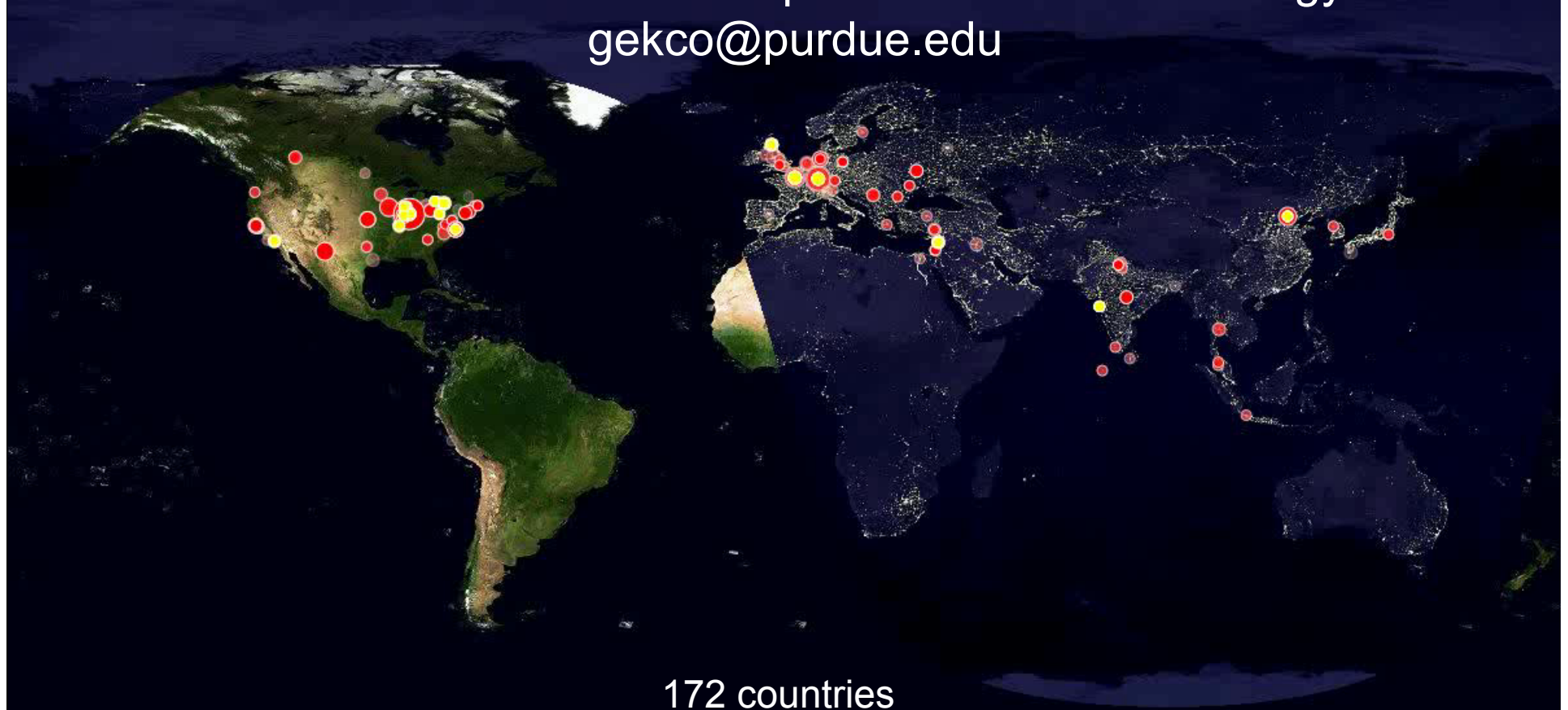


Exploring the Impact of nanoHUB.org on Research and Education Users

Gerhard Klimeck

Director Network for Computational Nanotechnology

gekco@purdue.edu



172 countries

nanoHUB usage 2010-02-06 18:00:00

nanoHUB and HUBzero Team



Gerhard Klimeck

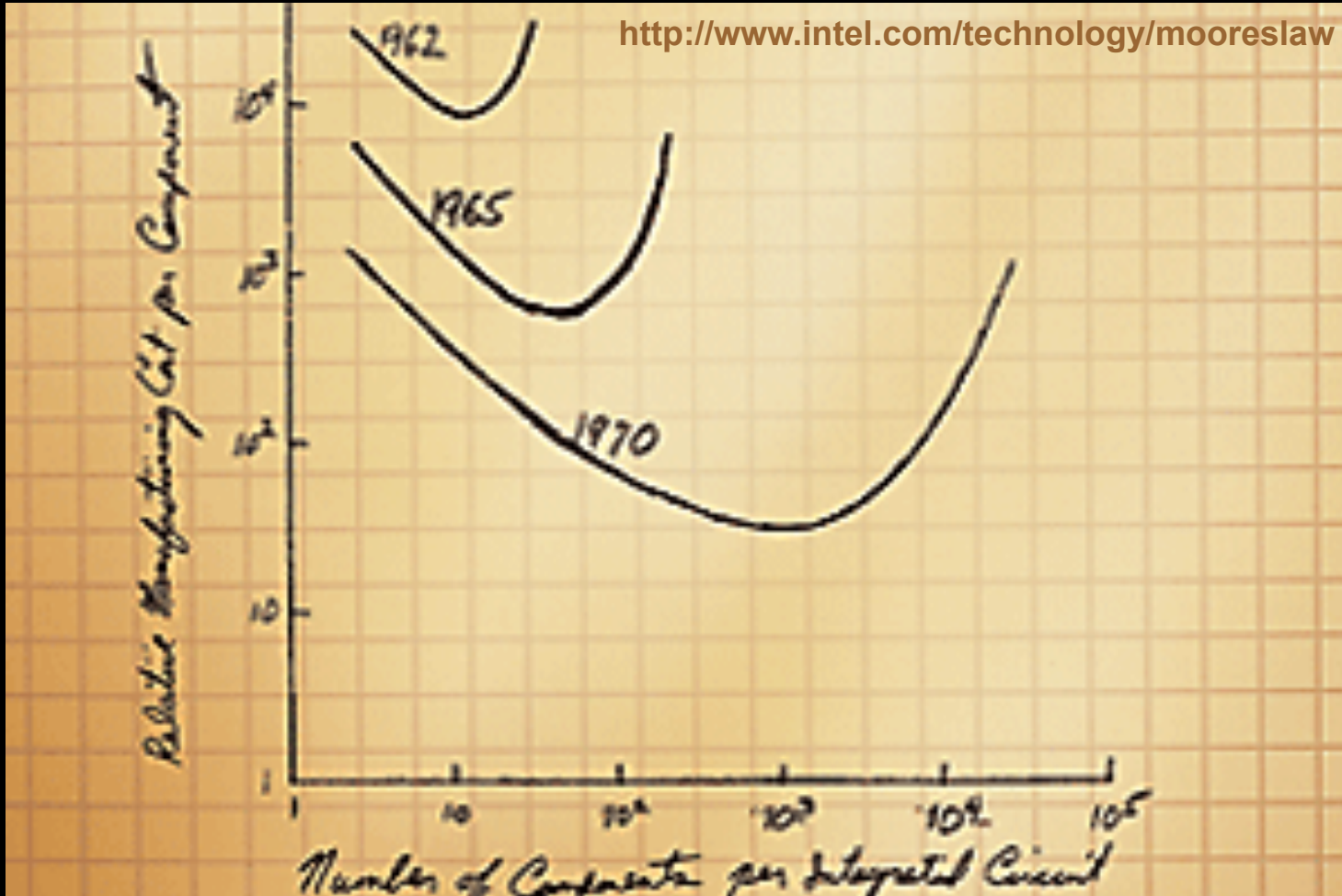


Research Group
@Purdue
@NASA JPL 1998-2003
@Texas Instruments 1994-1998



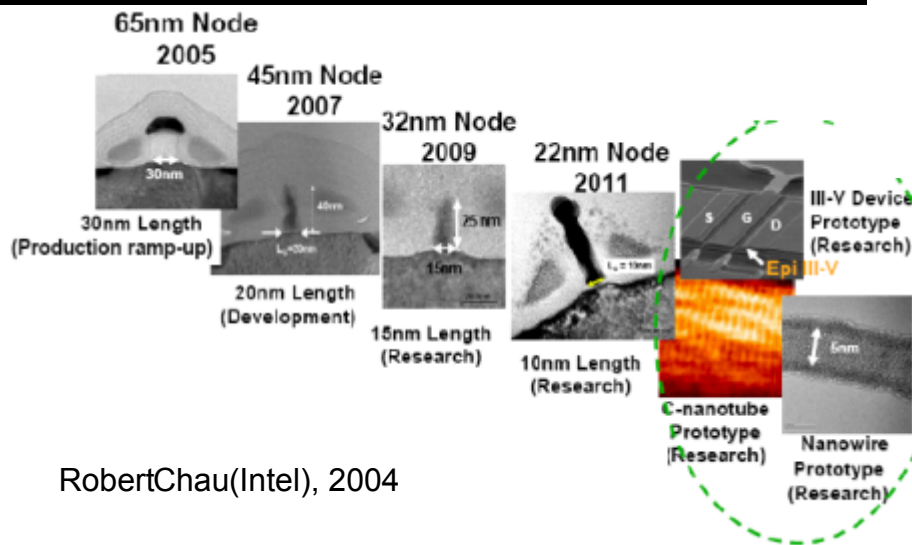
1965 Gordon Moore

Relative Manufacturing Cost per Component



Number of Components per Integrated Circuit

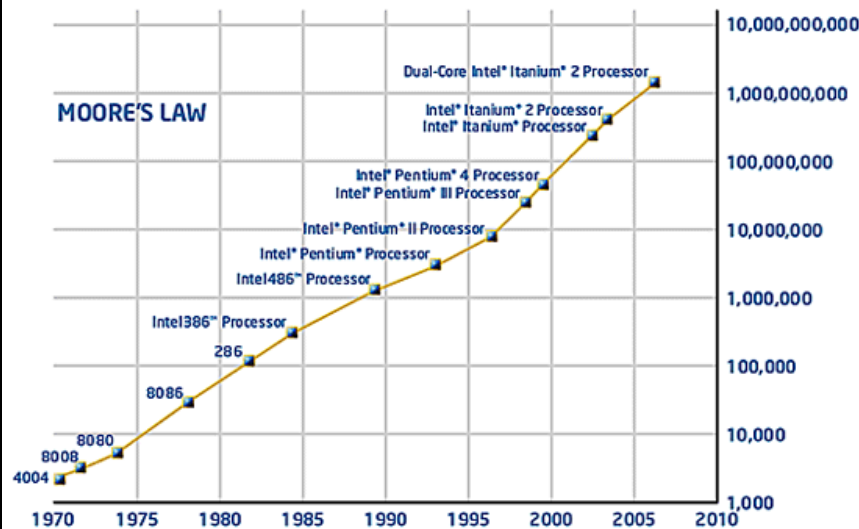
Intel in 2009



Device Size:
Tens of nanometers

Stanford SUPREM

<http://www.intel.com/technology/mooreslaw/index.htm> transistors



Device Integration:
>2 Billion

Berkeley SPICE

Berkeley

Simulation Program with Integrated Circuit Emphasis.



Ronald
A. Rohrer



Laurence
W. Nagel



Donald O.
Pederson

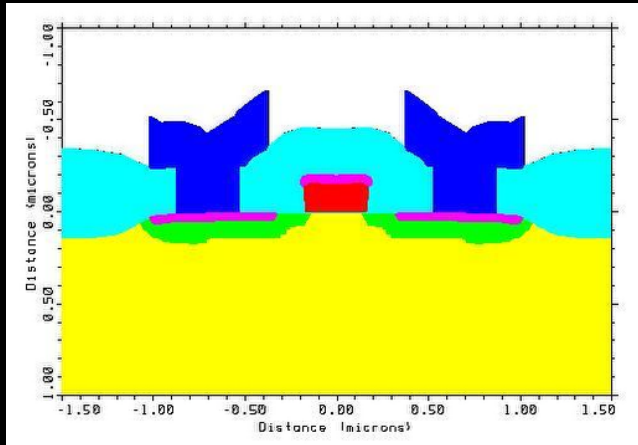
<http://www.omega-enterprises.net/>

from: Larry Nagel, BCTM '96

- Started as a class project
- Developed as a teaching tool
- Quality control: pass Pederson
- Dissemination:
 - ▶ Public domain code
 - ▶ Pederson carried tapes along
 - ▶ Students took it along to industry and academia
- ▶ Released 1972

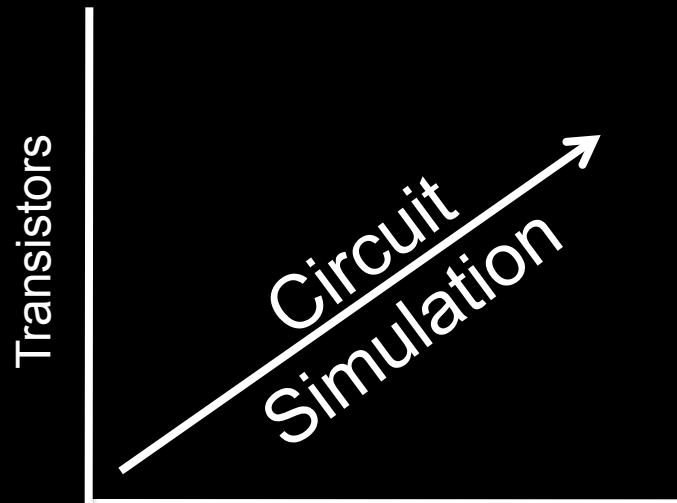
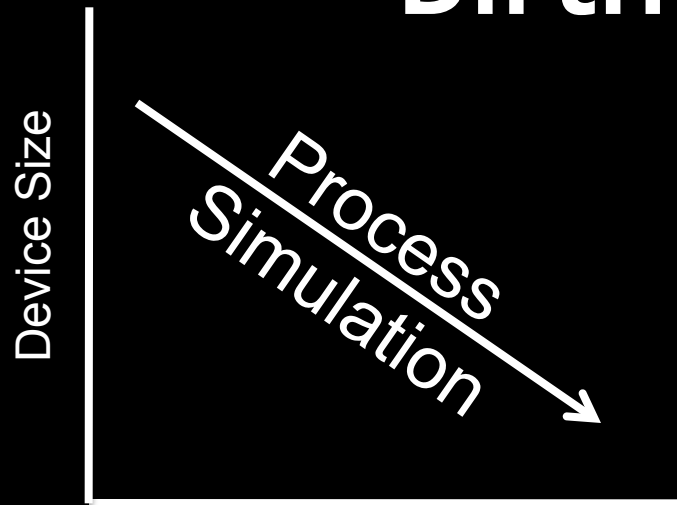
Stanford

SStanford UUniversity PRocEss MModeling



- Stanford wanted to mimic Berkeley success
- Combine various existing models
- Dissemination:
 - ▶ Public domain code
 - ▶ Community workshops
 - ▶ Students took it along to industry and academia

Birth of an Industry



Intel Capitalization:
\$85B
Total Industry:
\$280B

Years

What's Next?

Nano Initiatives

Device Size

nano-scale
structures

Transistors

Billions of nano
structures

Years

Research

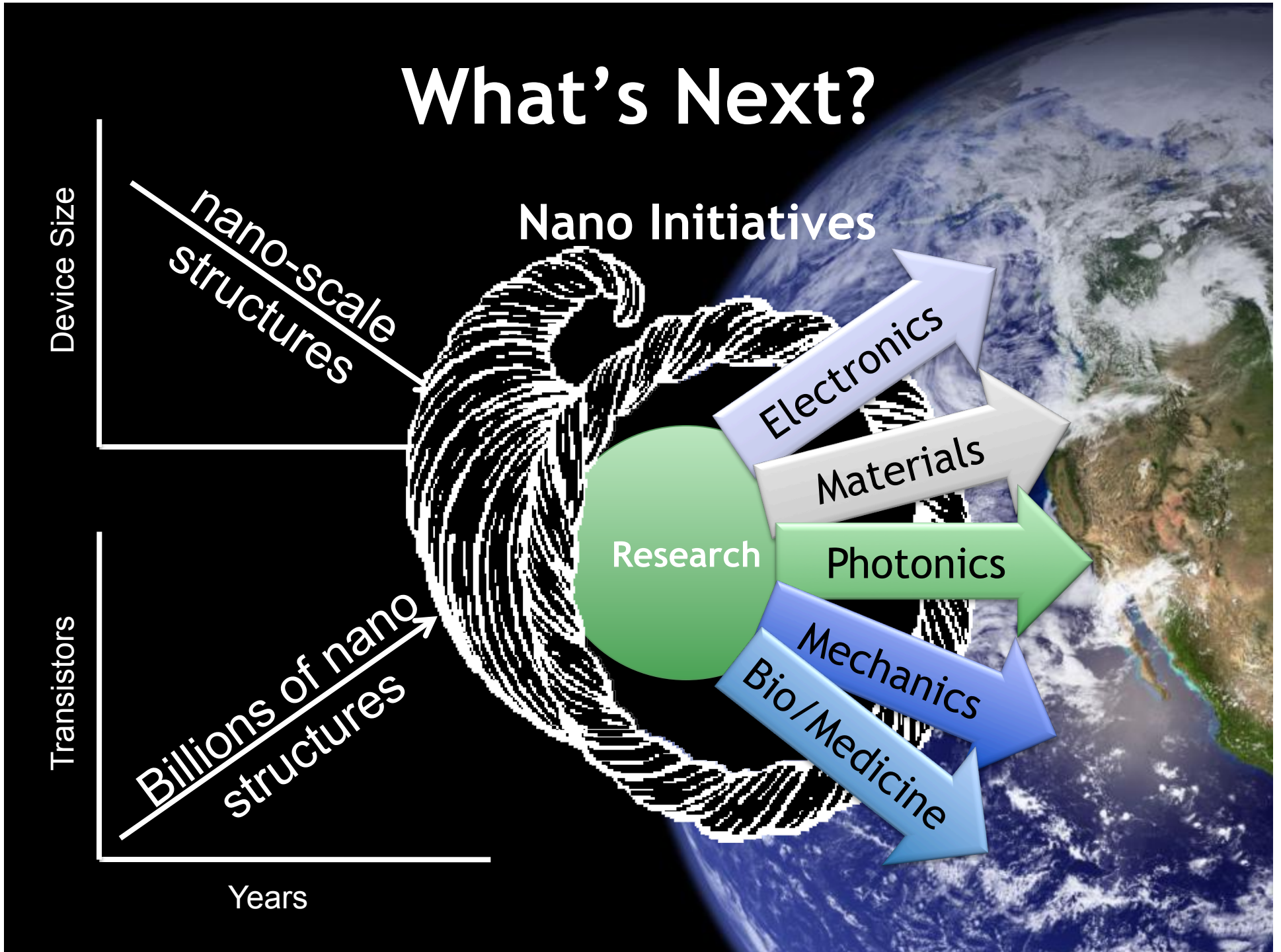
Electronics

Materials

Photonics

Mechanics

Bio / Medicine



What's Next?

Nano Initiatives

Device Size

nano-scale
structures

Transistors

Billions of nano
structures

Years

Research

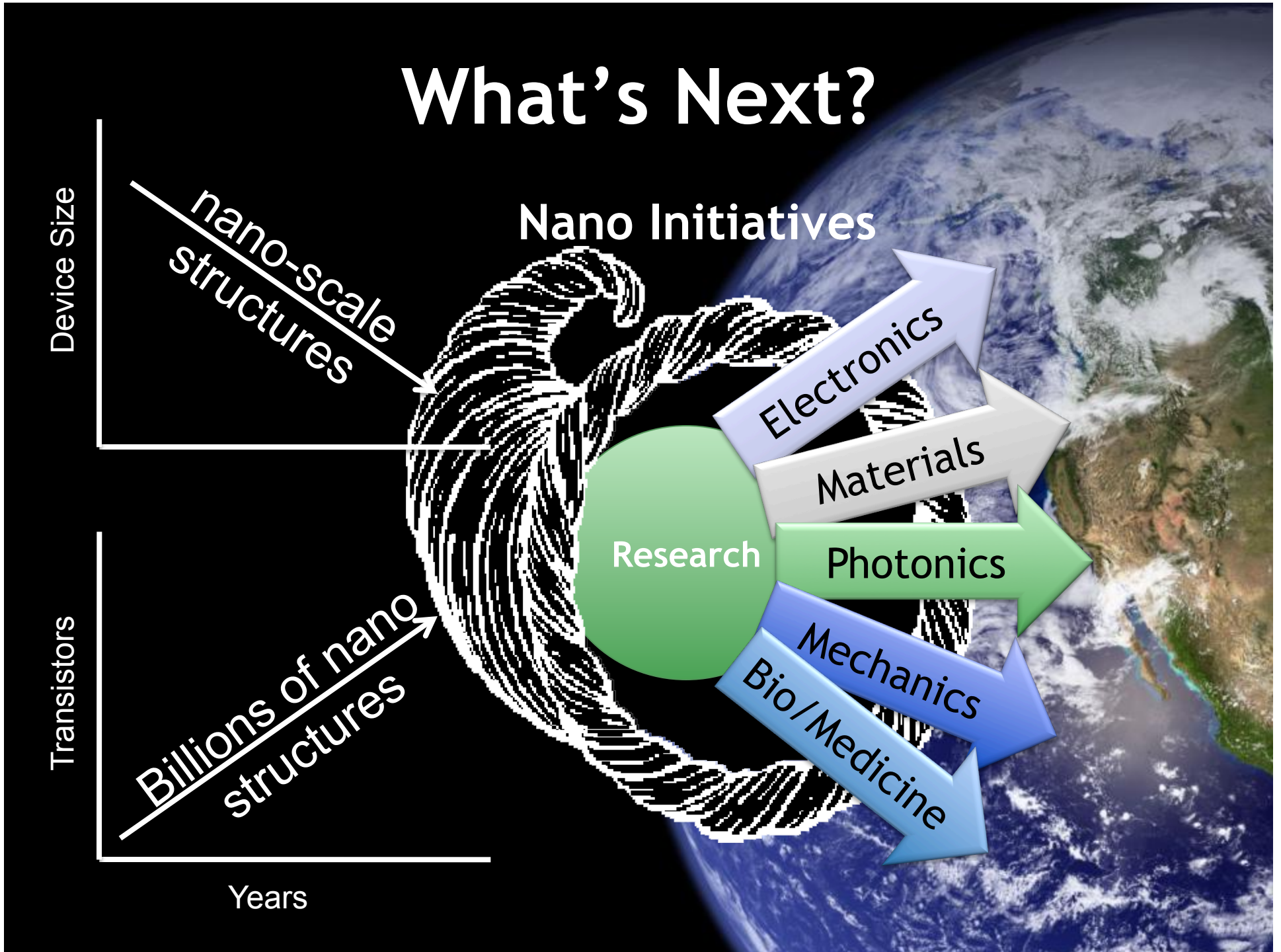
Electronics

Materials

Photonics

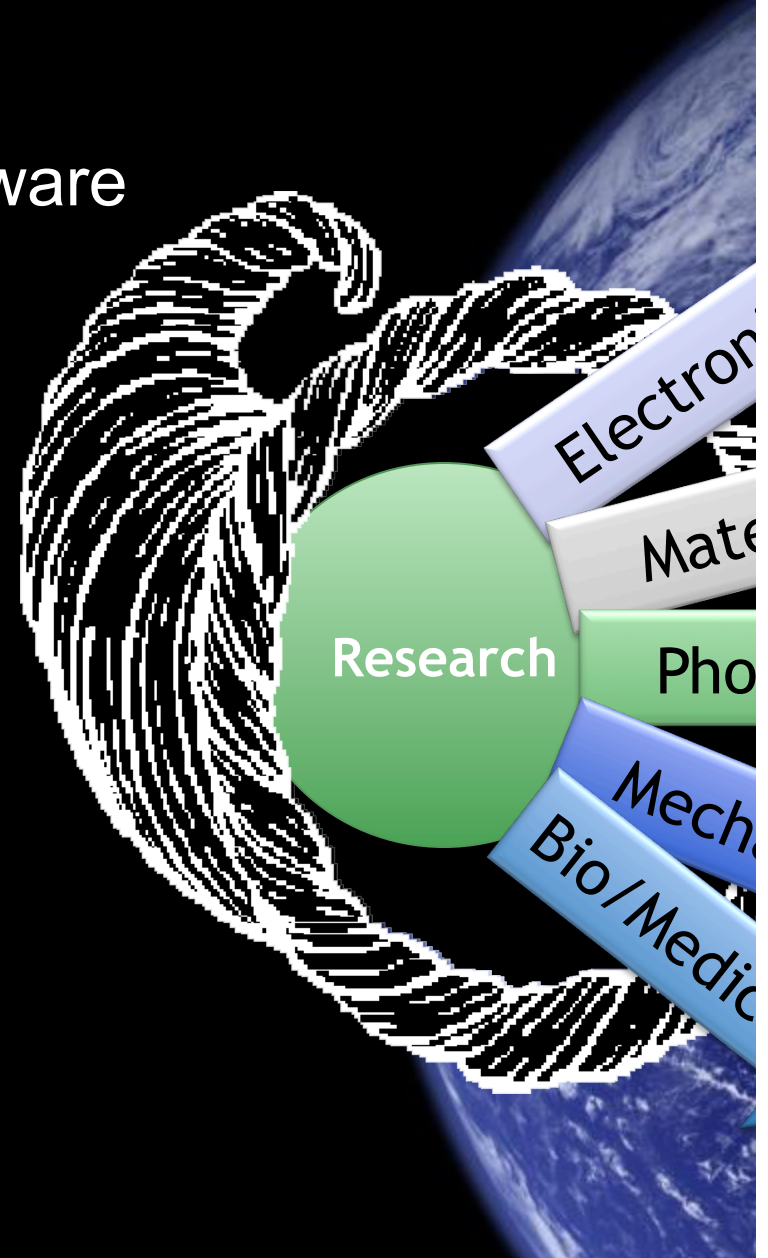
Mechanics

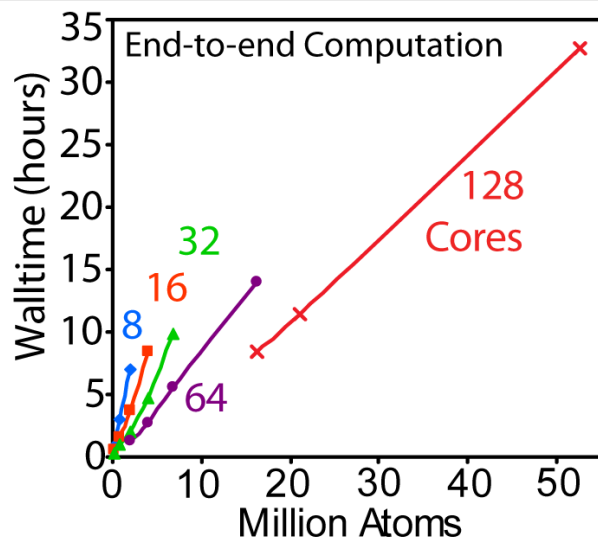
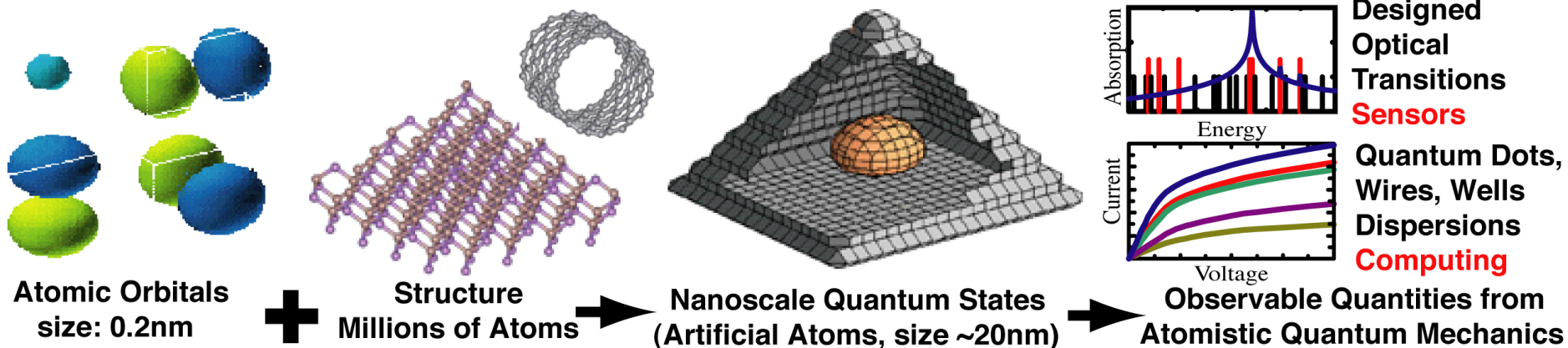
Bio/Medicine



Goals - Impact Metrics

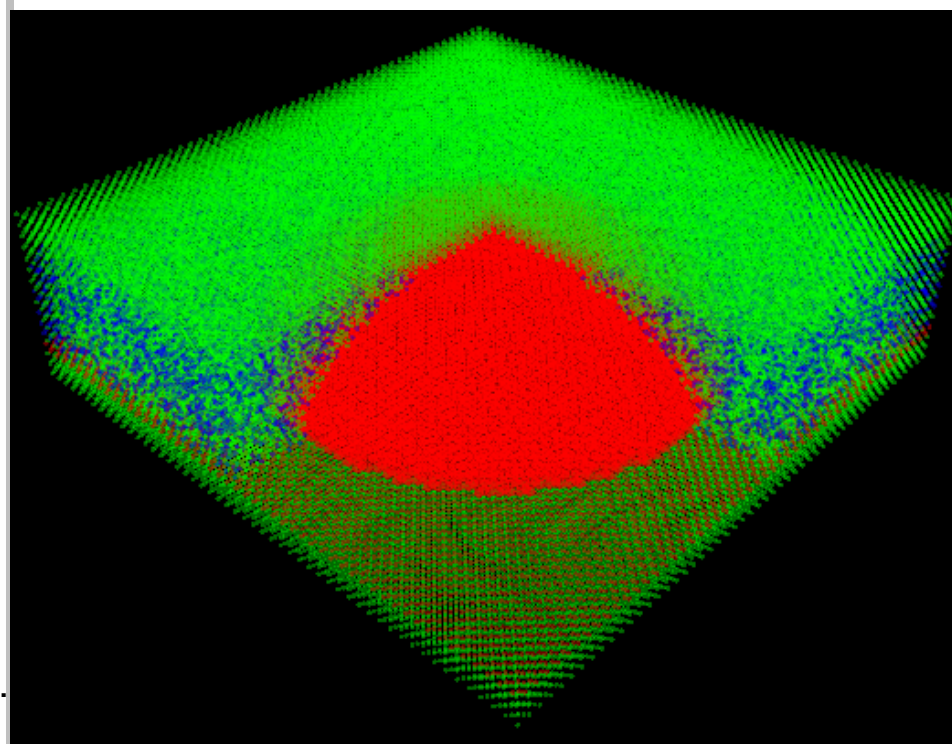
- Services:
 - Modeling and Simulation Software
 - Seminars, tutorials, classes
- Goals:
 - Knowledge transfer
 - Use in class rooms
 - Knowledge generation
 - Use in research
 - Use by experimentalists
 - Economic impact
 - Use in Industry
 - Professional Development / Community building



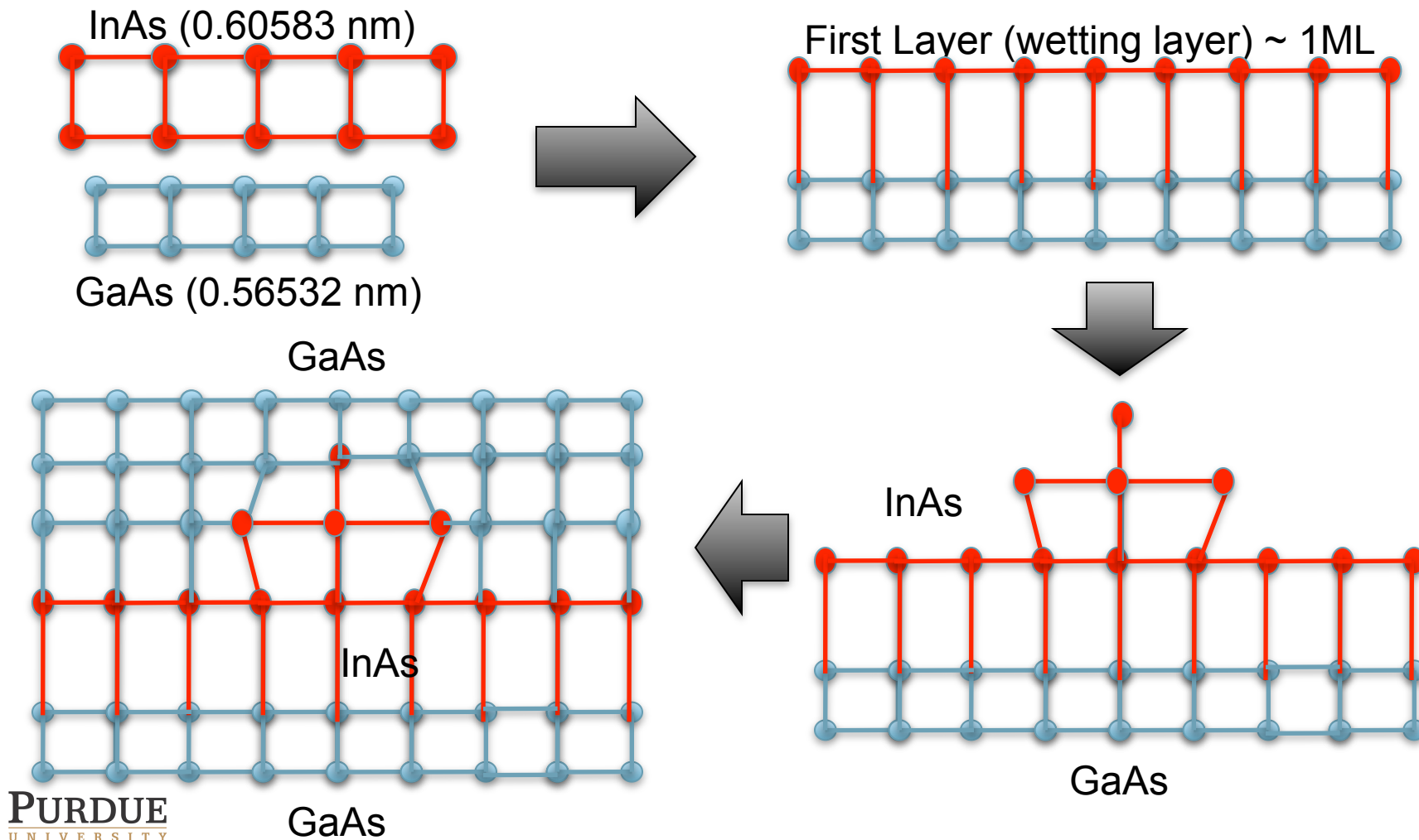


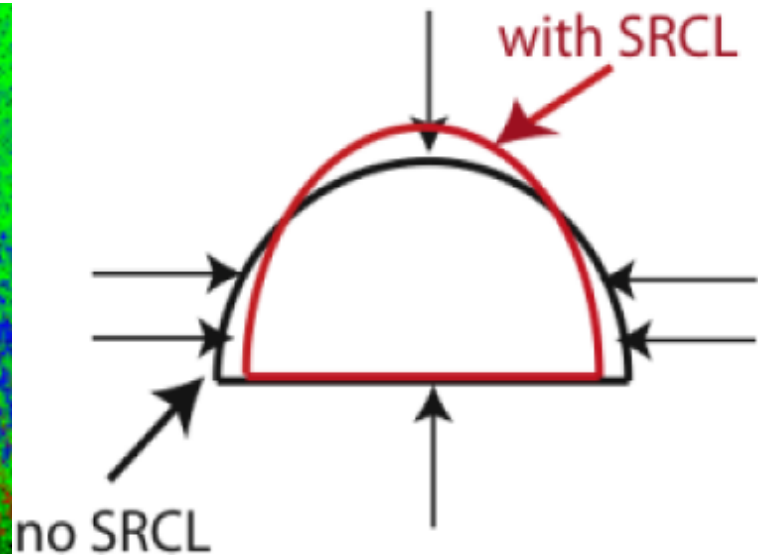
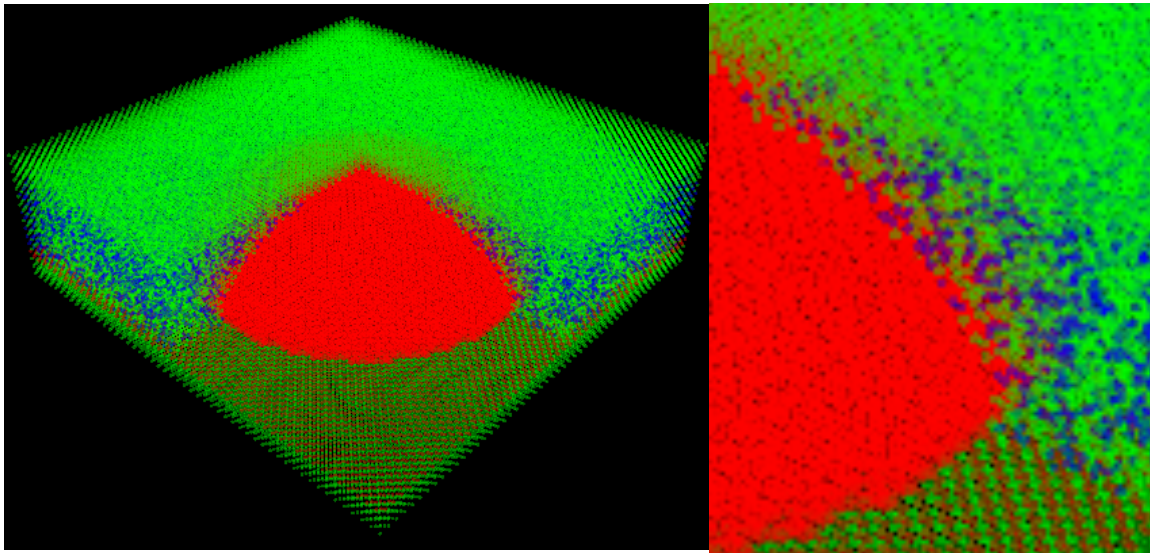
Demonstration / Capability / Impact:

- 52 million atom electronic structure (101nm)³.
- Quantum dots, nanowires, quantum computing...



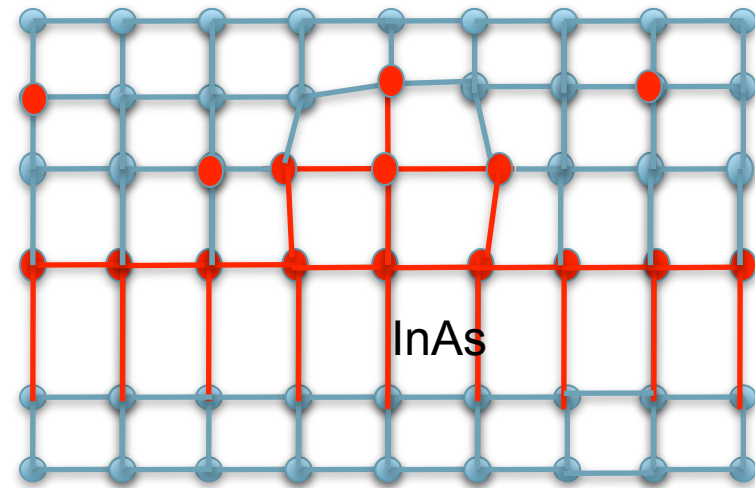
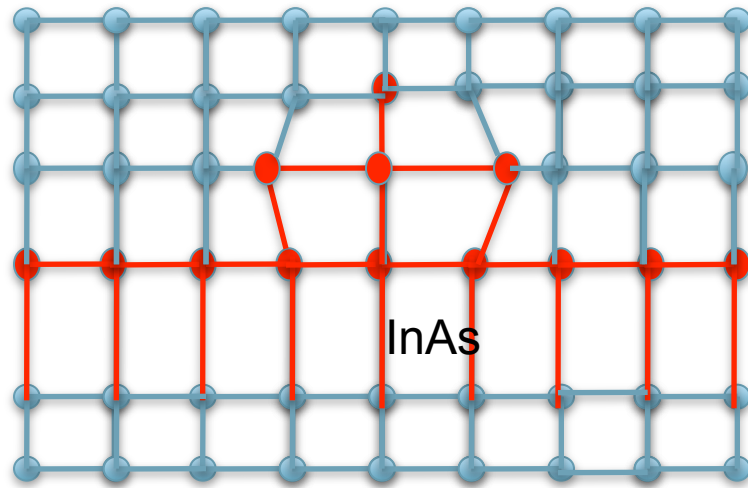
Self-Assembly Process → InAs deposition on GaAs substrate





GaAs

GaAs



GaAs

GaAs

Objective:

- Optical emission at $1.5\mu\text{m}$ without GaN
- Understand experimental data on QD spectra in selective overgrowth
- 17 experimental data points – growths Tatebayashi, et al, *Appl. Phys. Lett.*, V78. 3469.

Approach:

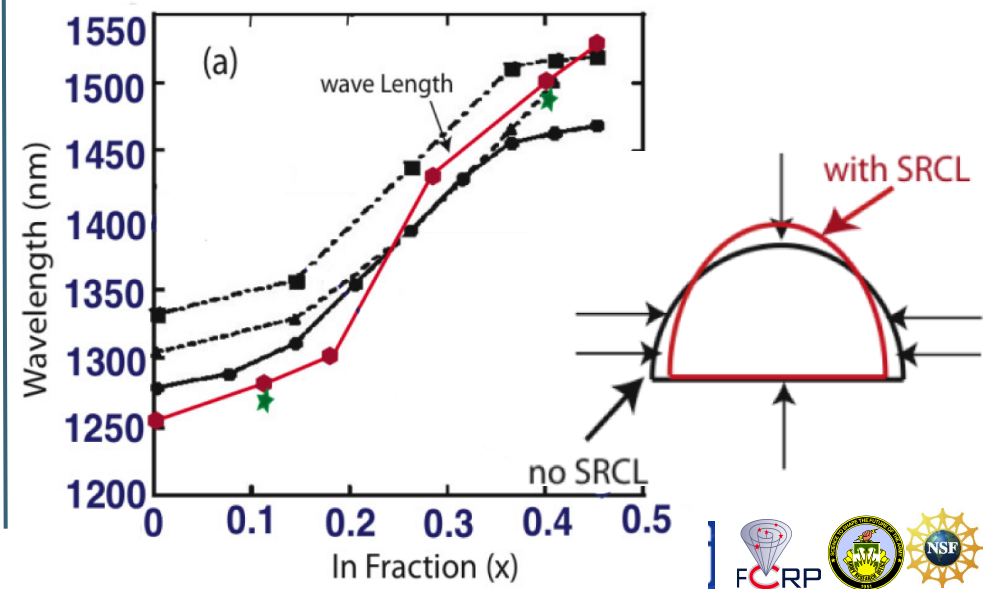
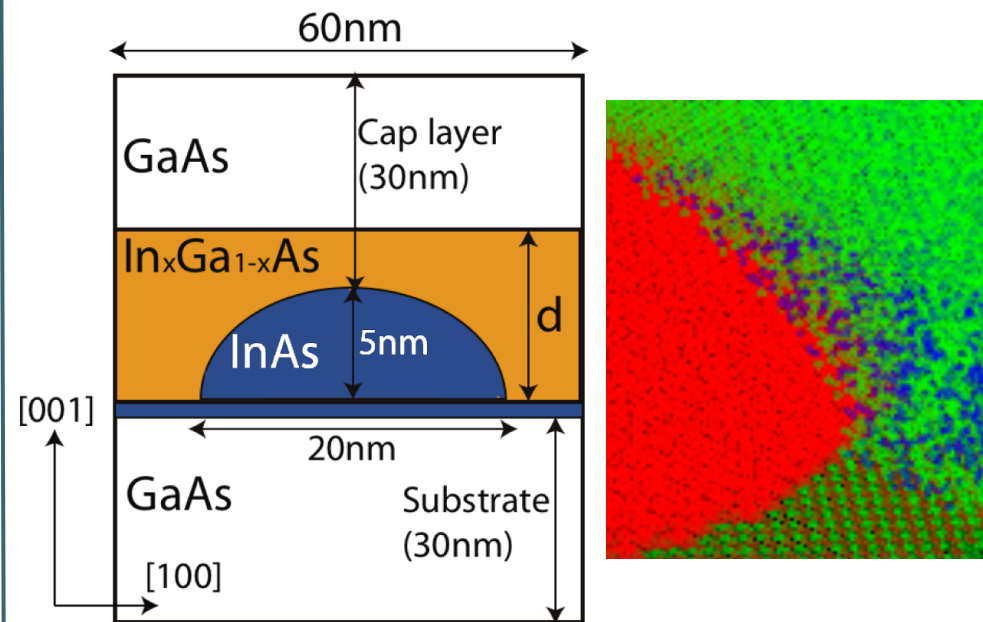
- Model large structure
 - 60nm x 60nm x 60nm

0 million atoms

- No changes to the previously published TB & VFF parameters

Result:

- Theory (red line) matches a sequence of 17 experiments (black dots/lines)
 - Bi-modal In-As, Ga-As bond distrib.
 - change in quantum dot aspect ratio
- Quantitative model of complex system



Overcoming barriers to quantum mechanics simulations in physics, chemistry, biology, and materials to migrate nano-science to nano-technology.

Algorithms, Computing,
Middleware, Service

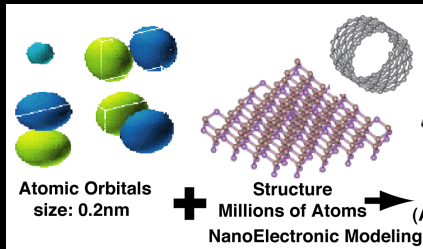
Open, available,
usable
by real users



Impact on Research

Impact on Education

Example: NEMO3D -

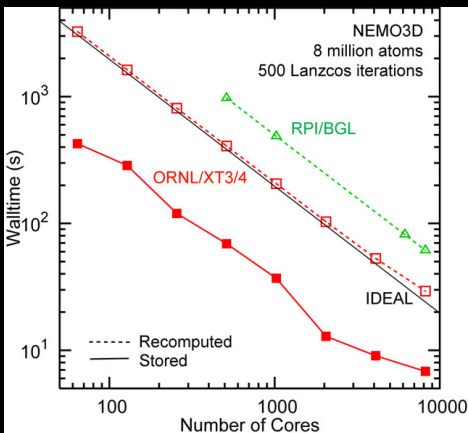
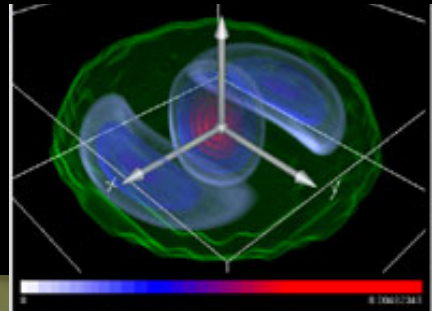


Algorithms, Computing, MiddleWare, Service



NCN / nanoHUB.org

Develop & Deploy
Methods, Tools, and Training
atomistic → mesoscopic → systems



Towards Peta-Apps
each atom on
nanoHUB H/W

- 8,192 cores IBM B/G and Cray XT3/4

Impact on

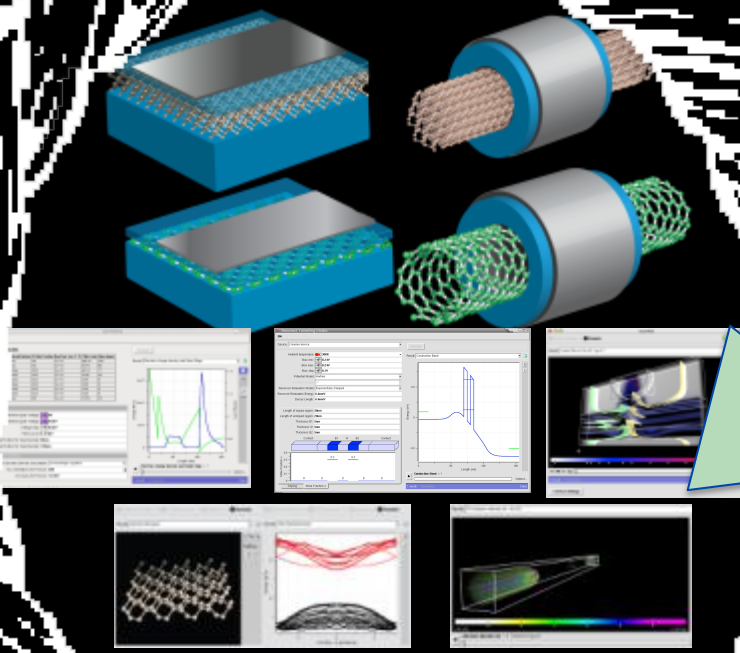


NEMO 3-D at 7 tutorials
SC05, SC06, SC07, TG06, TG7,
Nano06, NMD06, NEMS07,
>130 educators

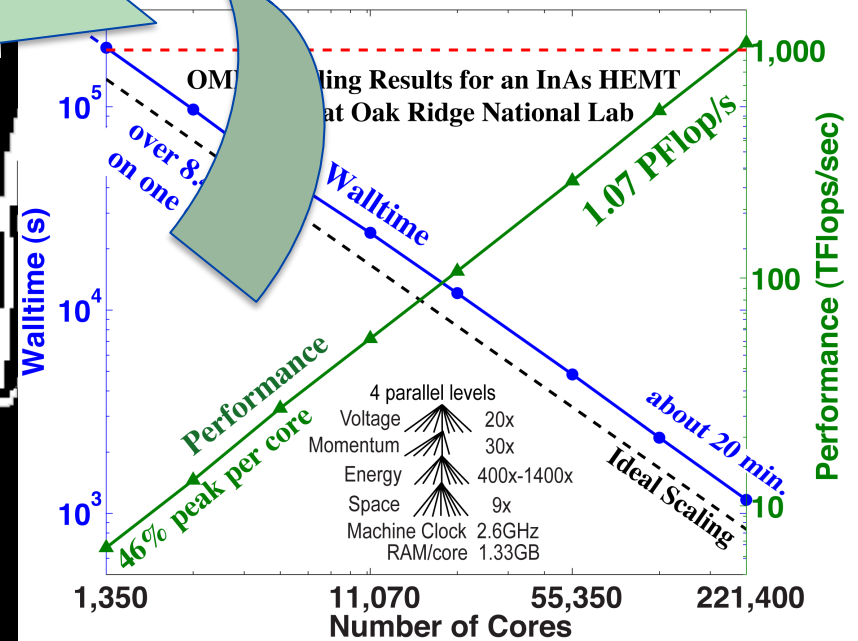
Electronic Structure & Electron Quantum Transport Simulations

NEMO & OMEN

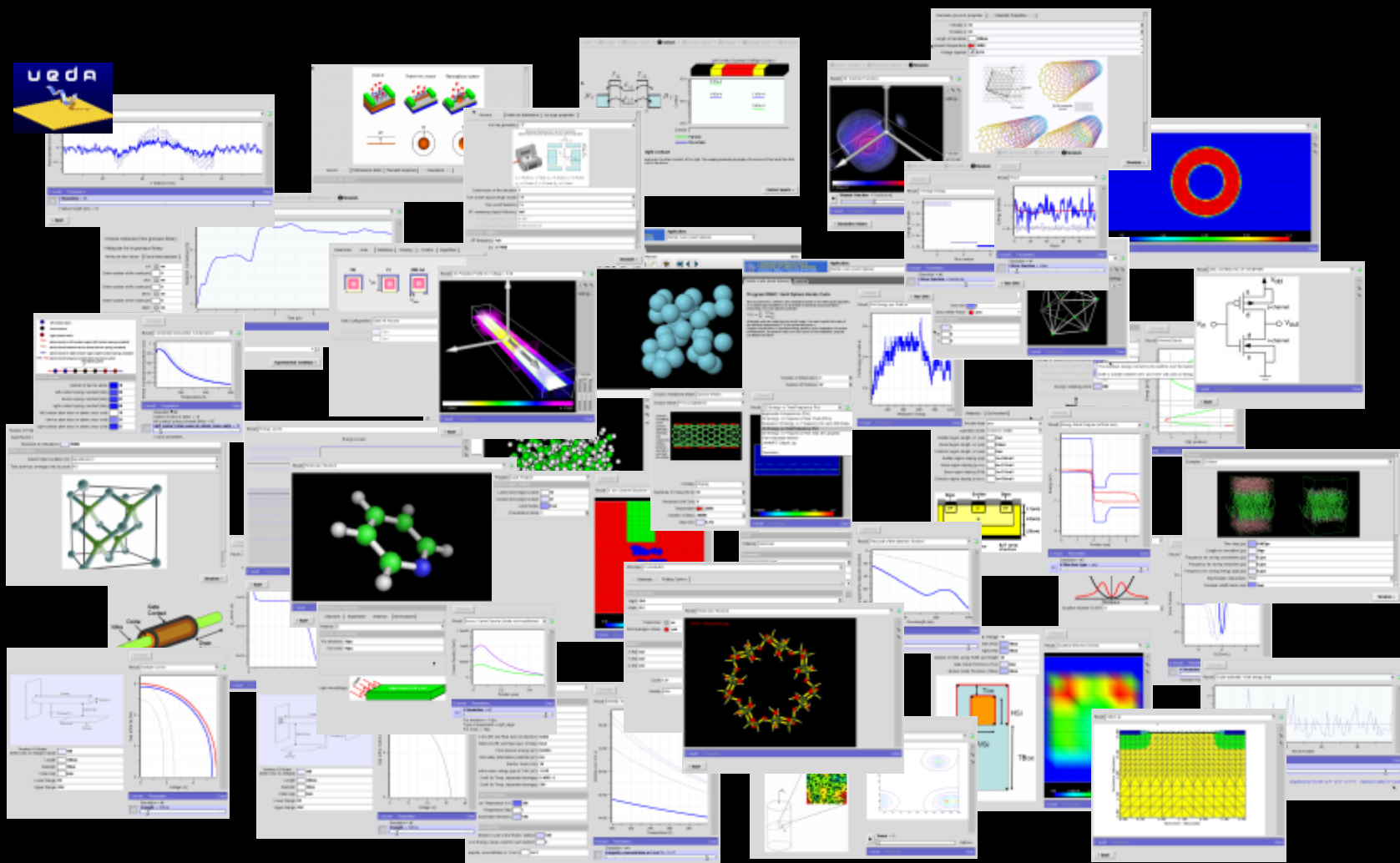
Runs on fastest computer in the world



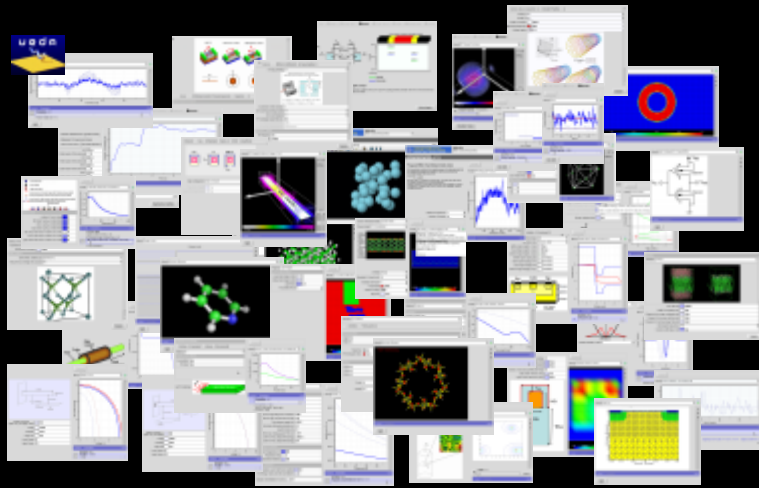
Runs 6 tools in nanoHUB
 >6,700 users
 >100k sims



Over 190 tools online!



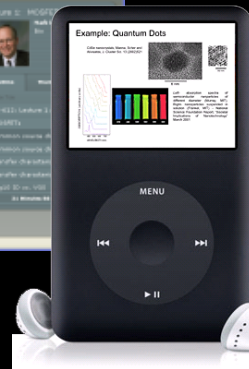
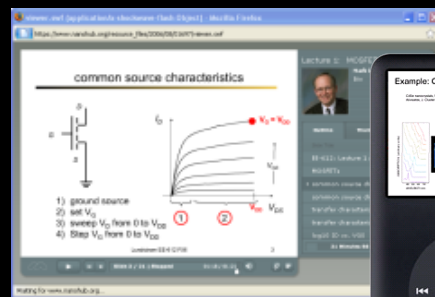
Over 2,300 Resources!



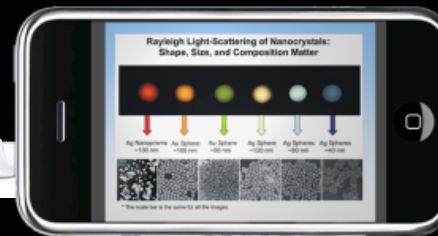
180 tools



43 courses



1,700 seminars and teaching materials



It Happens Here

The screenshot shows the nanoHUB.org website in a browser window. The browser's address bar displays "http://nanohub.org/". The website header includes the logo "nanoHUB.org" with the tagline "ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY" and "an NCN project". Navigation links include Home, My HUB, Resources, Members, Explore, About, Support, and a Help icon. A search bar and buttons for "Login" and "Register" are also present.

The main content area features a "now on iTunes U" banner with a music player interface. Below this, four key features are highlighted: "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", and "SHARE & PUBLISH tools and research through our easy upload process". A world map graphic is accompanied by the text "Over 100,000 users annually" and links for "Detailed statistics" and "Who's online?".

The page is divided into three columns:

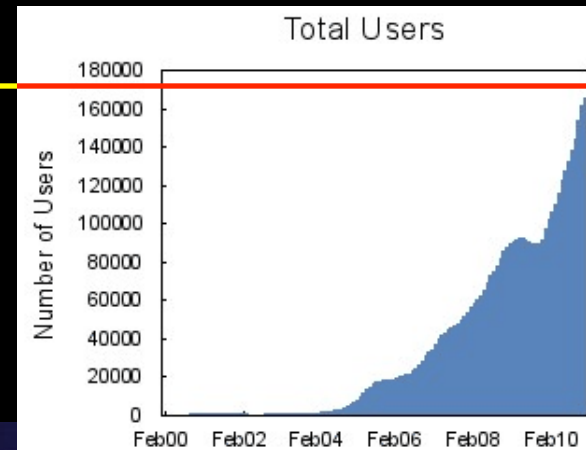
- RESOURCES:** Includes a search bar, a list of popular tags (e.g., nanoelectronics, course lecture, material science, nanotransistors, research seminar, nano/bio, hosted/produced by NCN@Illinois, devices, quantum transport, tutorial, molecular electronics, nano electro-mechanical systems, transistors, NEGF, nanophotonics, carbon nanotubes, education/outreach, uuc, nanomedicine, Illinois, ABACUS, NCN Supported, band structure, MOSFET, materials), and a "More..." link. It also lists categories like Animations, Courses, Downloads, Learning Modules, Notes, Online Presentations, Publications, Series, Teaching Materials, Tools, Workshops...
- FEATURED:** Lists featured content such as "Drift-Diffusion Lab: Simulate single semiconductor characteristics - in Tools", "Illinois ECE 460 Optical Imaging, Chapter 3: Imaging - in Teaching Materials", "James Leary, Purdue University, West Lafayette - Contributions: 26, Average resource ranking: 8.38", "ANTSU—Assembly for Nanotechnology Survey Courses - in Topics", "ECE 495N: Fundamentals of Nanoelectronics - featured on iTunes U", and "Why is Fermi level referred to as electrochemical potential - asked by Anonymous, in Answers".
- NOTABLE QUOTE:** Features a quote: "All of the tools on nanoHUB are easy to use, amazingly comprehensive and accurate." attributed to "Onur Ates, Graduate Student, Arizona State University - in Notable Quotes".

A "NEW IN RESOURCES" section lists recent additions: "Overview of How People Learn Framework to Support Instructional Design in Online Presentations, Apr 19, 2010", "PN junction in Animations, Apr 17, 2010", and "Local density of states in Animations, Apr 17, 2010". A link "See what else is new" is provided.

Nano App Store

170,000 users worldwide

As much traffic as www.purdue.edu
Users at all Top 50 US Engr Schools
19% of all .edu domains

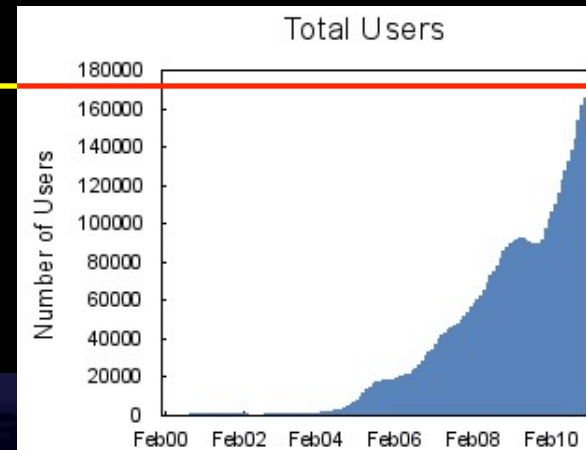


172 countries

Nano App Store

170,000 users worldwide

As much traffic as www.purdue.edu
Users at all Top 50 US Engr Schools
19% of all .edu domains



Sociology

How do Users Behave?

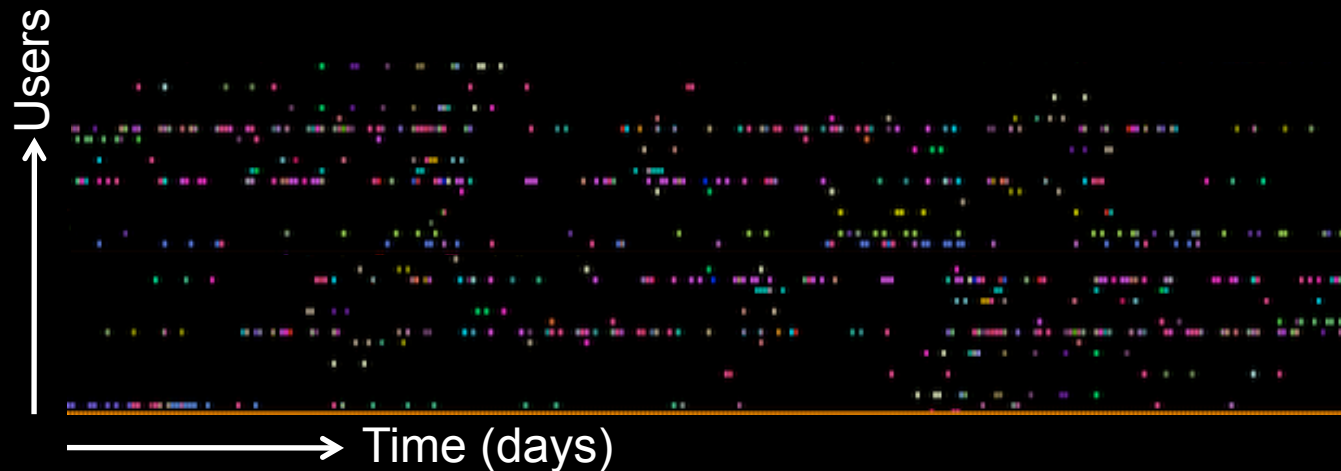
- Questions:
 - How many students in the class?
 - Which tools?
 - Intensity of use
 - Sustained use
 - Percentage of service: Education vs. Research use
- Some Statistics
 - 8,600 users ran 345,000 simulations Academic Year 2009/2010
 - 116 classes / 97 institutions in Academic Year 2009/2010
 - Info Obtained from self-registration, manual follow-up
 - 575 citations in the literature
 - Info obtained from Google Scholar and manual analysis

Sociology

How do Users Behave?

- Questions:
 - How many students in the class?
 - Which tools?
 - Intensity of use
 - Sustained use
 - Percentage of service: Education vs. Research use
- Can we get answers? Automatically?
=> Improve Services
 - Better tool classification
 - Customize web page for users, customize learning experience
 - Computational resource provisioning
- Broaden user base

The nanoHUB Matrix



Each dot represents simulation activity on a particular day
The color of the dot indicates a particular tool

We will look backwards into history
for each user in the past 12 months
And plot ALL their activities

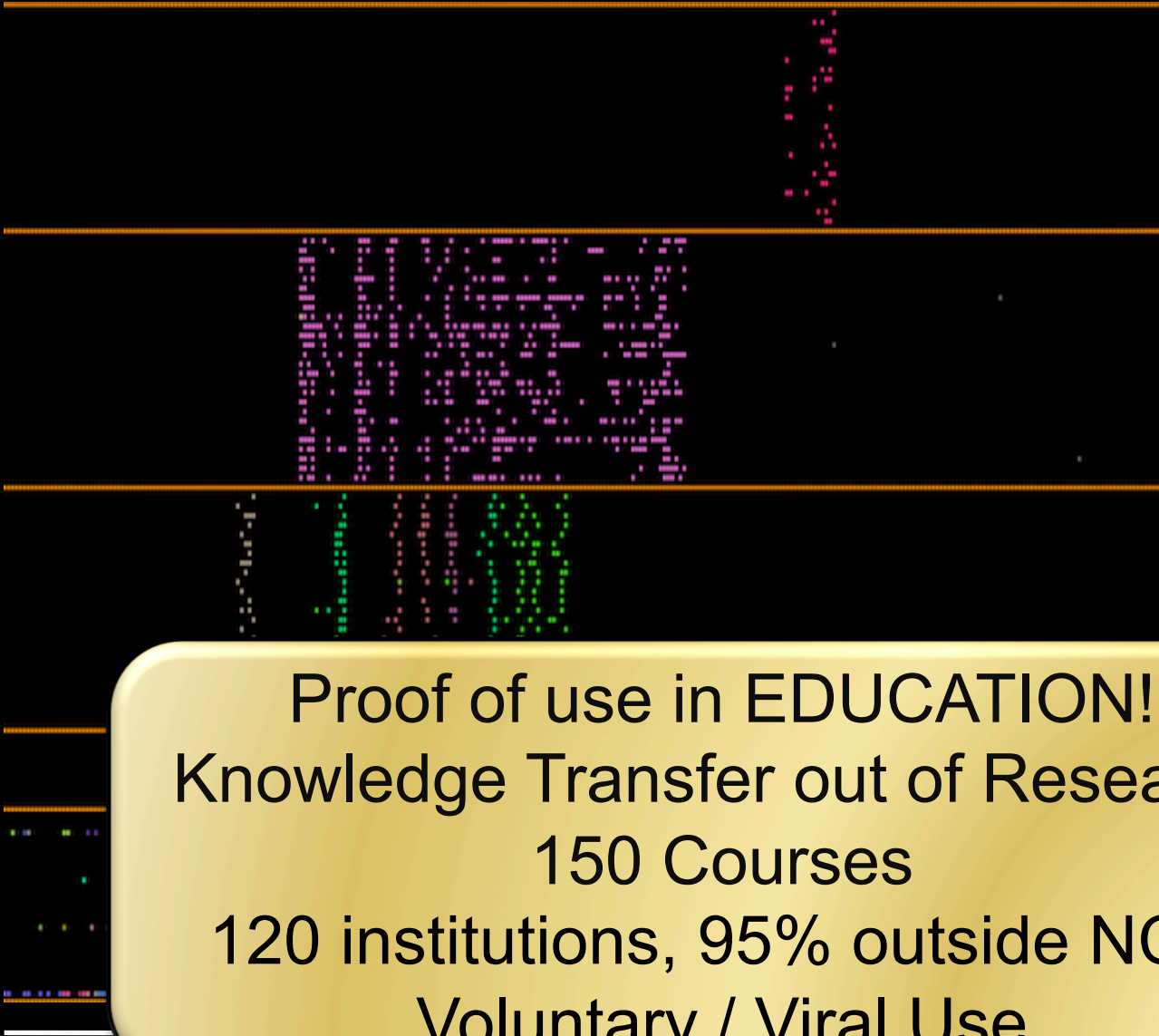
2010-06-30

6 users

1 days of history

The nanoHUB Matrix

Formal Education vs. Research



single tool,
single use /
homework

single tool,
sustained,
intense

multiple tools,
sustained,
periodic

tools,
class

ch,
study

Users ↑

Proof of use in EDUCATION!
Knowledge Transfer out of Research
150 Courses
120 institutions, 95% outside NCN
Voluntary / Viral Use

Research Impact

Device Size

nano-scale
structures

Transistors

Billions of nano
structures

Years

Research

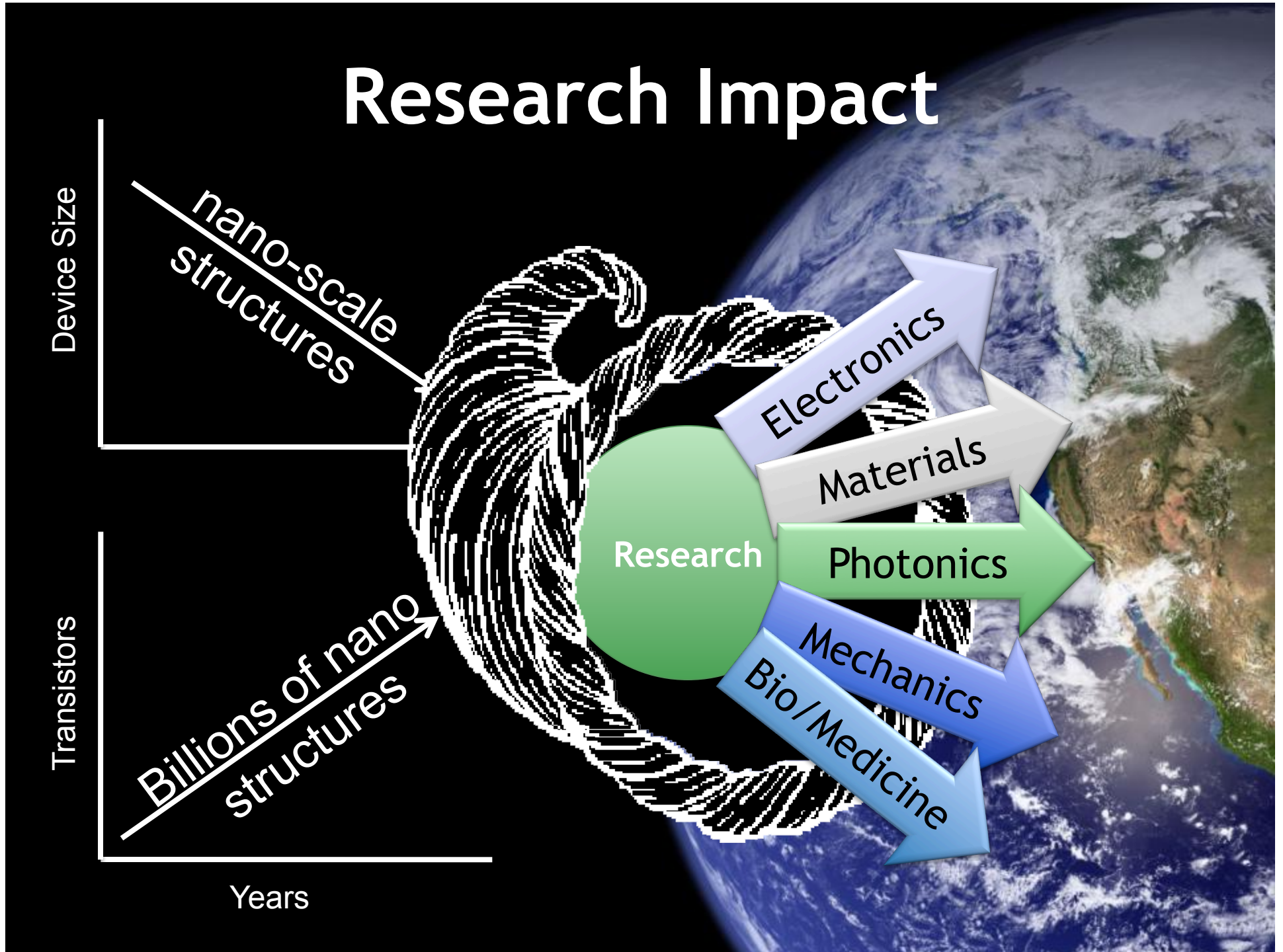
Electronics

Materials

Photonics

Mechanics

Bio / Medicine



719 nanoHUB Citations

1 citation is a paper

1 line is common author

56% outside NCN

1,400

Over 1,400 authors

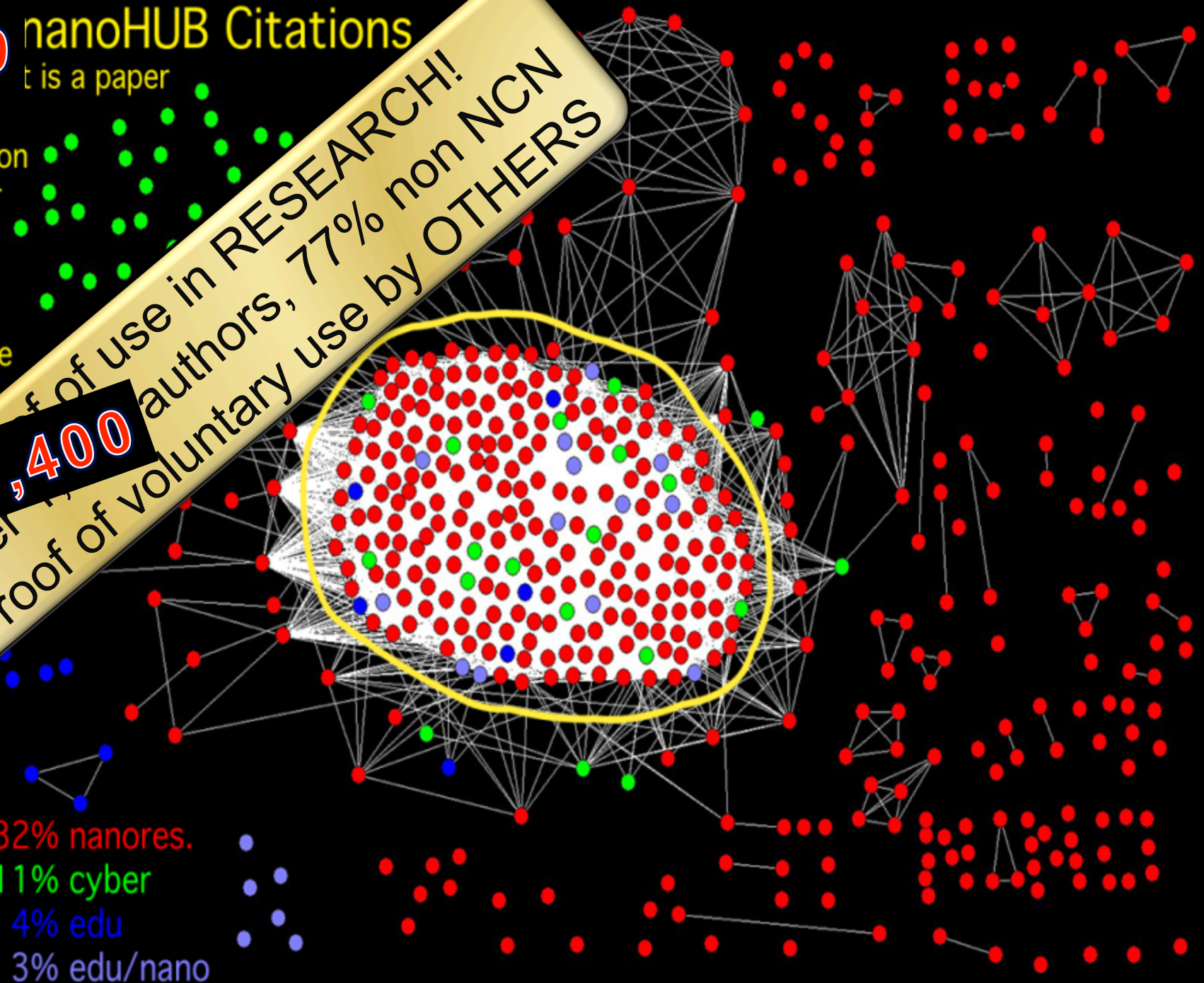
Proof of use in RESEARCH!
Proof of voluntary use by OTHERS

469 82% nanores.

62 11% cyber

24 4% edu

20 3% edu/nano

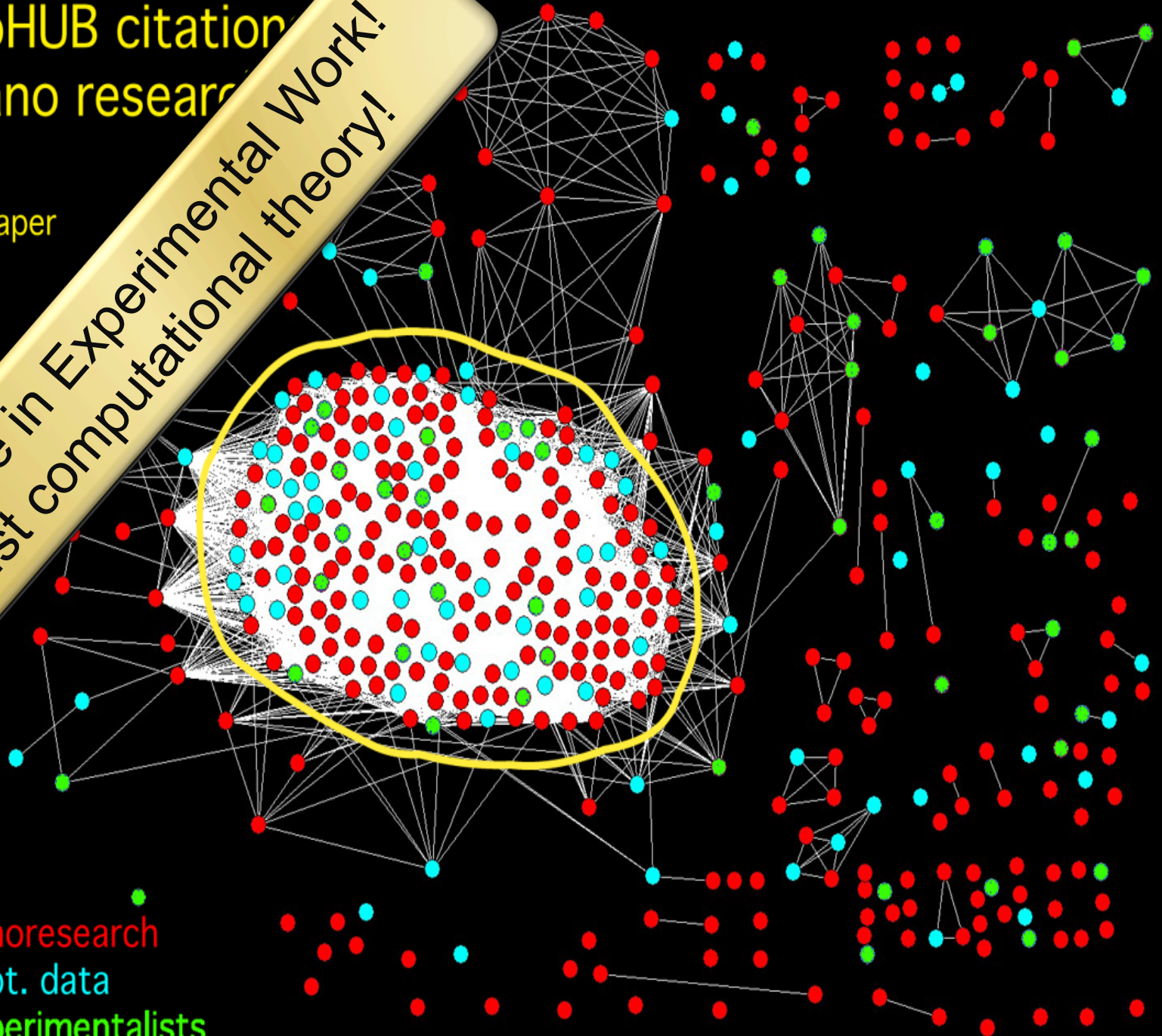


575 nanoHUB citation
469 in nano research

each dot is a paper
line is
common
author

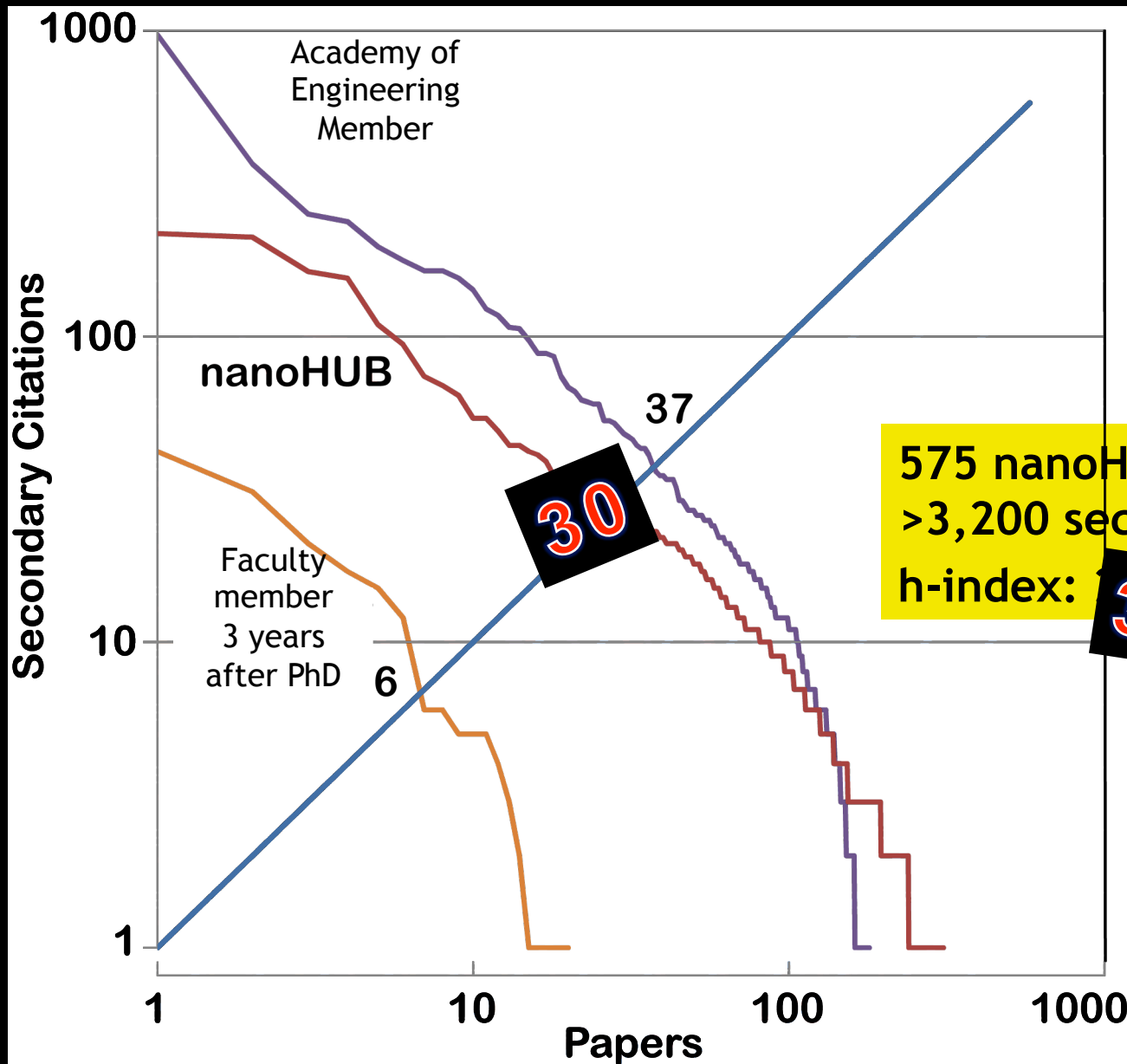
Proof of use in Experimental Work!
Not just computational theory!

469 82% nanoresearch
142 30% expt. data
55 12% experimentalists



719 nanoHUB Citations

Research: Publish or Perish



575 nanoHUB citations
>3,200 secondary citations
h-index: 30

30

30

6

Industry Impact

Device Size

nano-scale
structures

Transistors

Billions of nano
structures

Years

Research

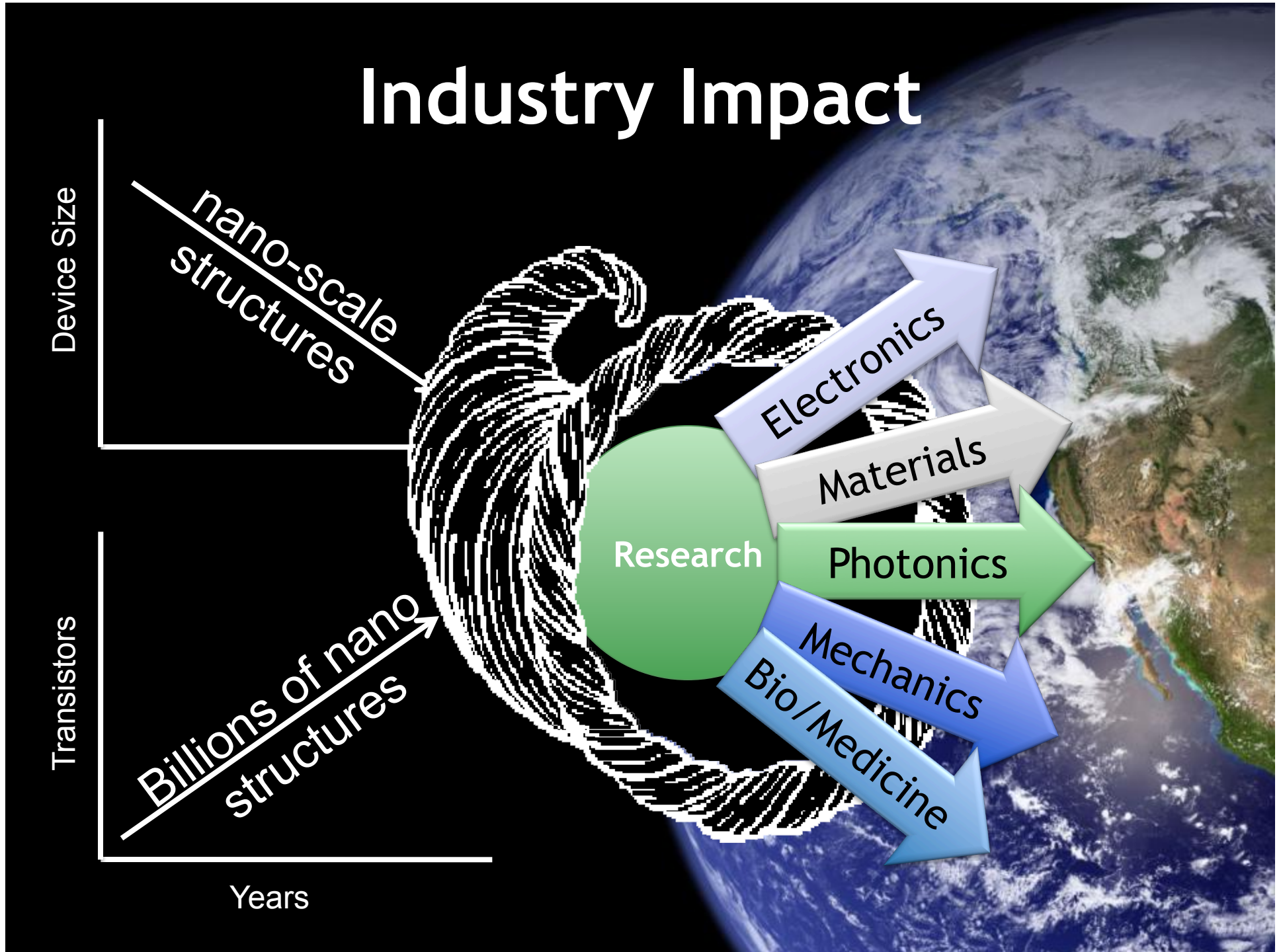
Electronics

Materials

Photonics

Mechanics

Bio / Medicine



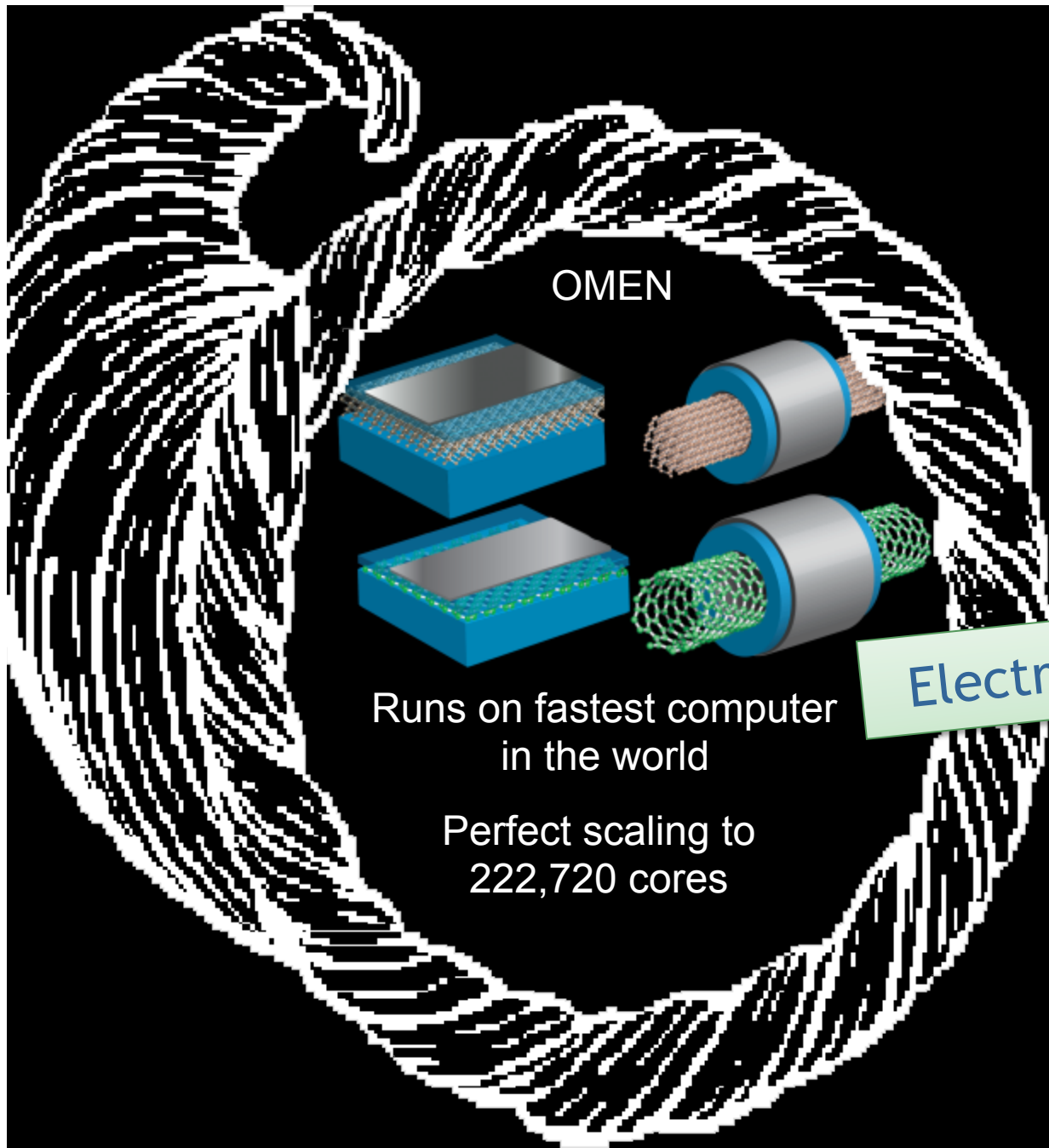
Papers by Industrial Authors

8.7%

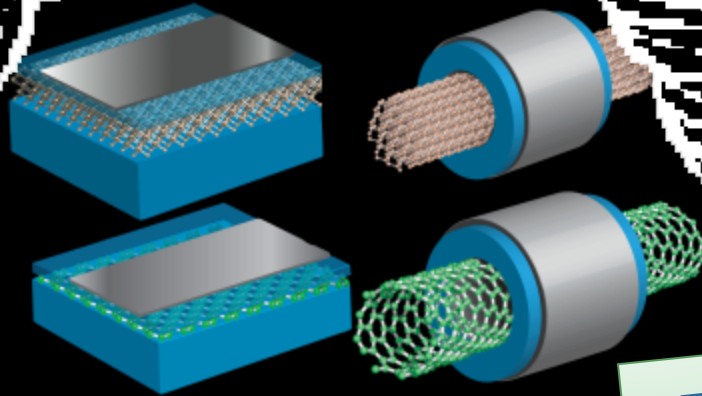


Publications

- 46 papers total
- 41 papers in nano



OMEN



Runs on fastest computer
in the world

Perfect scaling to
222,720 cores

Electronics



Mark Stettler, PhD.
Mgr. TCAD, Oregon

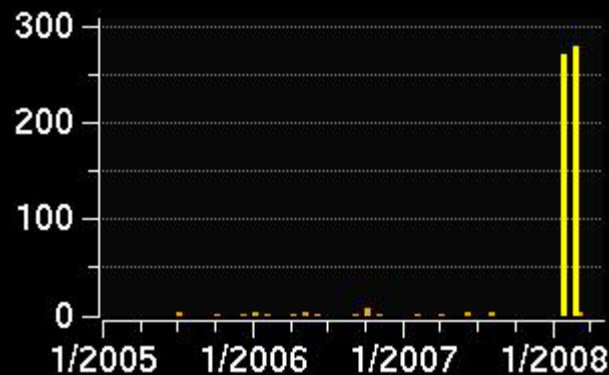


Dmitri Nikonov, PhD.
Mgr. Strategic Research, CA

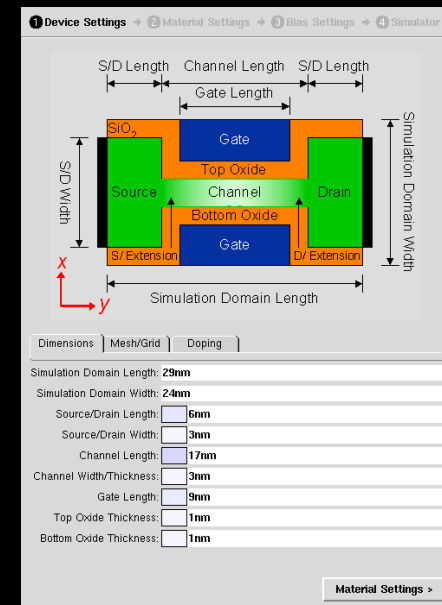
Texas Instruments => Patent

Dr. R. Chris Bowen
Texas Instruments

I used the tool in a mode ... far away from the original intent of the simulator. ... The insight that "nanoFET Lab" provided was convincing enough for me to begin more detailed simulations at Texas Instruments and to ultimately develop a patent application.



■ Simulation Runs ■ Web Visits



nanoFET Lab

3 AFM Manufacturers:

- Training / Virtual Instrument
- Research



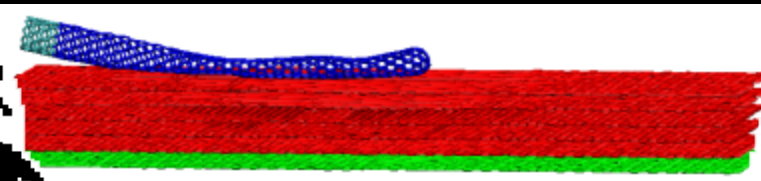
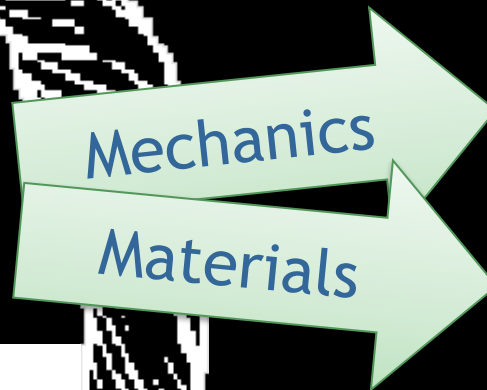
Mechanics



I have been using VEDA ...
... found it to be extremely useful. ...
... enabled us to make better choices in designing new probes.
... used VEDA as a check on other calculations.

Roger Proksch
Asylum Research

New Partnership



Virtual Atomistic
Tip and Surface

Fund tool development

Molecular Dynamics
(virtual surfaces)



VEDA
(Virtual AFM)

Community Building Professional Development

Device Size

nano-scale
structures

Transistors

Billions of nano
structures

Years

Tools
Researchers
Publications

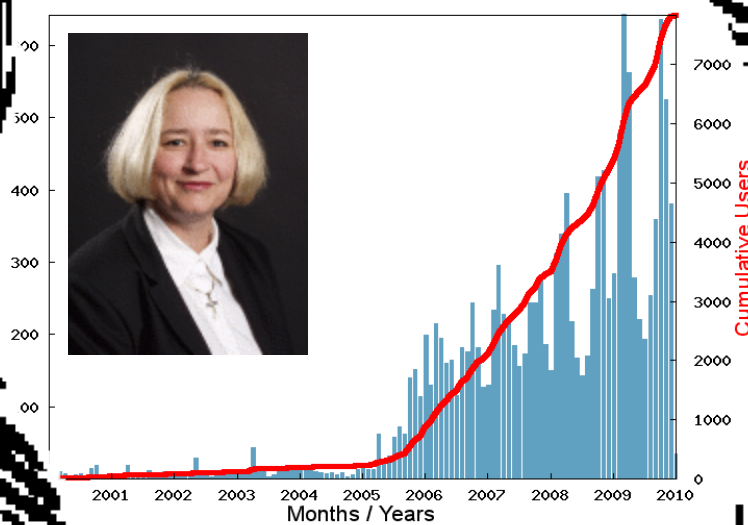


Next Generation Publications Research Incentives

Tool Usage \gg reading papers

Dragica Vasileska

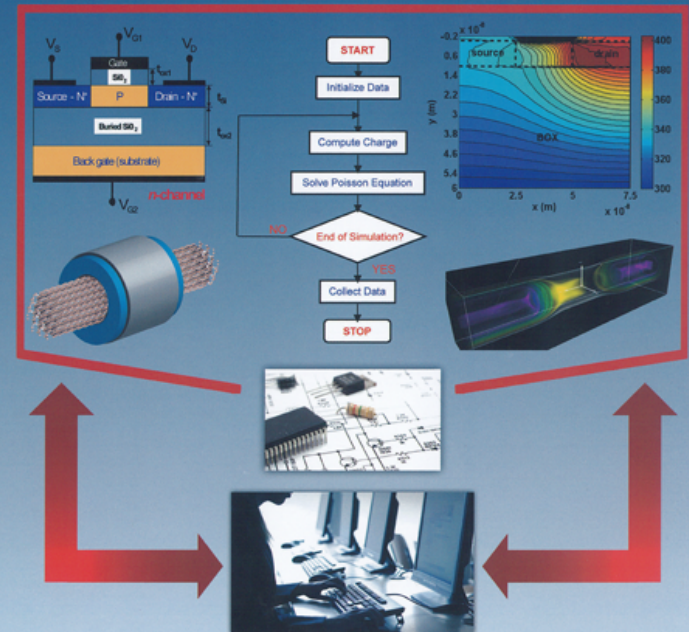
Users of Simulation Tools Authored by Dragica Vasileska (7,835 Users)



17 tools
 \rightarrow 7,835 users
 \rightarrow 115 citations

Computational Electronics

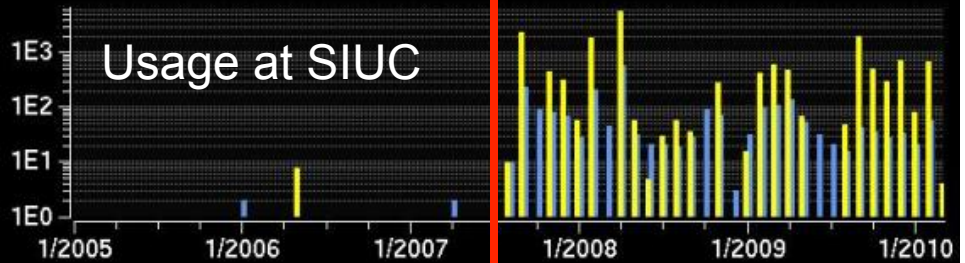
Semiclassical and Quantum
Device Modeling and Simulation



Dragica Vasileska · Stephen M. Goodnick · Gerhard Klimeck

Next Generation Faculty:

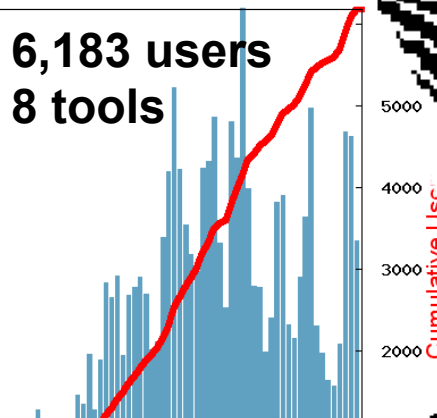
Shaikh Ahmed



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



6,183 users
8 tools



Post Doc
at Purdue

Faculty at
SIUC

- Infused nanoHUB into existing classes
- Built a new 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.

Glafkos Galanos
Chair, Dept. of Electr. and Comp. Eng, SIUC

nanoHUB on iTunes U



Nov 2009 start

350 content items today

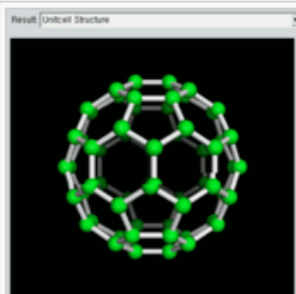
55,000 downloads

~10,000 downloads/month

Wikipedia Contributions

ਨੈਨੋਤਕਨੀਕ **Punjabi**

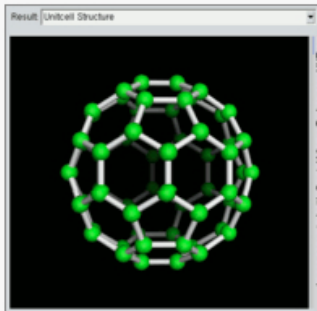
ਨੈਨੋਤਕਨੀਕ ਜਾਂ ਨੈਨੋਪ੍ਰੋਦਯੋਗਿਕੀ, ਵਿਵਹਾਰਕ ਸੀਮਾ ਦੇ ਅੰਦਰ ਵੈੱਬ ਨੈੱਟਵਰਕ ਦੇ ਰੂਪ ਵਿੱਚ ਡੇ ਅਣੂਆਂ ਦੇ ਗੈਰ ਕੋਵਲੈਂਟ ਪ੍ਰਭਾਵ ਤੇ ਕੇਂਦਰਤ ਹੈ। ਇਨ੍ਹਾਂ ਦਿਸ਼ਾਵਾਂ ਵਿੱਚ ਖੋਜ ਦੇ ਕੀ ਨਤੀਜੇ ਹੋਣਗੇ। C₆₀, ਜਿਨੂੰ ਬਕਿਬਾਲ ਵੀ ਕਹਿੰਦੇ ਹਨ, ਜੋ ਕਾ



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 spe parte di queste molecole sono isolanti quando superano la l conduttivo, in particolare la grafite (recuperata dal carbone) è un semi-metallo, una categoria compresa fra metalli e ser atomo. Fra ogni foglio, le interazioni sono abbastanza debo



Veduta ruotante di cristallo C₆₀ di Fullerene Buckminster.

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

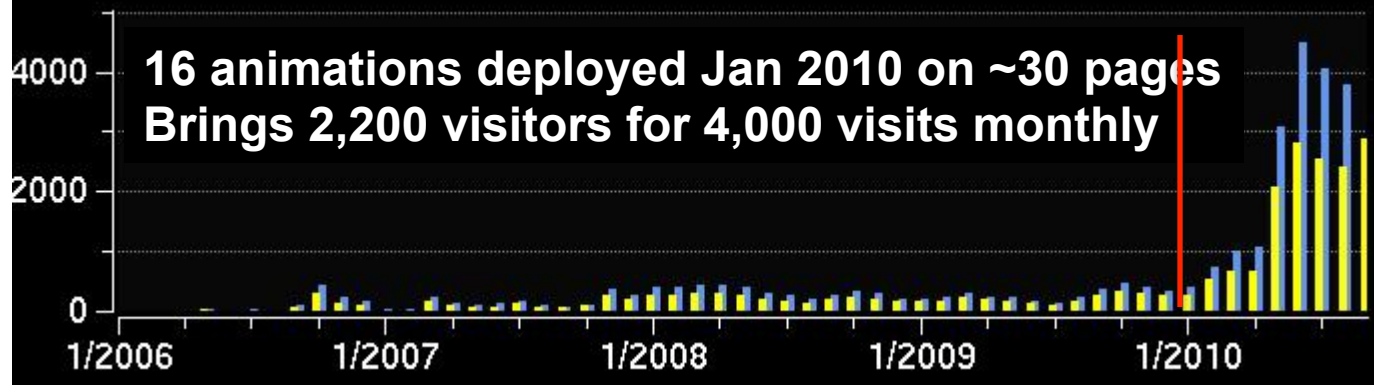
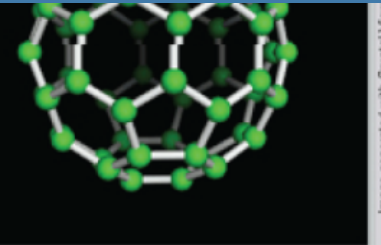
Geschichte [Bearbeiten]



rotierende Struktur von C₆₀



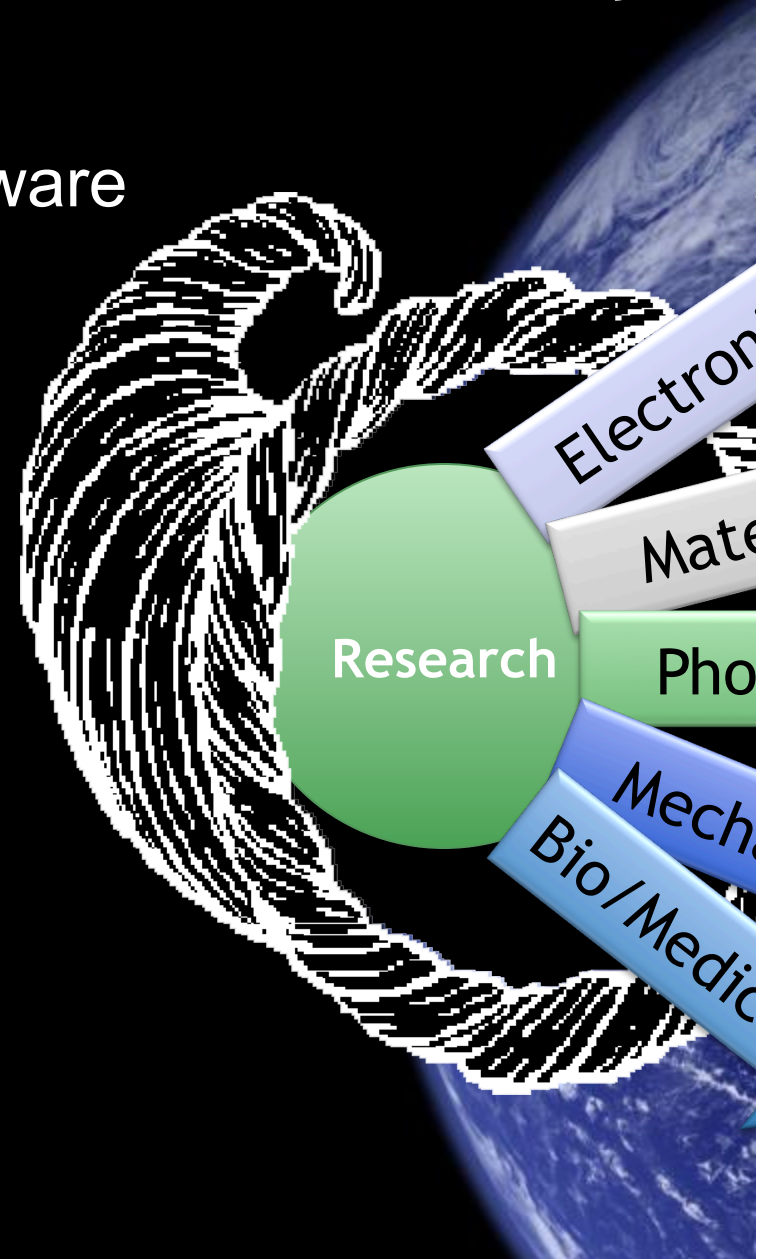
Nanotubi di carbonio **German**

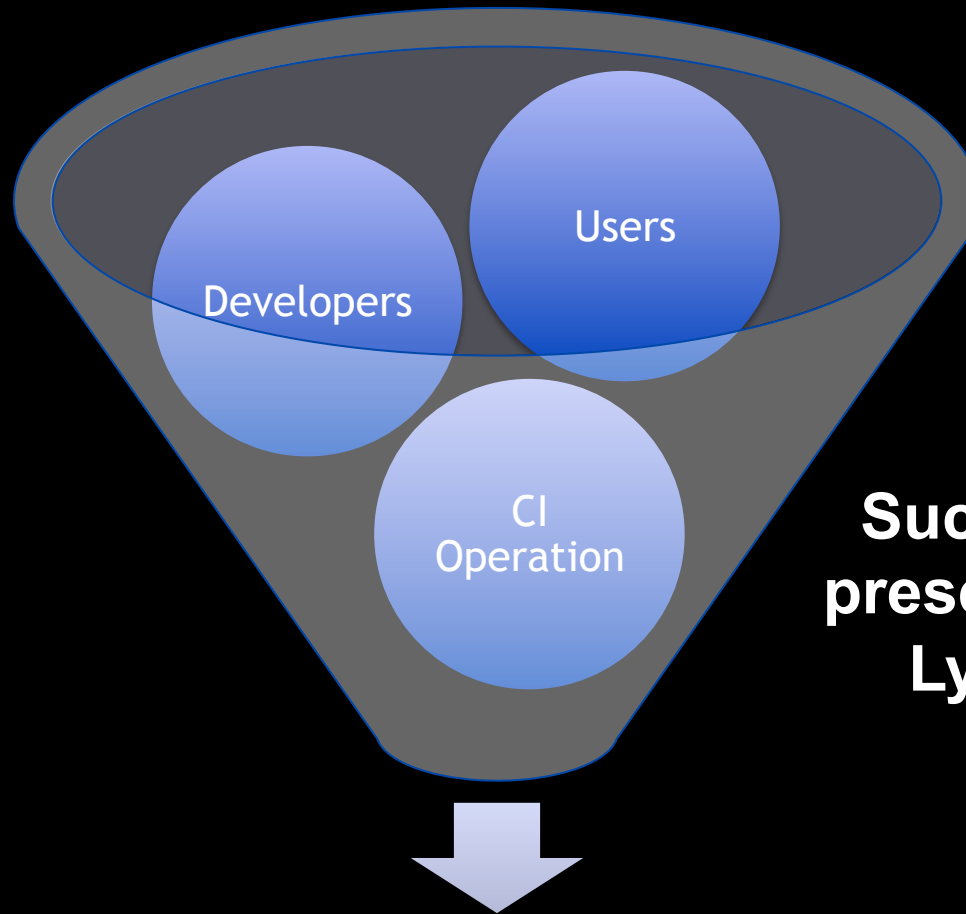
rotating view of Buckminster fullerene

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Requirements



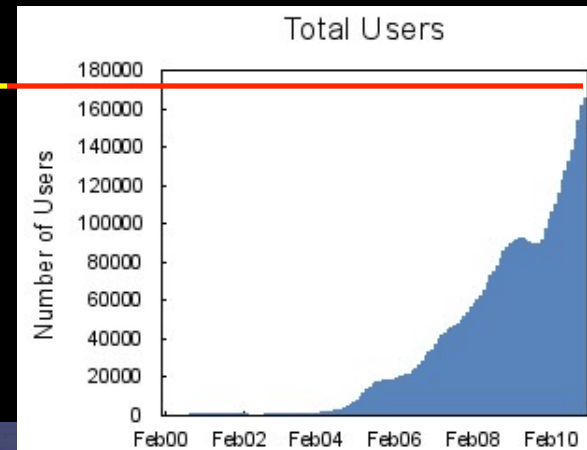
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