity of interest:
angle of failure initiation



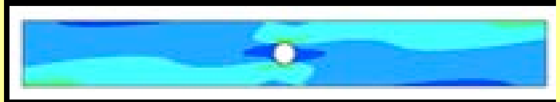
Work of Koslowski and Pipes groups

Failure angle prediction vs. experiments

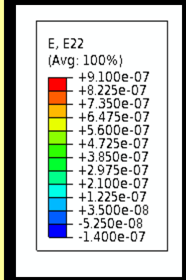


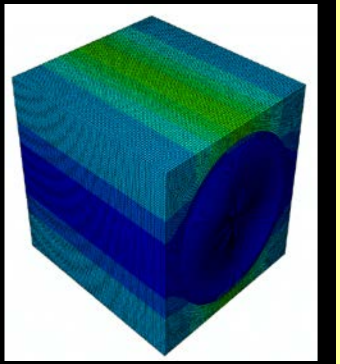
- Theoretical predictions agree in average with experiment
- We are interested in deviations around the average

Micromechanical enhancement

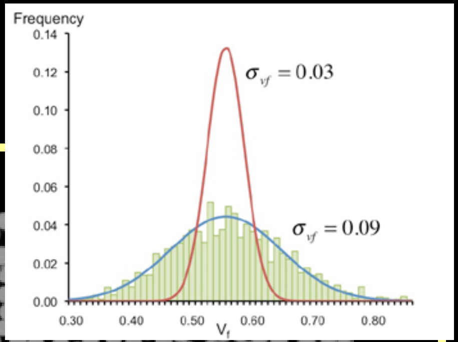


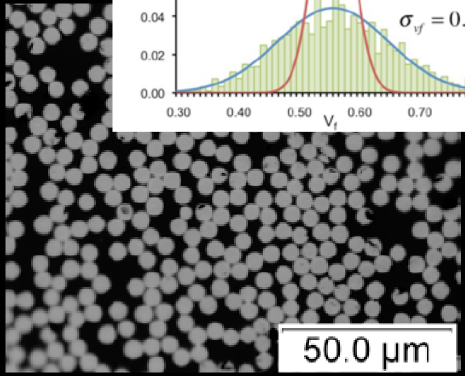
FEM simulations with homogenized properties



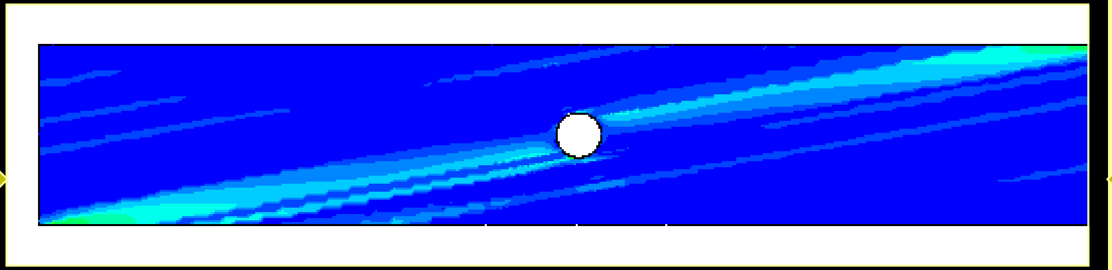


RVE simulations





Variability in volume fraction



Micro Mechanical enhanced solution

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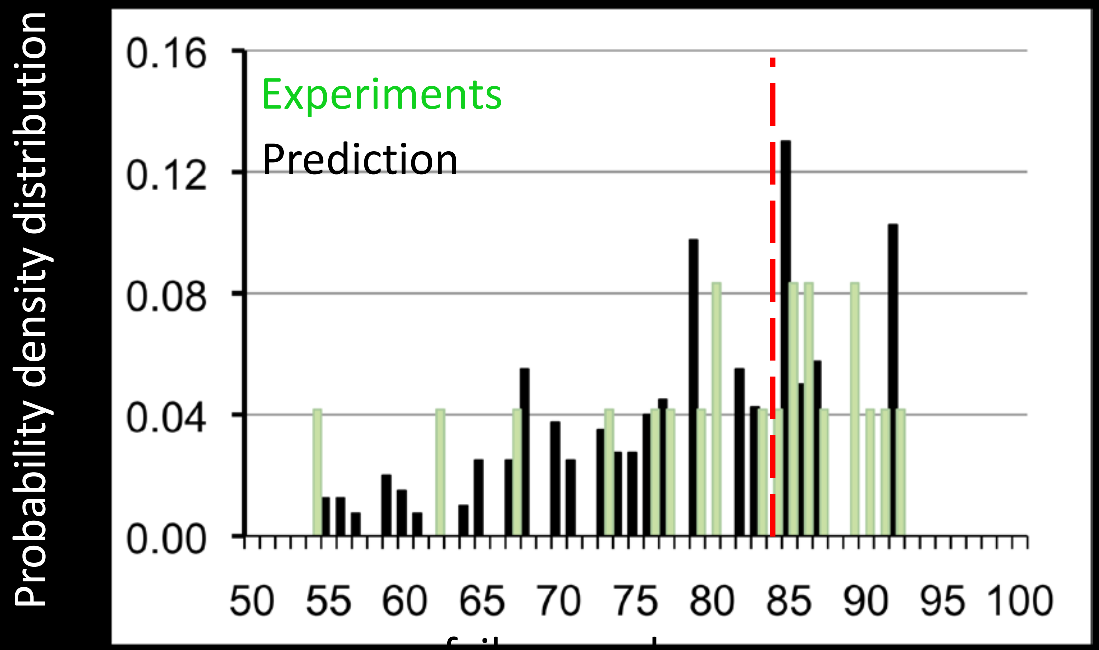
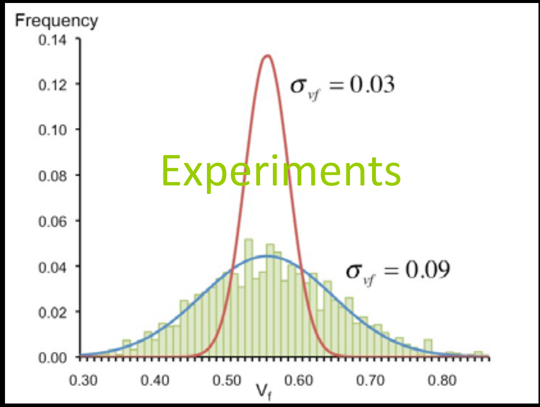
Variability in failure angle

Acknowledging microstructural variability captures distribution of experimental failure angles





Mendoza Jasso, Goodsell, Ritchey, Pipes, Koslowski, *Composites Science and Technology*, **71** (16) 1819-1825, 2011.
Mendoza Jasso, Goodsell, Pipes and Koslowski, *JOM*, **63** (9) 43-48, 2011.
Mendoza-Jasso and Koslowski, Composites Structures, 102, 148-153, 2013

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Thanks

STARnet

National Science Foundation
WHERE DISCOVERIES BEGIN

nanoHUB.org
an NCN project

NNSA
National Nuclear Security Administration

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
UNITED STATES AIR FORCE

OFFICE OF NAVAL RESEARCH
S&T

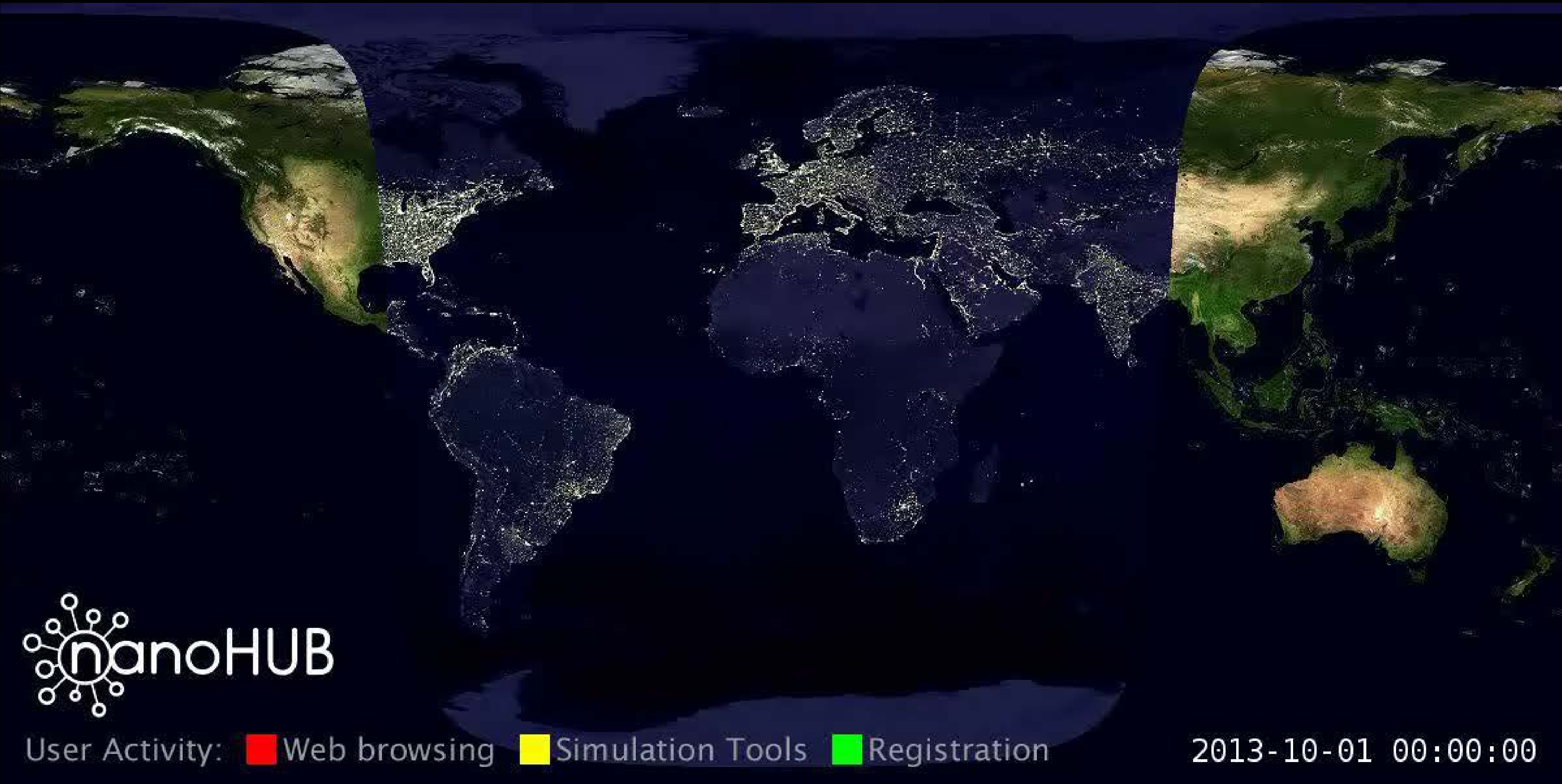
DEFENSE THREAT REDUCTION AGENCY
UNITED STATES OF AMERICA

DOW

BOEING

Office of Science

Educación y simulaciones en nanoHUB



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