Mythbusting Scientific Knowledge Transfer with nanoHUB.org

Gerhard Klimeck, Purdue University, gekco@purdue.edu

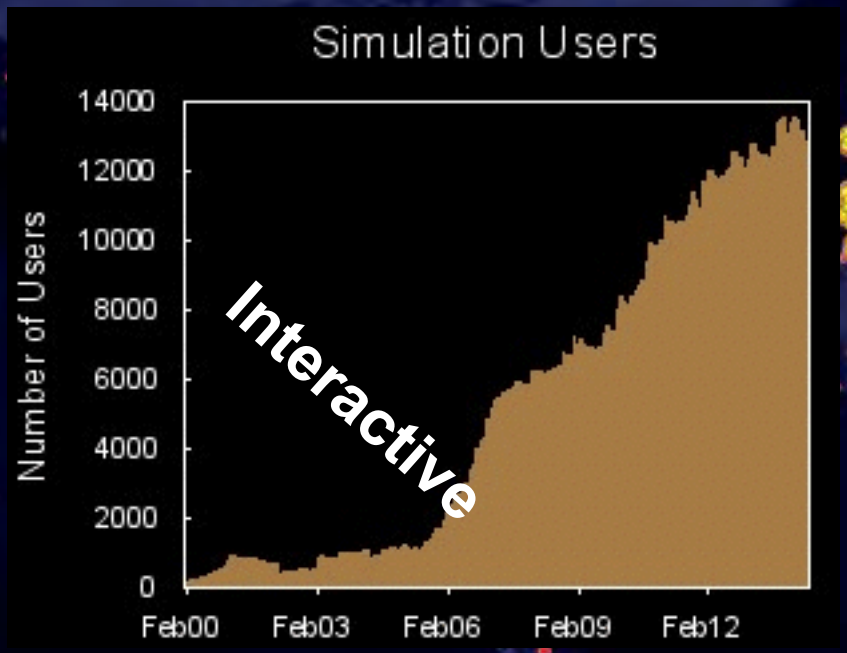
PURDUE UNIVERSITY

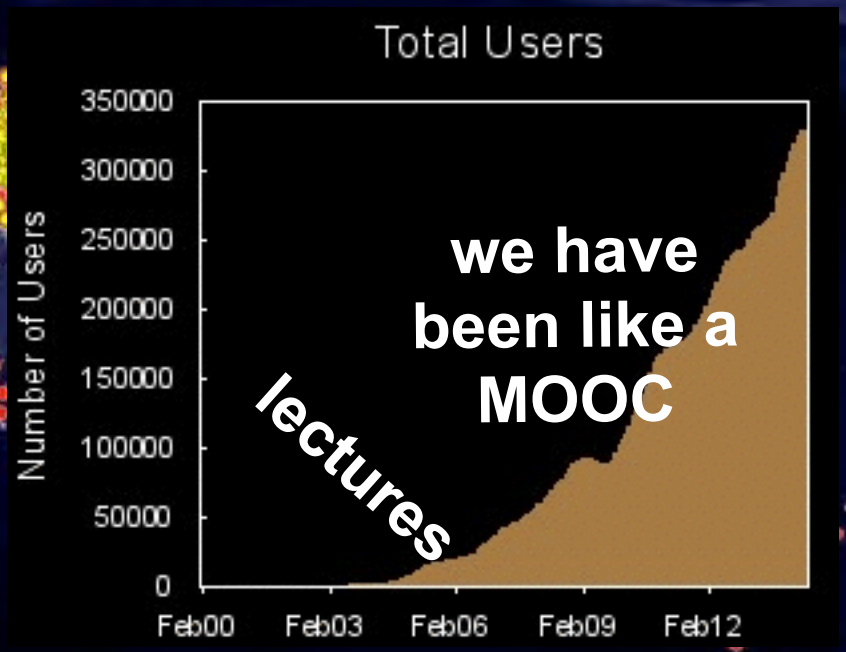
Documenting with Real Data

Research<=>Education, Collaborative, Global Impact

The Essence of a Research University

Gerhard Klimeck, Purdue University, gekco@purdue.edu



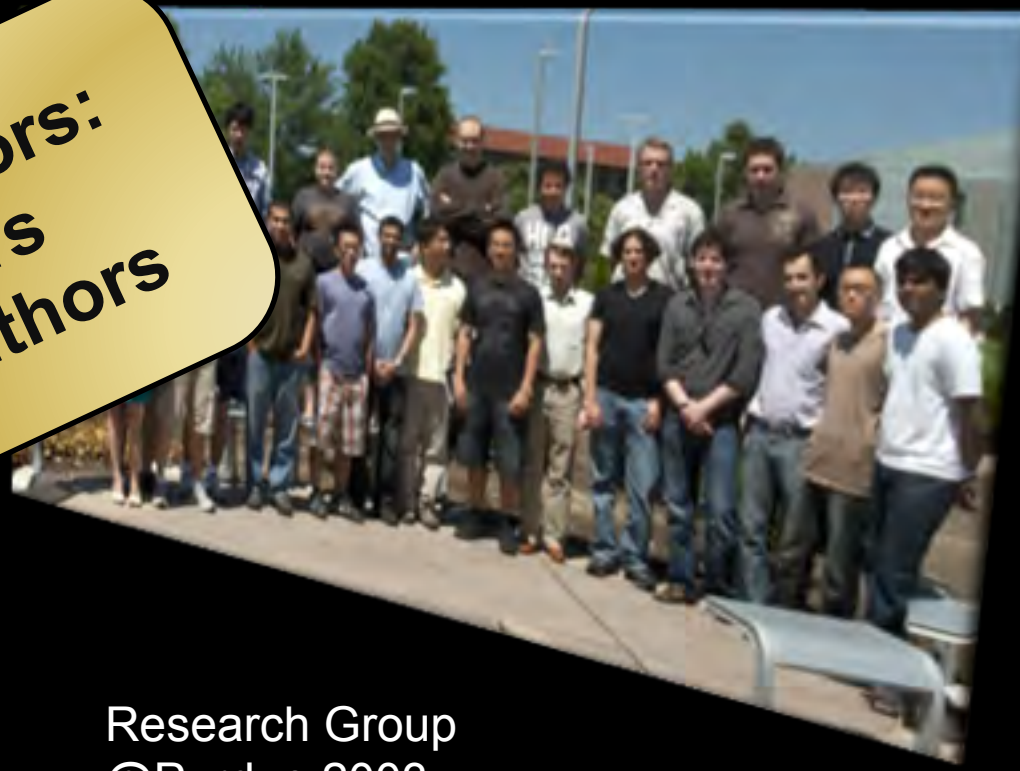


Over 13,000 / 330,000 Users Annually

PURDUE UNIVERSITY

Thanks to

nanoHUB contributors:
380+ tool authors
1,080+ content authors

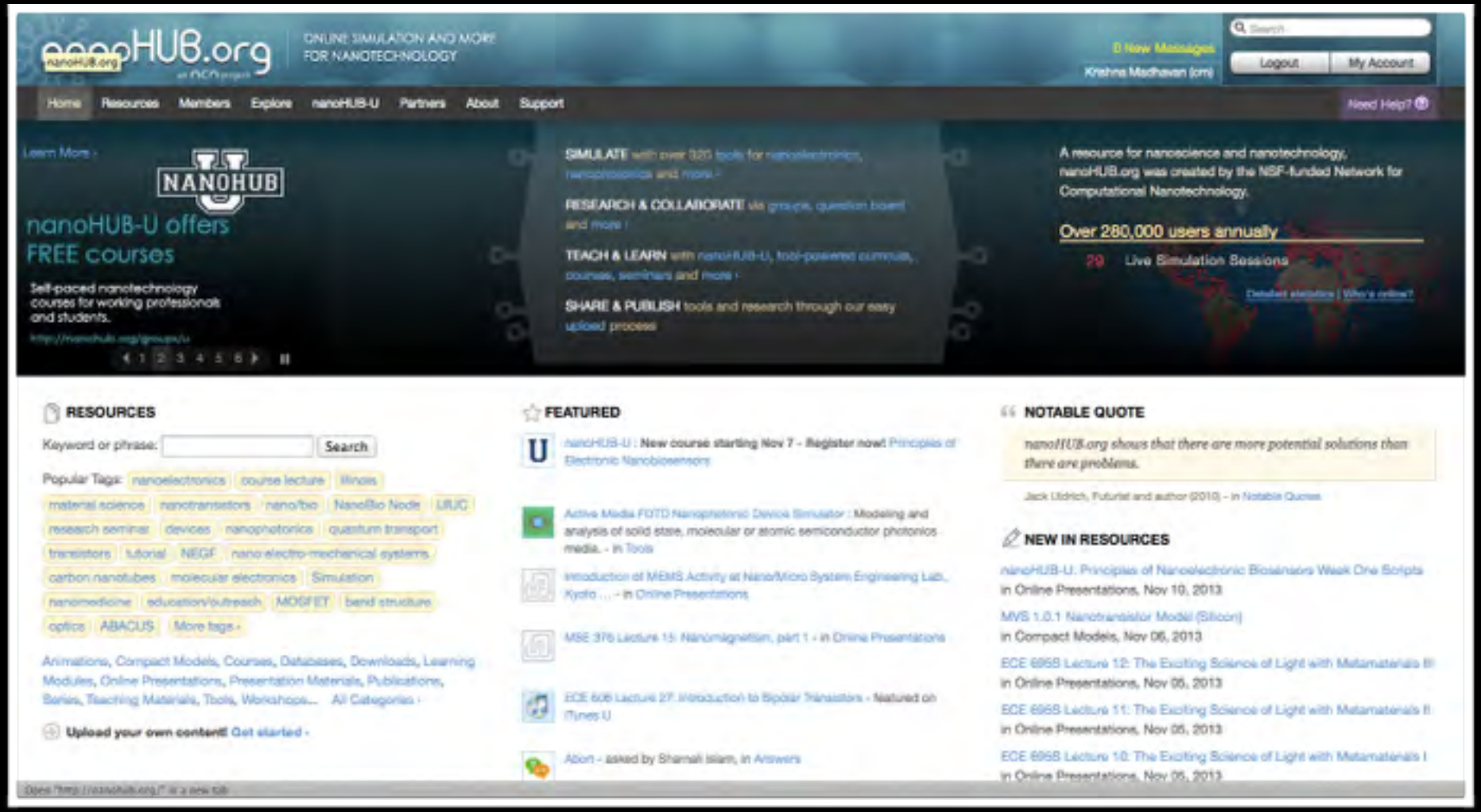


Research Group
@Purdue 2003-....
@NASA JPL 1998-2003
@Texas Instruments 1994-1998

nanoHUB and HUBzero Team

nanoHUB

more than a web site

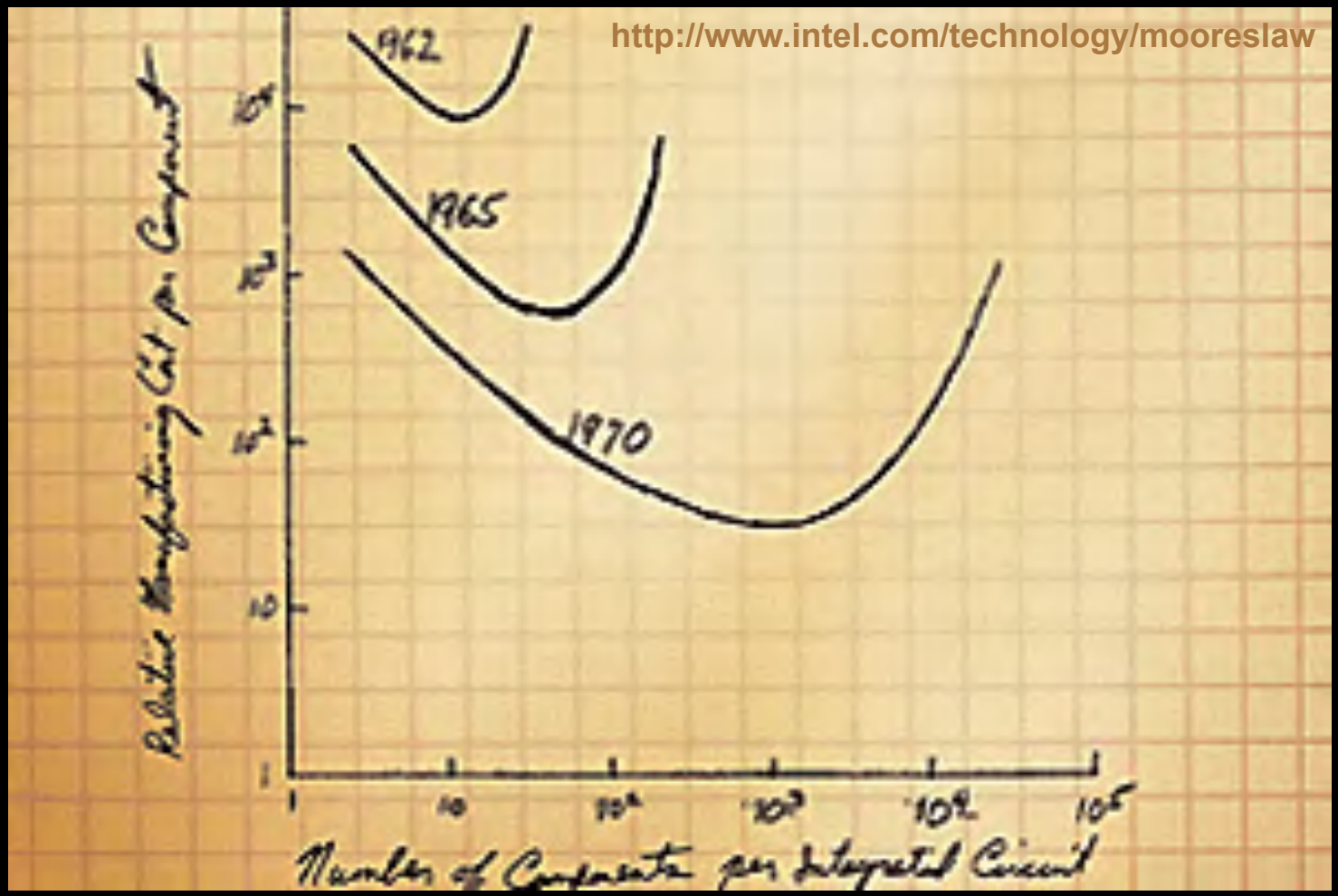


It’s FREE !!!

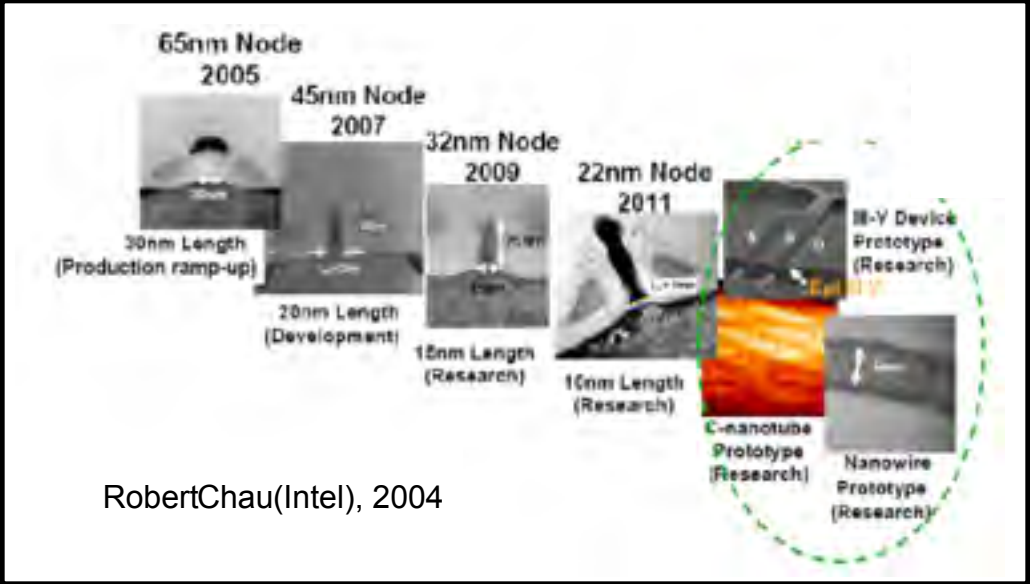
Yes, really !!!

Users do not pay anything!

1965
Gordon Moore



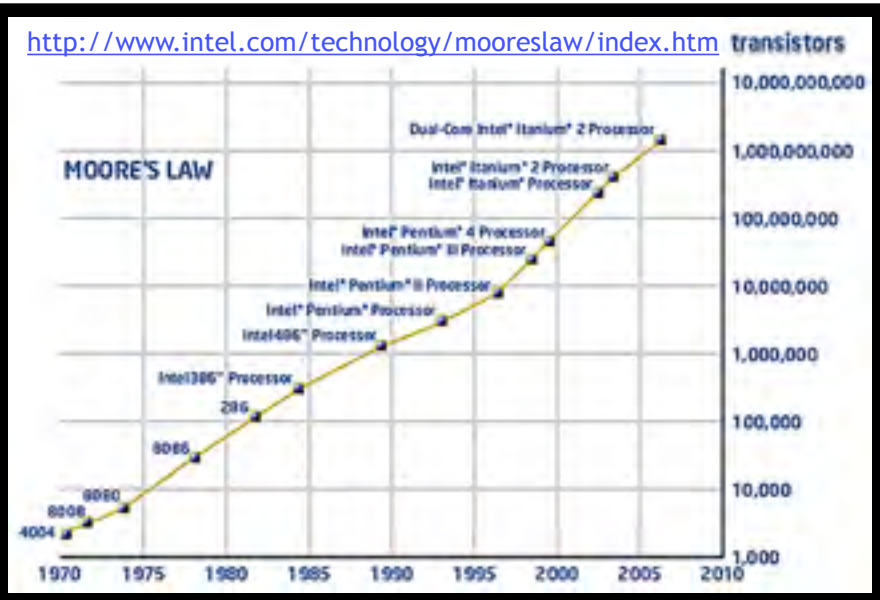
Moore's Law



RobertChau(Intel), 2004

Device Size:
Tens of nanometers

Stanford SUPREM



Device Integration:
>2 Billion

Berkeley SPICE

Berkeley

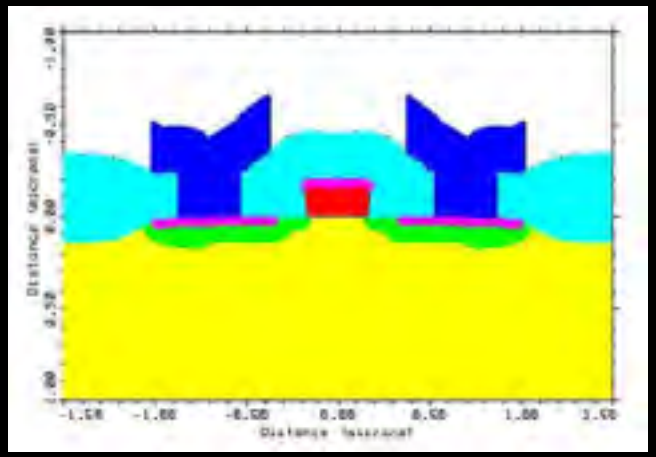
Simulation Program with Integrated Circuit Emphasis.

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

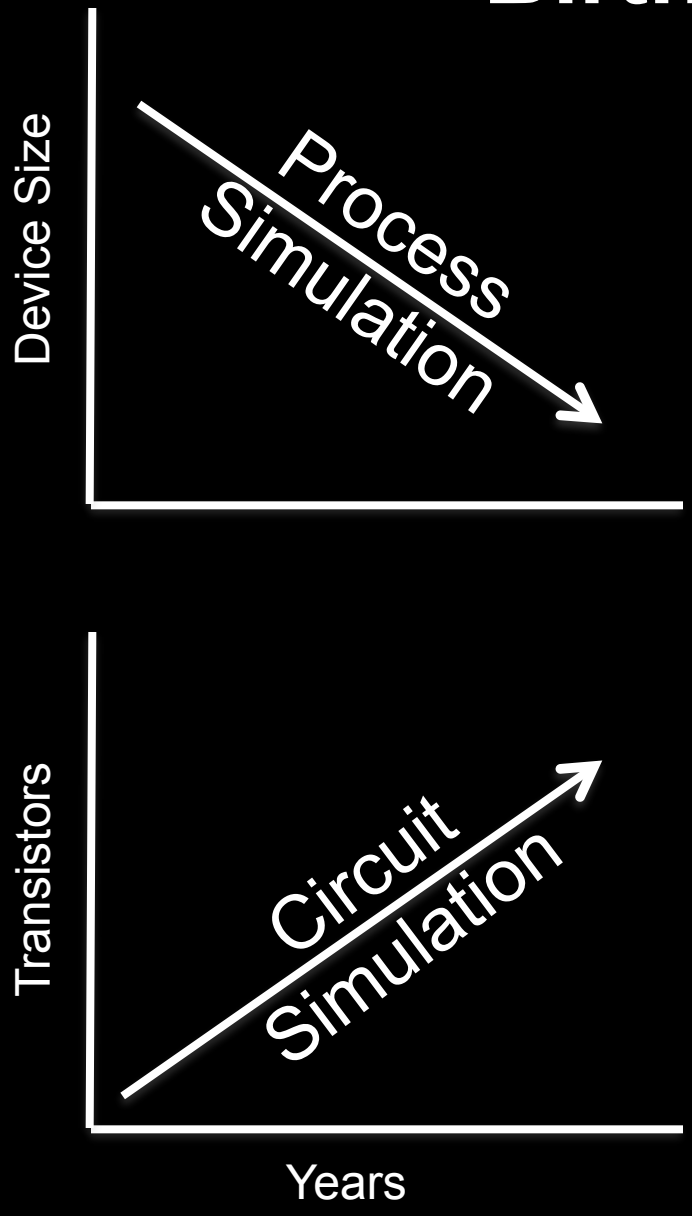
- Released 1972

Stanford
Stanford University PRocEss Modeling



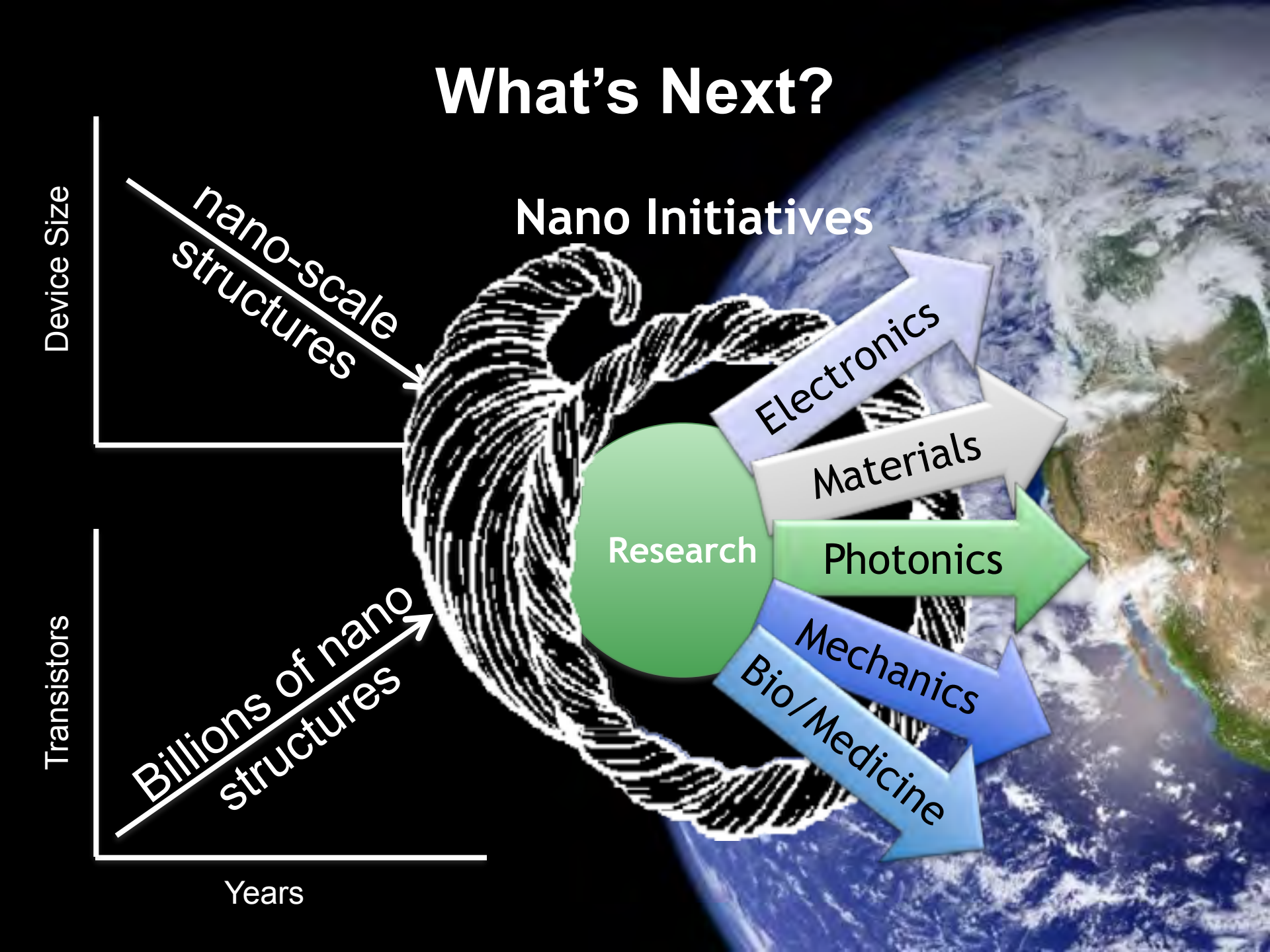
- Stanford wanted to mimic Berkeley success
- Combine various existing models
- Dissemination:
  - Public domain code
  - Community workshops
  - Students took it along to industry and academia

Birth of an Industy

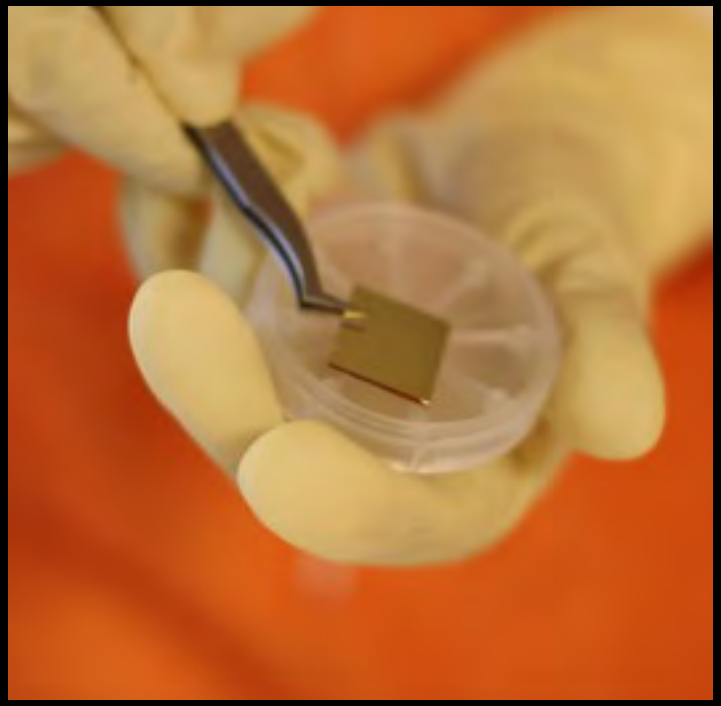


Intel Capitalization:
$85B
Total Industry:
$280B

What's Next?

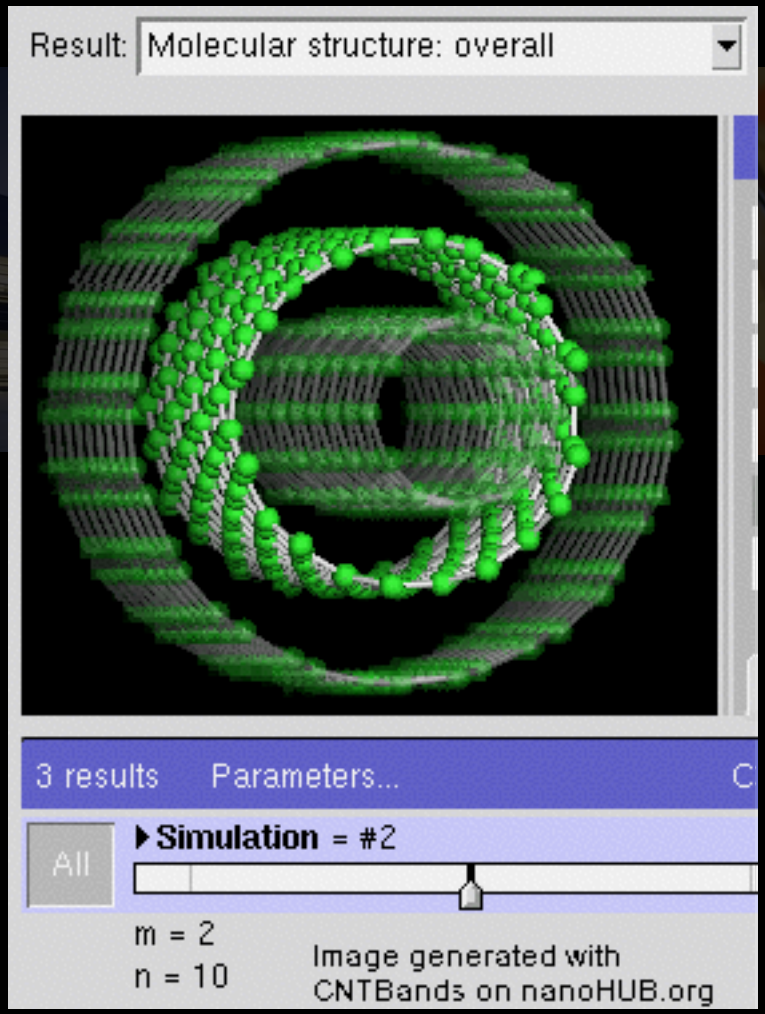

Device Size
nano-scale structures
Transistors
Billions of nano structures
Years
Nano Initiatives
Research
Electronics
Materials
Photonics
Mechanics
Bio/Medicine

Nanotechnology

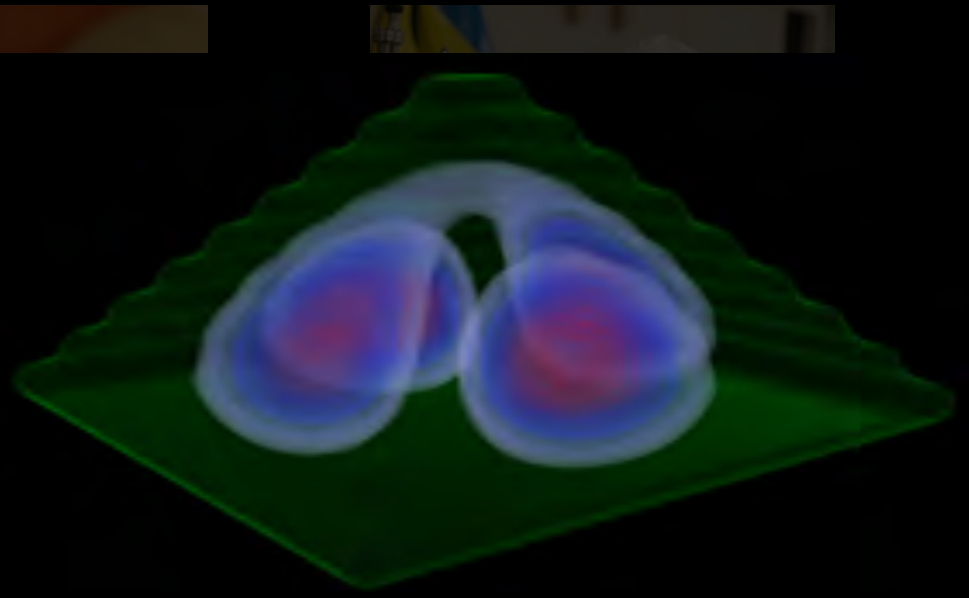


Extensive Facilities

Nano Models

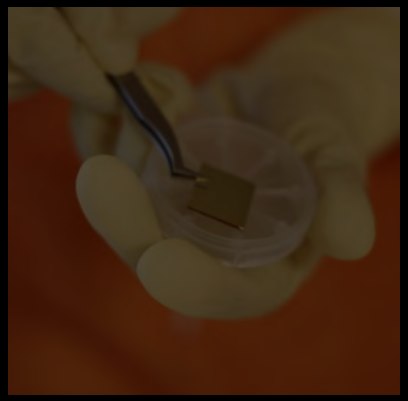


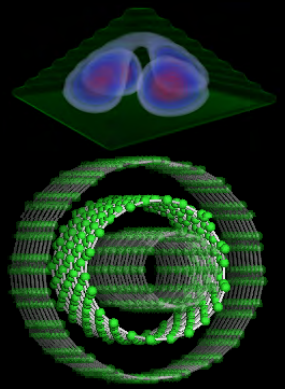
Carbon Nanotubes



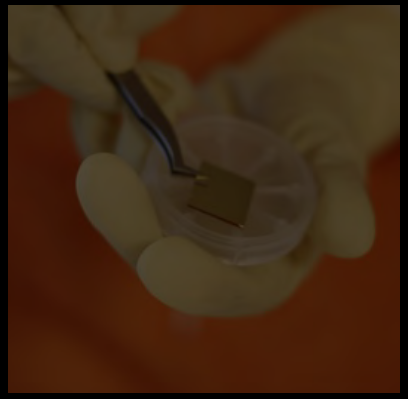
Quantum Dots
Artificial Atoms

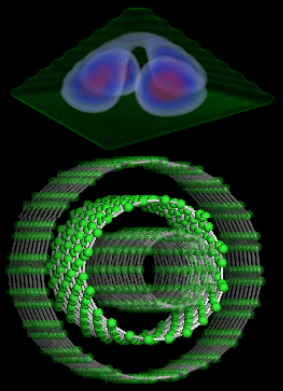
Computational Nano



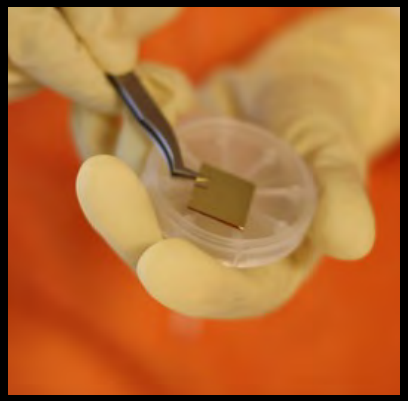


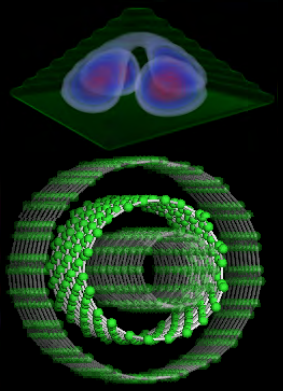
Computational Nano



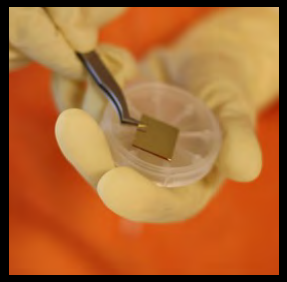


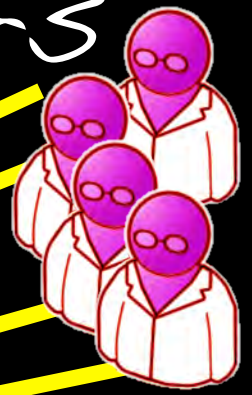
Different Worlds

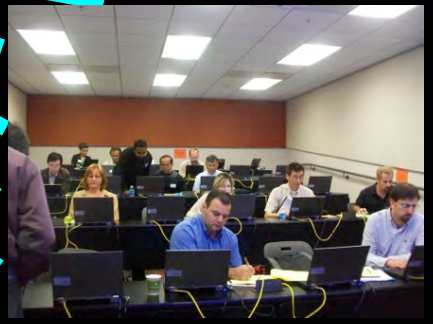




Imagine Breaking Barriers





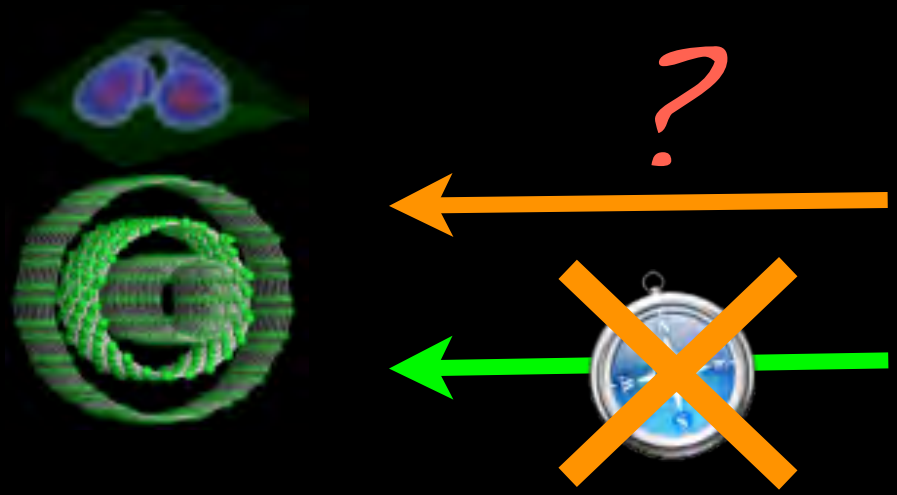


Easy use

No Install

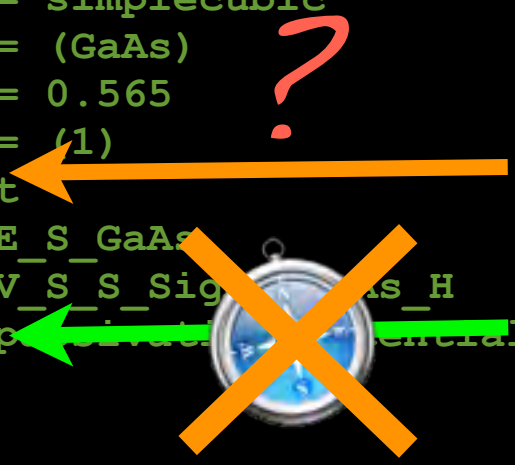
Any Browser

Why is this so hard?



Most research codes
are written by one user
for one user

```
Structure
{
    Material
    {
        name                    = GaAs
        tag                     = substrate
        crystal_structure       = simplecubic
        atoms                   = (GaAs)
        Lattice:a_lattice       = 0.565
        regions                 = (1)
        Bands:TB:s:param_set                          = nanohub
        Bands:TB:s:nanohub:E_S_GaAs                   = 12.1307935176
        Bands:TB:s:nanohub:V_S_S_Sig                  = -20
        Bands:TB:s:nanohub:p                          = 125
    }
    Domain
    {
        name                    = structure1
        type                    = pseudomorphic
        base_material           = substrate
        dimension               = (18.0,19.0,9.0)
        periodic                = (false, false, false)
        crystal_direction1      = (1,0,0)
        crystal_direction2      = (0,1,0)
        crystal_direction3      = (0,0,1)
        space_orientation_dir1  =  (1,0,0)
        space_orientation_dir2  =  (0,1,0)
        regions                 = (1)
        geometry_description    = simple_shapes
    }
```



User Hostile

1 Input → 2 Simulate

About this tool
Questions?

Number of States: 7

Surface passivation: yes

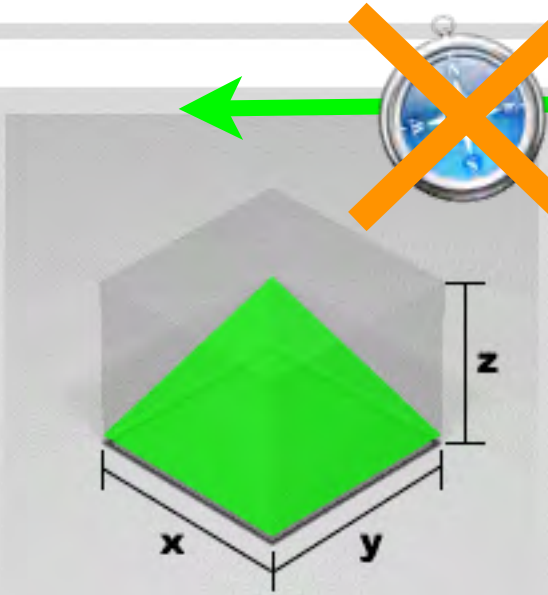
Device Structure | Light Source

Geometry: Pyramid

X dimensions: 10nm

Y dimensions: 10.5nm

Z dimensions: 5nm

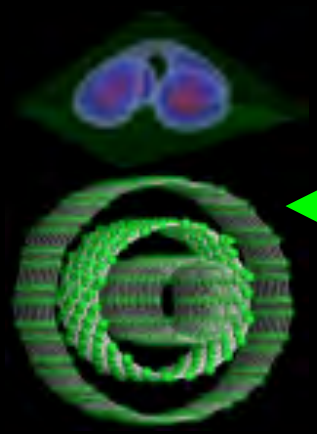


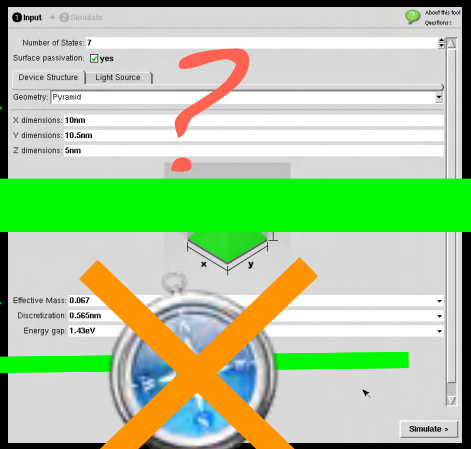
Effective Mass: 0.067

Discretization: 0.565nm

Energy gap: 1.43eV

Why is this so hard?





Most research codes

Accessible (no installation)

are written by one user

Developer Friendly

for one user

HUBzero

Rappture

User Friendly

Emerged Myths

User Friendly

Cannot use research codes for education

Must write own code to do research

Experimentalists cannot use research codes

Accessible (no installation)

NO End-to-end Science Cloud Possible

Developer Friendly

Building User Interfaces too Difficult

Must rewrite code for web deployment

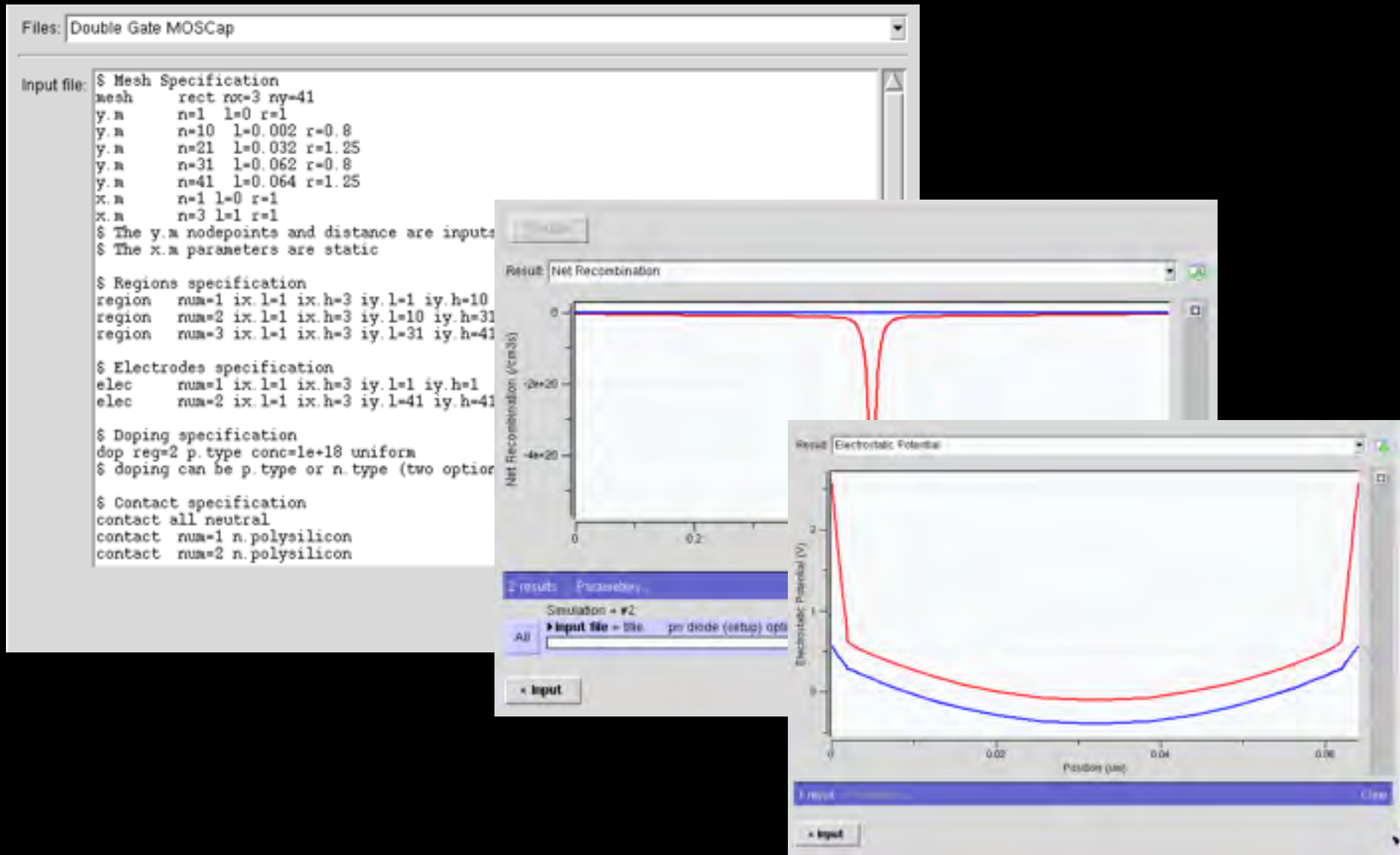
There is no incentive to share codes

Customers

Market

Suppliers

Step in the right direction: PADRE Industrial Tool – Bell Labs

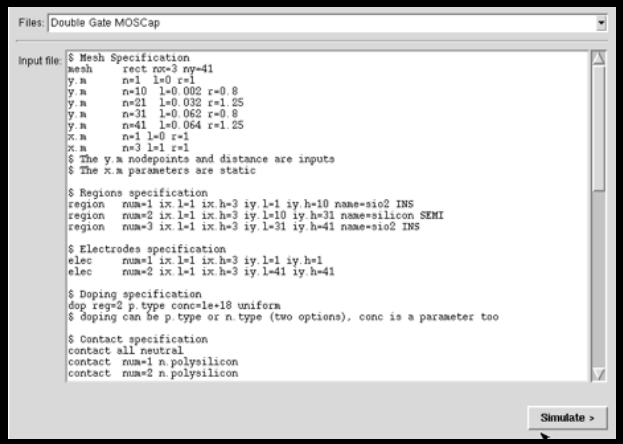


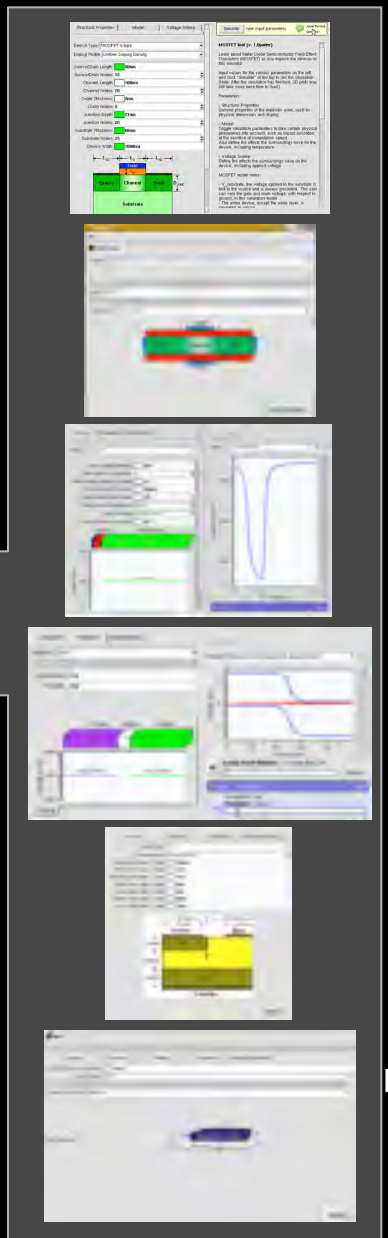
MOSFET: Running PADRE Simply

Impact of Simplified GUI Tools

945 Users,
41,285 jobs

6,649 Users,
104,282 jobs





MOSFET:
2,715 Users,
38,000 jobs

MUGfet:
240 Users,
3,600 jobs

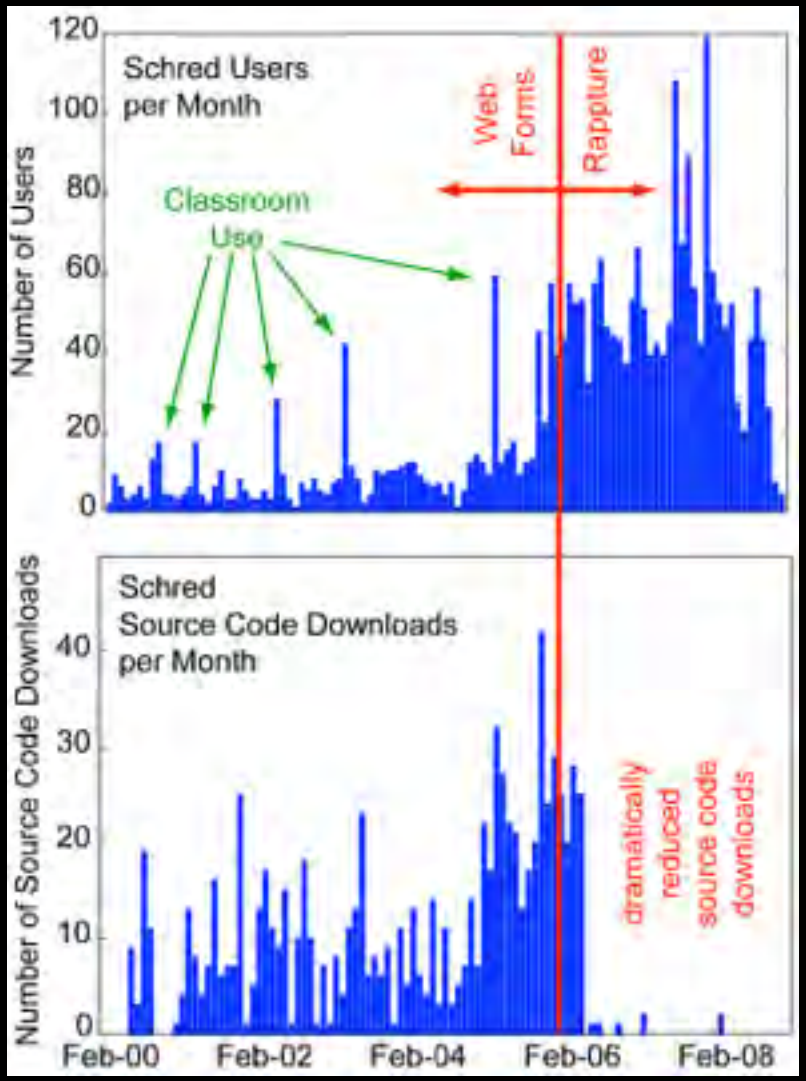
MOSCAP:
1,694 Users,
18,000 jobs

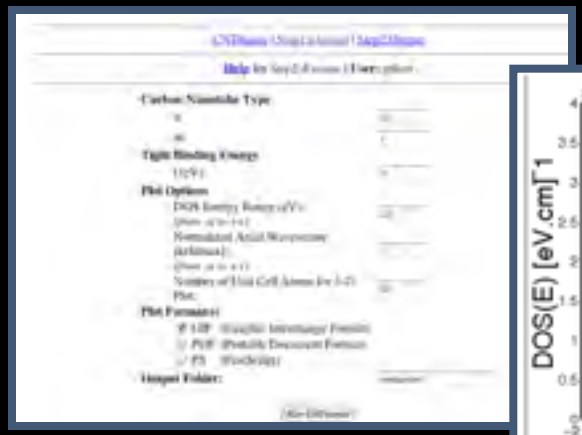
PN junction:
3,563 Users,
33,000 jobs

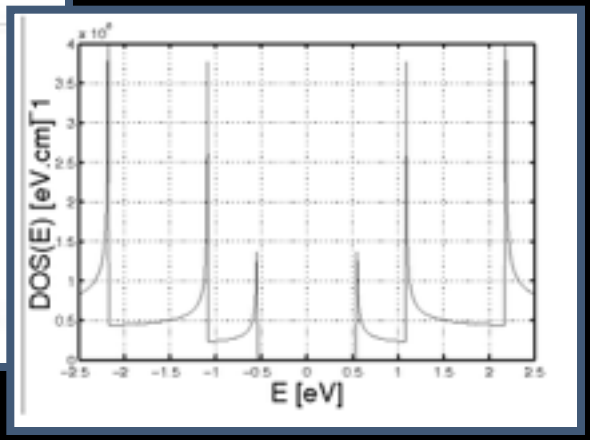
BJT:
557 Users,
3,000 jobs

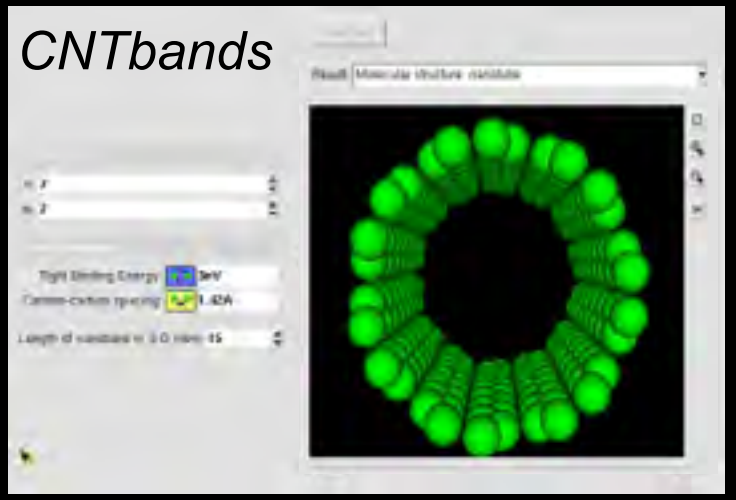
Drift-Diffusion:
721 Users,
7,400 jobs

Importance of a good GUI



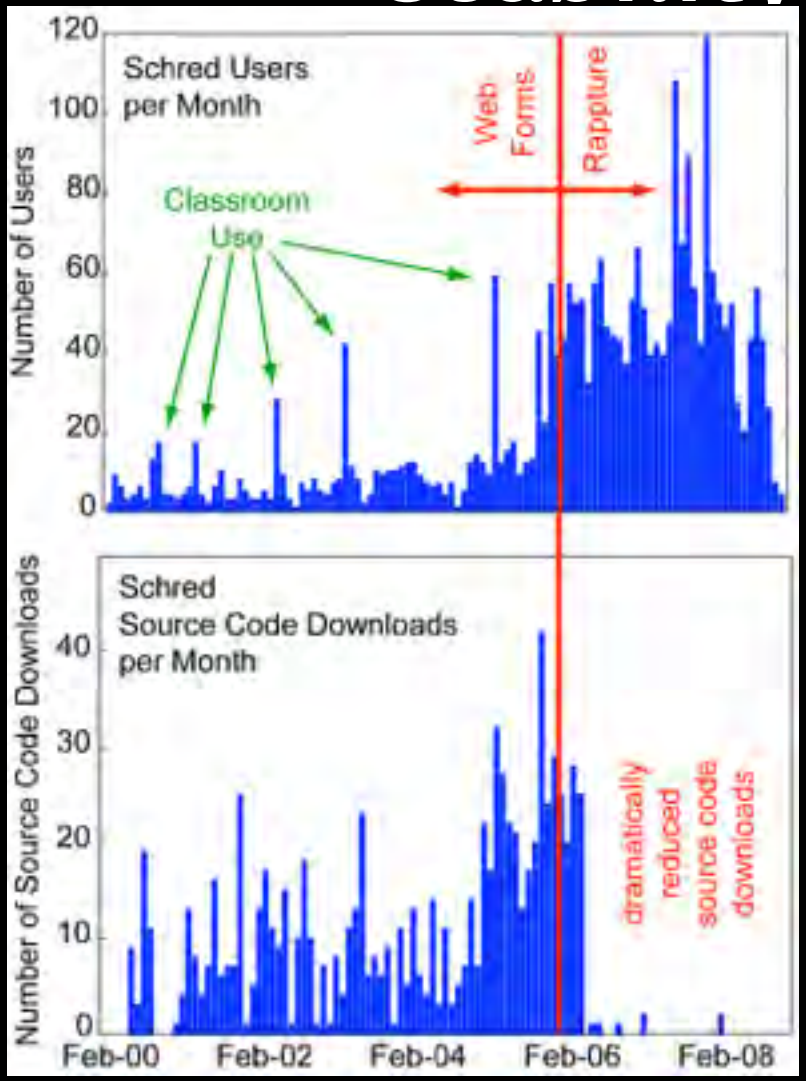






Same behavior across all similar converted tools

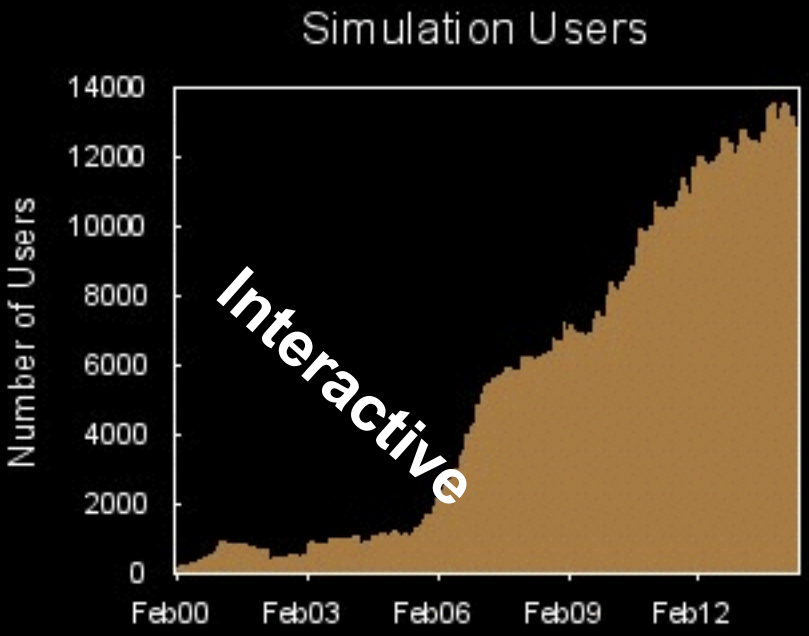
Balancing Usability and Capability



nanoHUB

iPhone / iPad

Balancing Usability and Capability

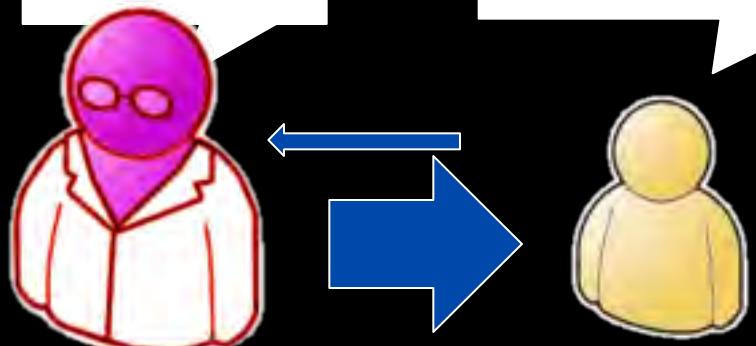


nanoHUB

iPhone / iPad

What else is different? Developer Experience?

Usual Science Gateway Process



Researcher

Web Developer

- **175 tools / 4 years: => $8M**
- $500k/tool
- NO new research!
- Not validated by researcher (disowned)
- Researcher has much better version
- Code rewrite takes 2-3 years

Many Proposals read alike

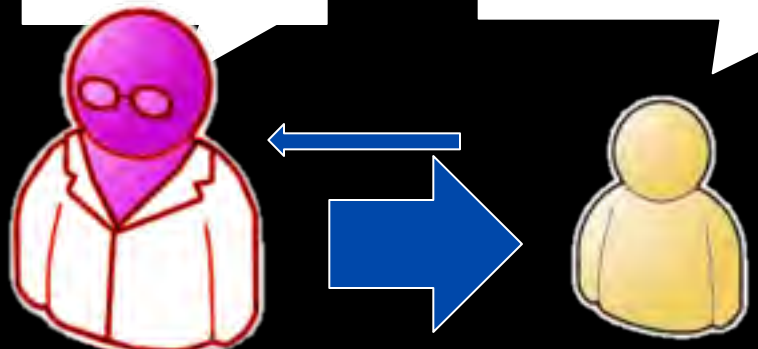
Usual Science Gateway Process

- 175 tools / 4 years:
  => ~~$8M~~
- $500k/tool

NSF

Customers / Users

- Scale back expectations
- Not research codes
- Toy applications
- Not deep research
- Maybe for education?

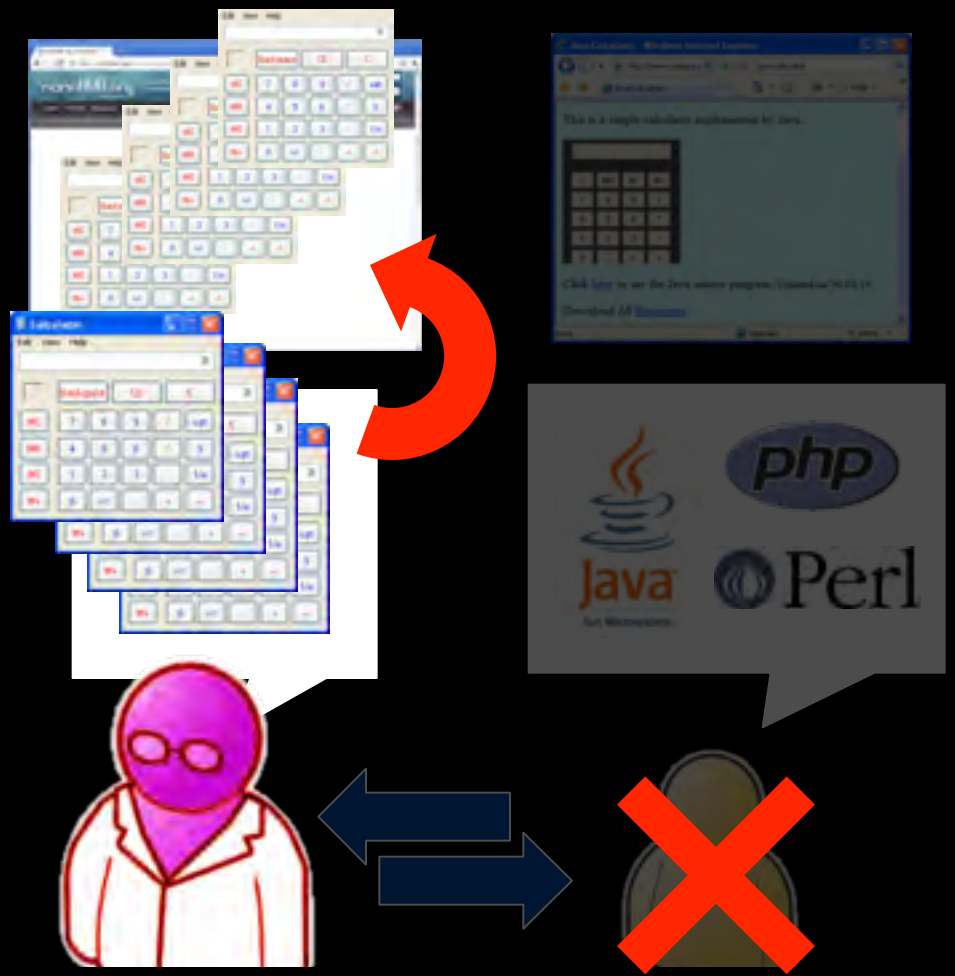


Researcher

Web Developer

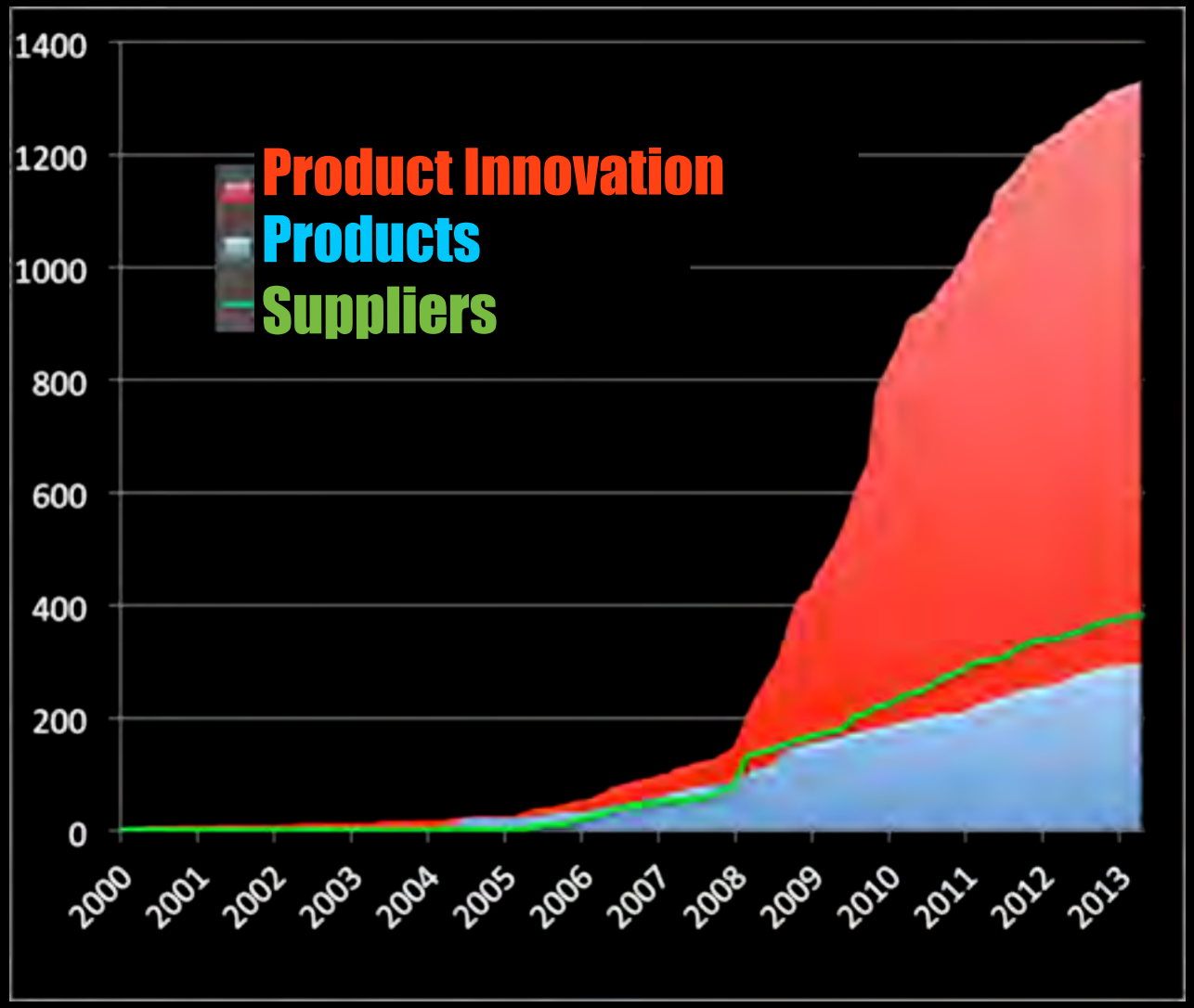
Generating a Bad Reputation

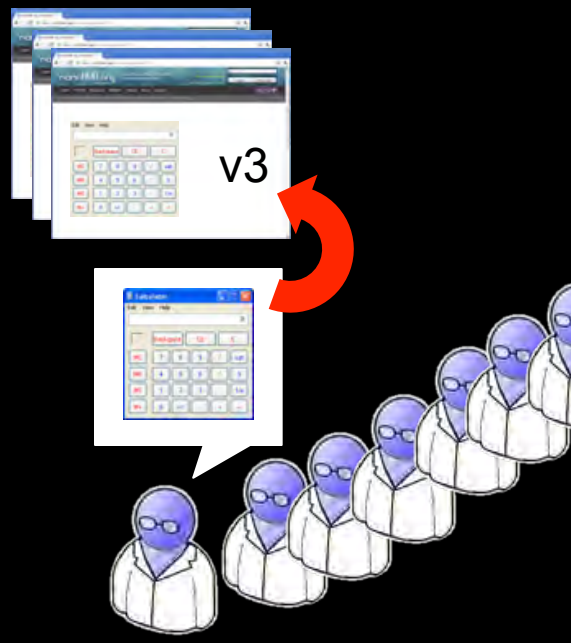
nanoHUB Process



- **175 tools / 4 years without $88M**
- Eliminate bottlenecks
  - No Middleman
  - No Rewrite
  - Retain ownership
- Rapid Deployment: 2-3 years → 1-2 weeks
- **Rappture** toolkit
- **HUBzero** Ecosystem

nanoHUB is different



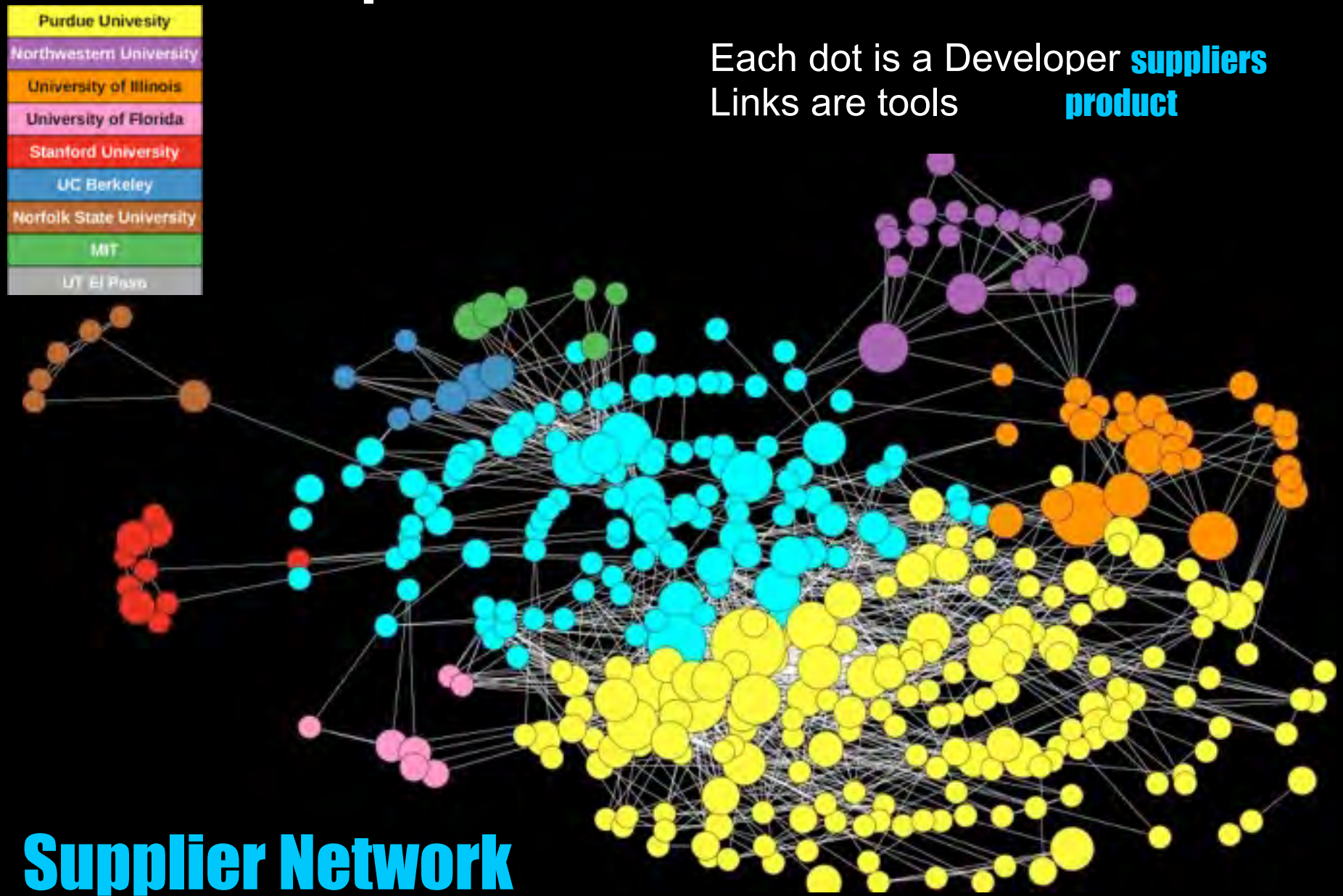


Continual Engagement

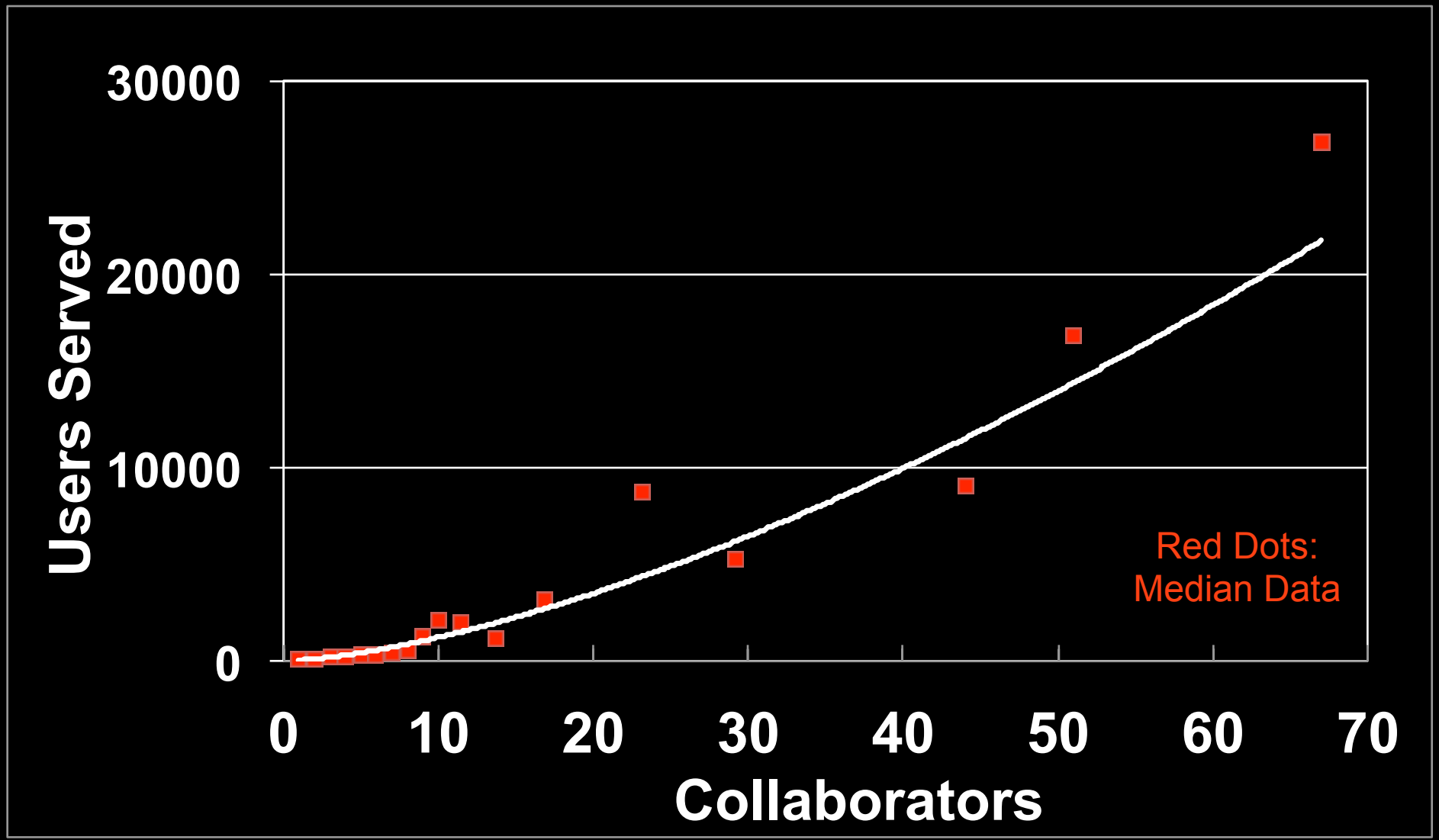
380+ Developers
NOT PAID by NCN

nanoHUB can prove it

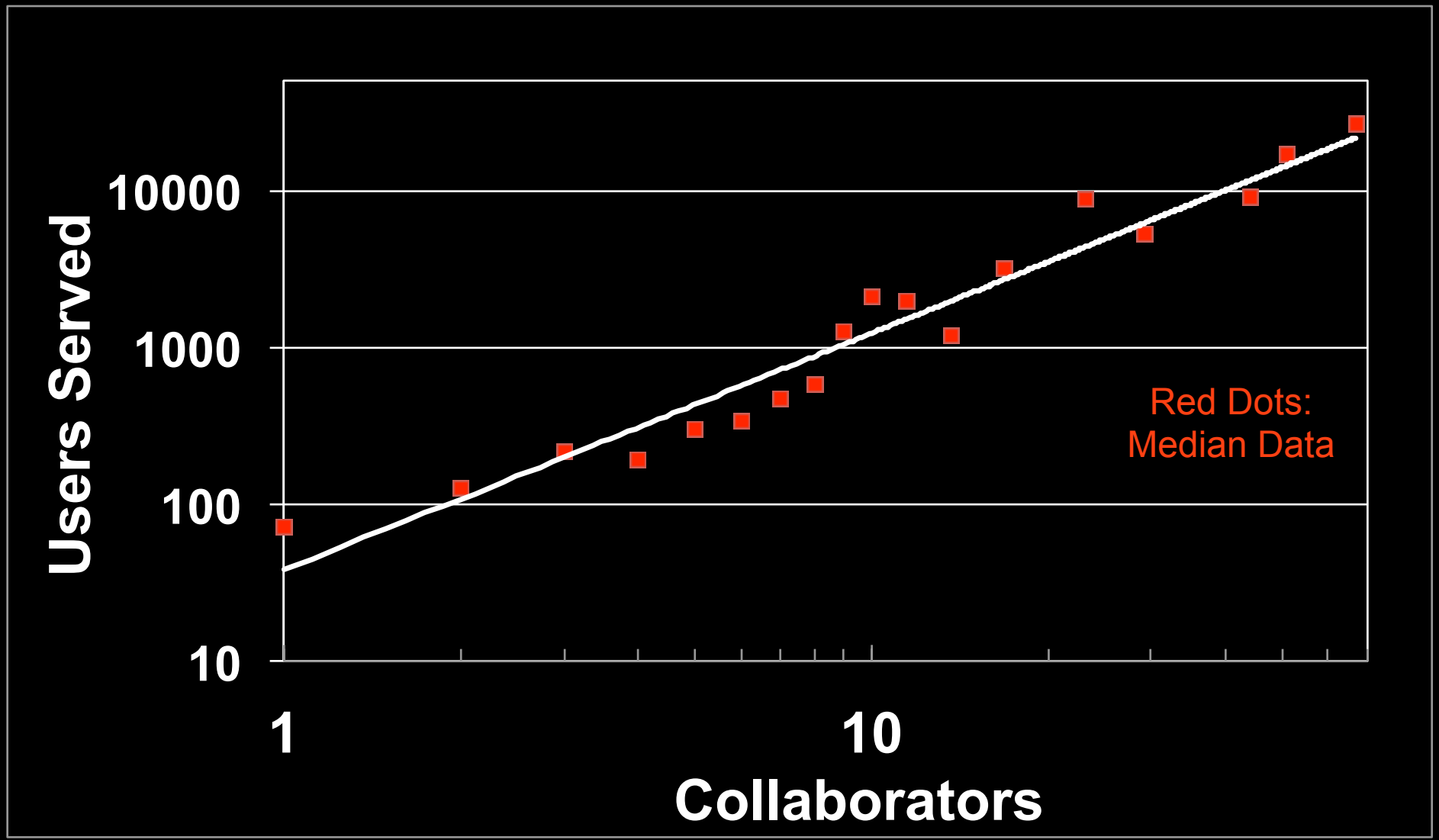
Developer Collaboration Network



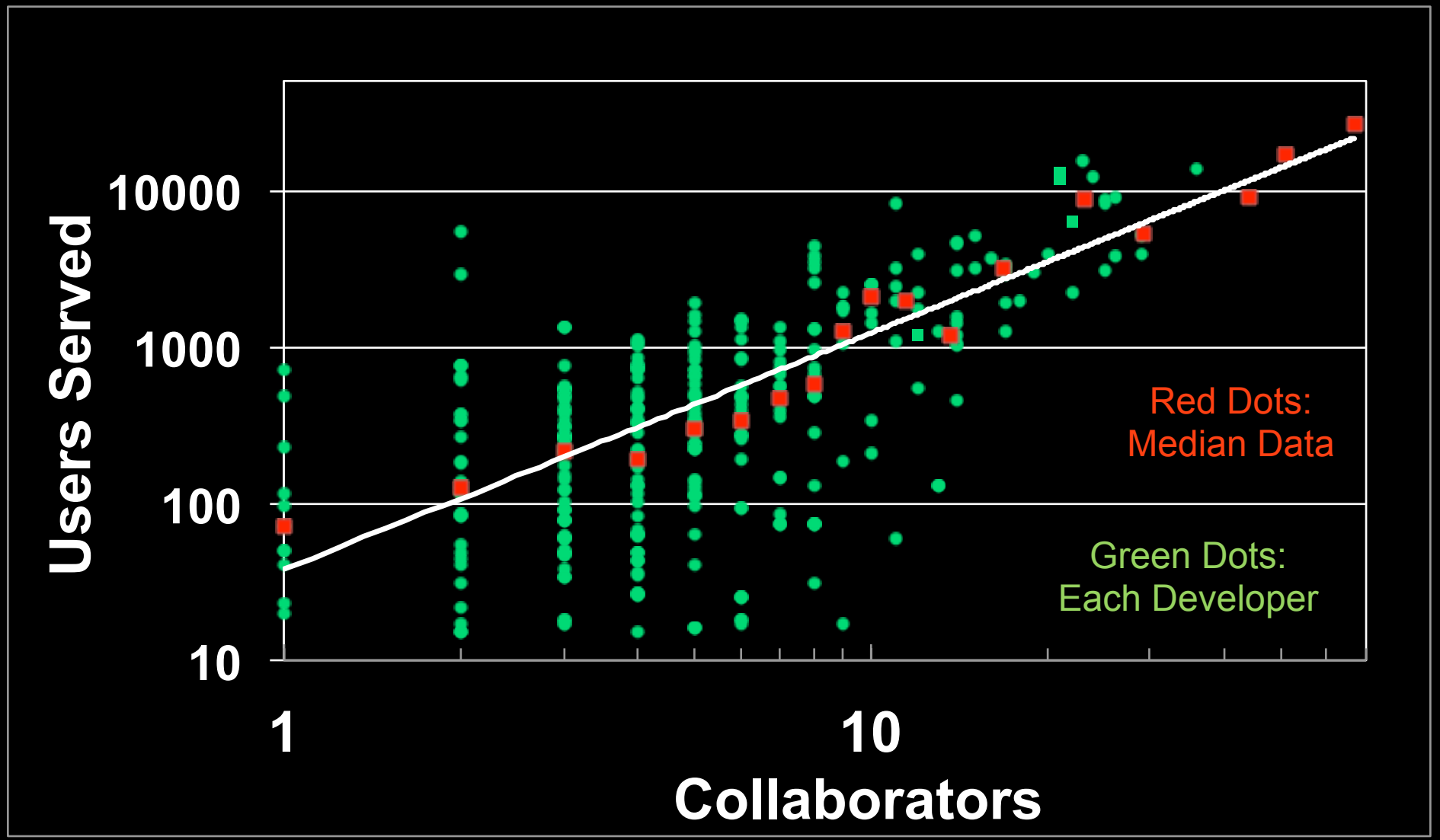
Developer Collaboration Impact



Developer Collaboration Impact

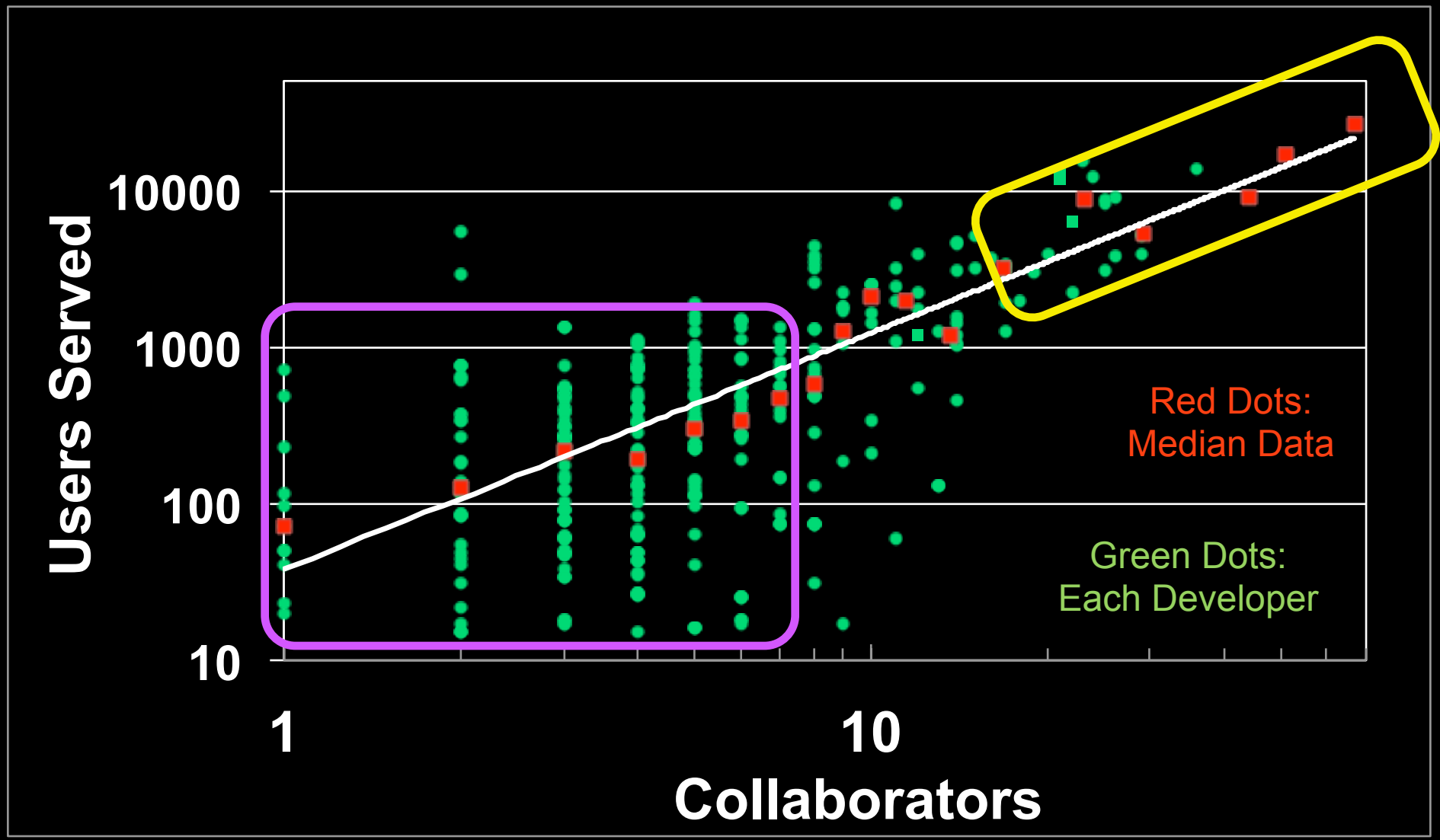


Developer Collaboration Impact



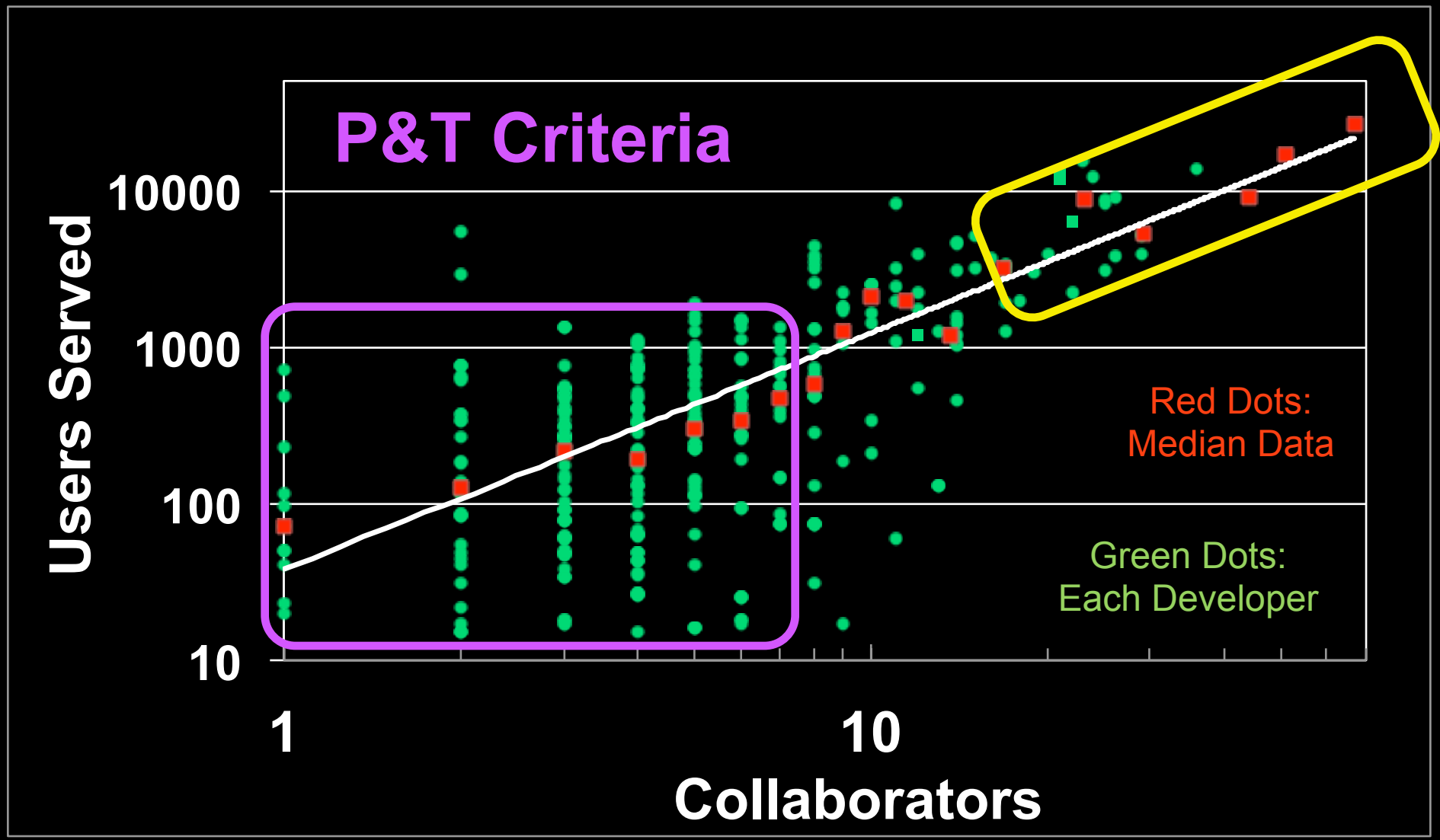
Small Collaborations: Scattered Success

Large Collaborations Predictable Success



Old Approach

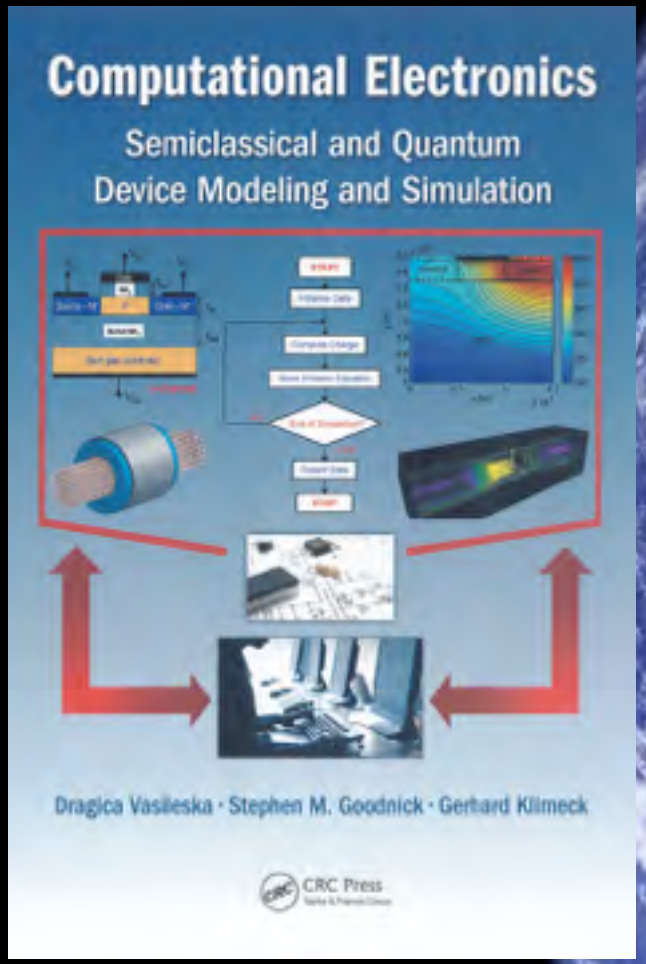
Surviving Universities



Next Generation Publications
Research Incentives

Great for Proposals
=> Proof of outreach

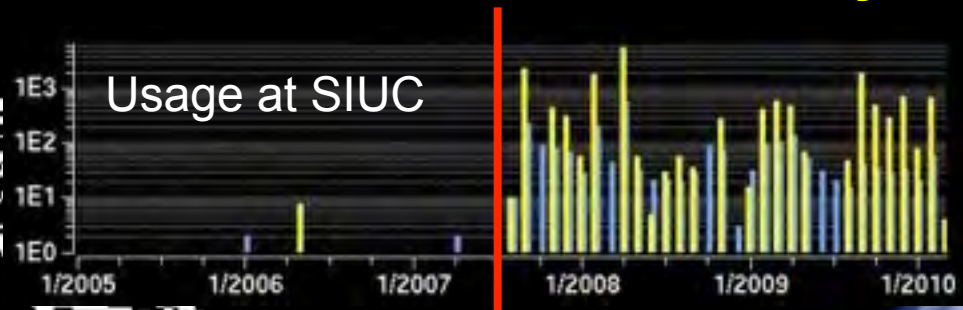
Dragica Vasileska



17 tools
➔ 11,570 users
➔ 123 citations

Next Generation Faculty:

Shaikh Ahmed



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
~10,000 downloads/month

In Good Company:
Stanford
MoMA, PBS stations
The New York Public Library,
Public Radio International,

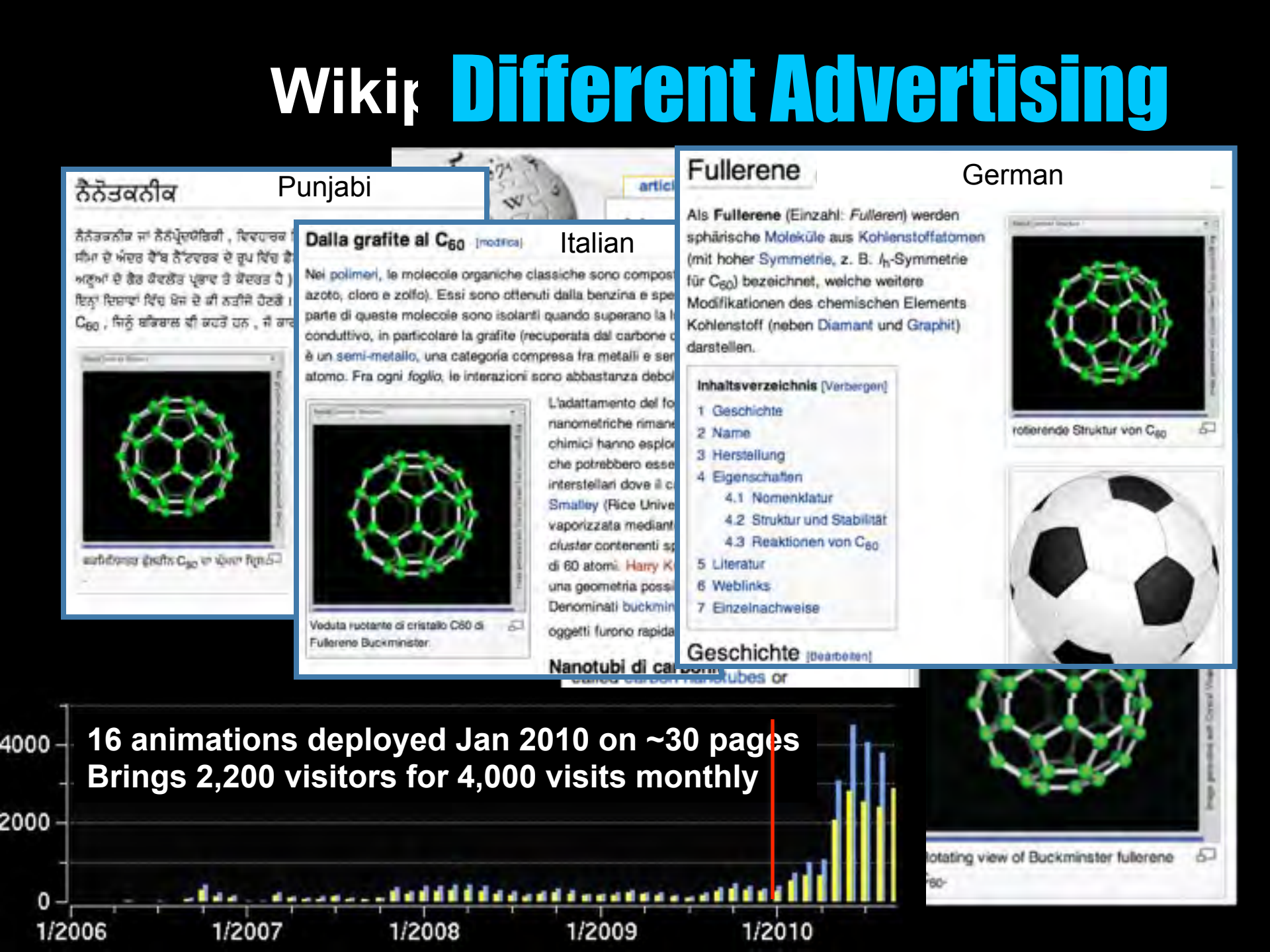
Leveraging New Markets

Wiki Different Advertising

Punjabi

Italian

German



16 animations deployed Jan 2010 on ~30 pages
Brings 2,200 visitors for 4,000 visits monthly

Suppliers

Myths Busted

User Interfaces too Difficult

Rewrite Code for Web Deployment

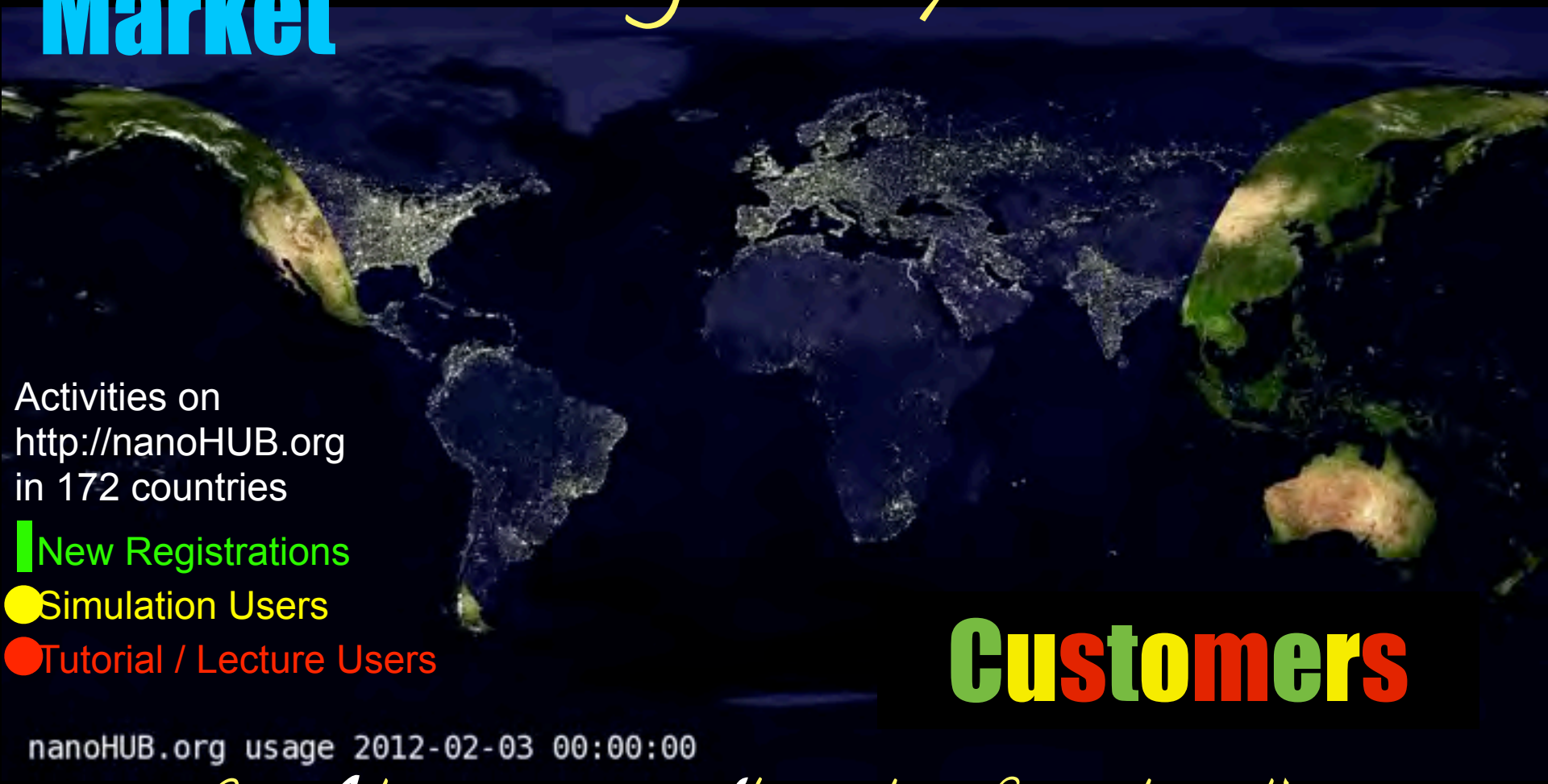
There is no incentive to share codes

HUBzero

Rappture

Emerged Myths

Market



Customers

Cannot use research codes for education

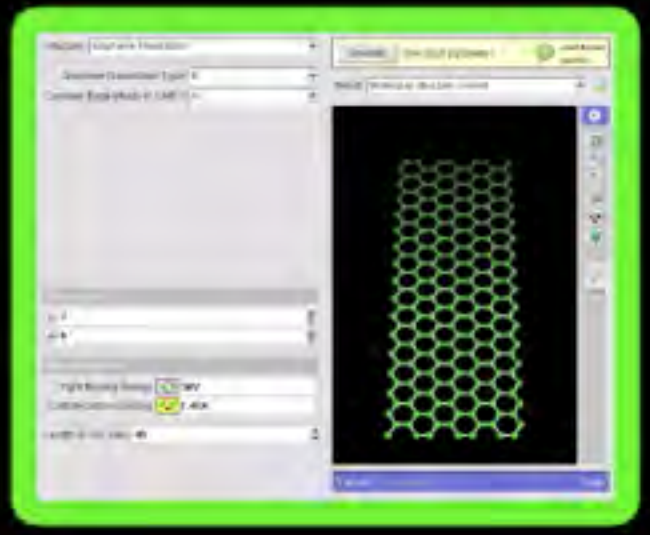
ACCeSSible (no installation)

Must write own code to do research

NO End-to-end Science Cloud Possible

Experimentalists cannot use research codes

User Behavior Analysis

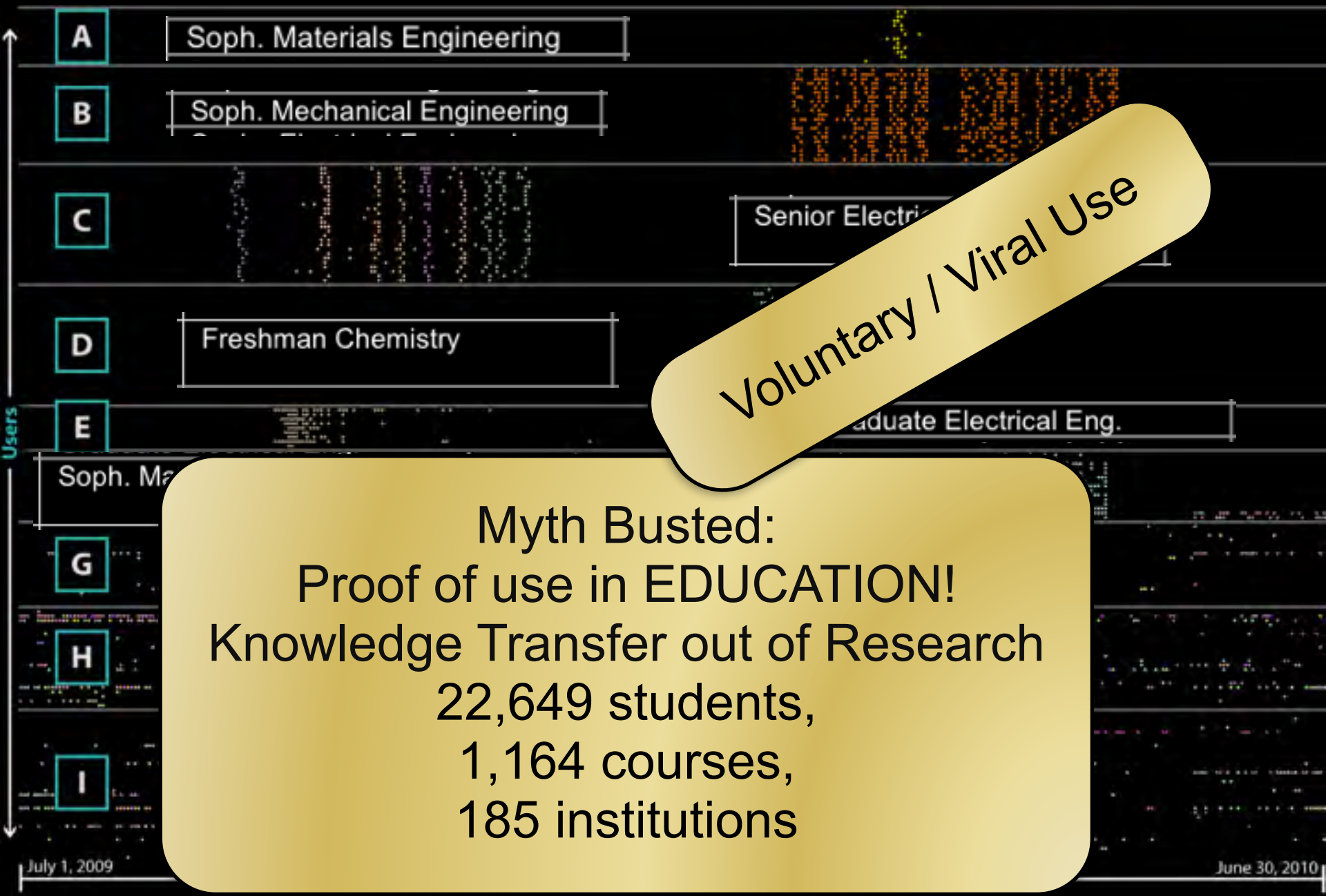


Users

Time (days)


nanoHub User Behavior
Users
Time (days)
2010-06-30
6 users
1 days of history

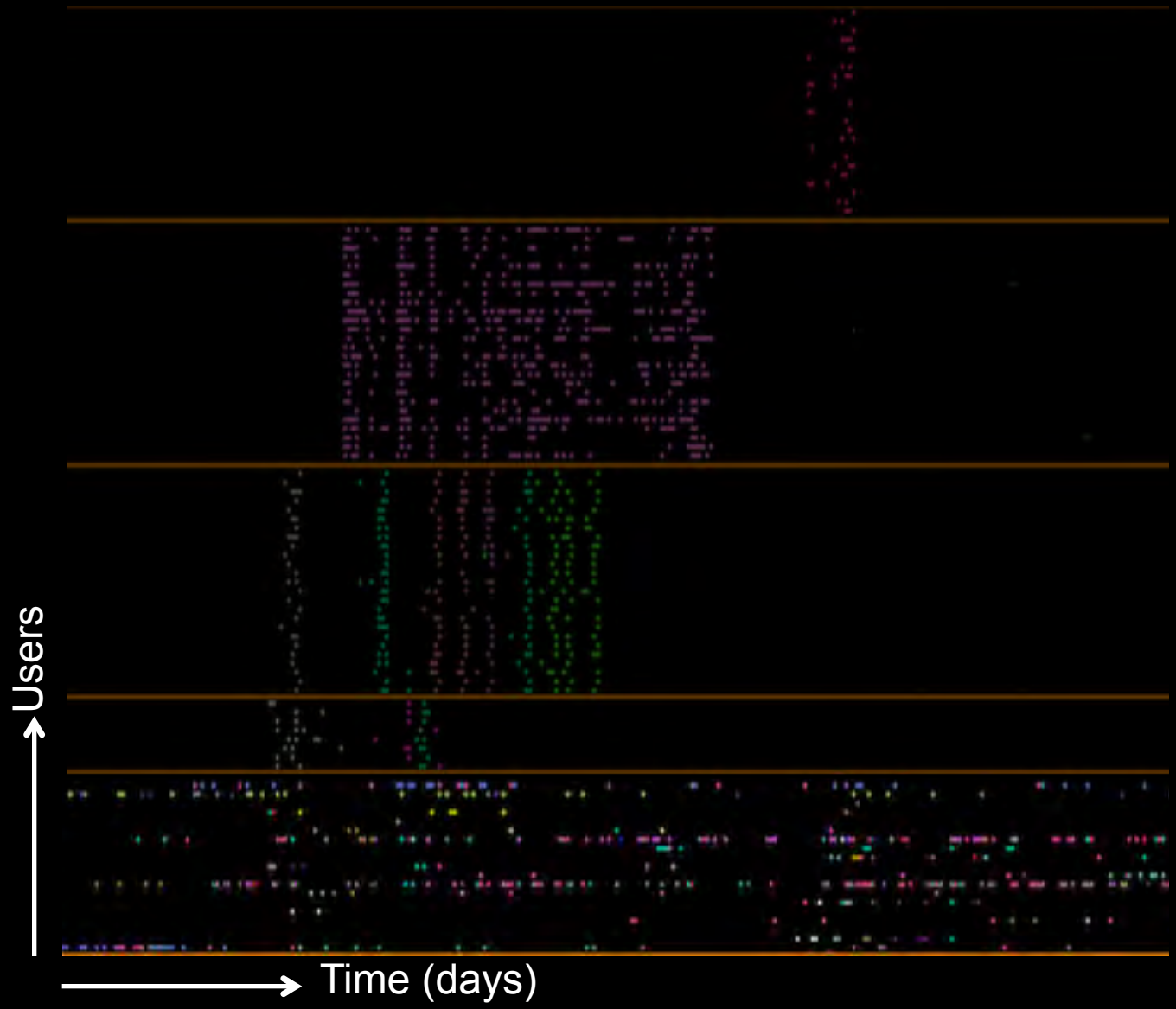
Formal Education vs. Research

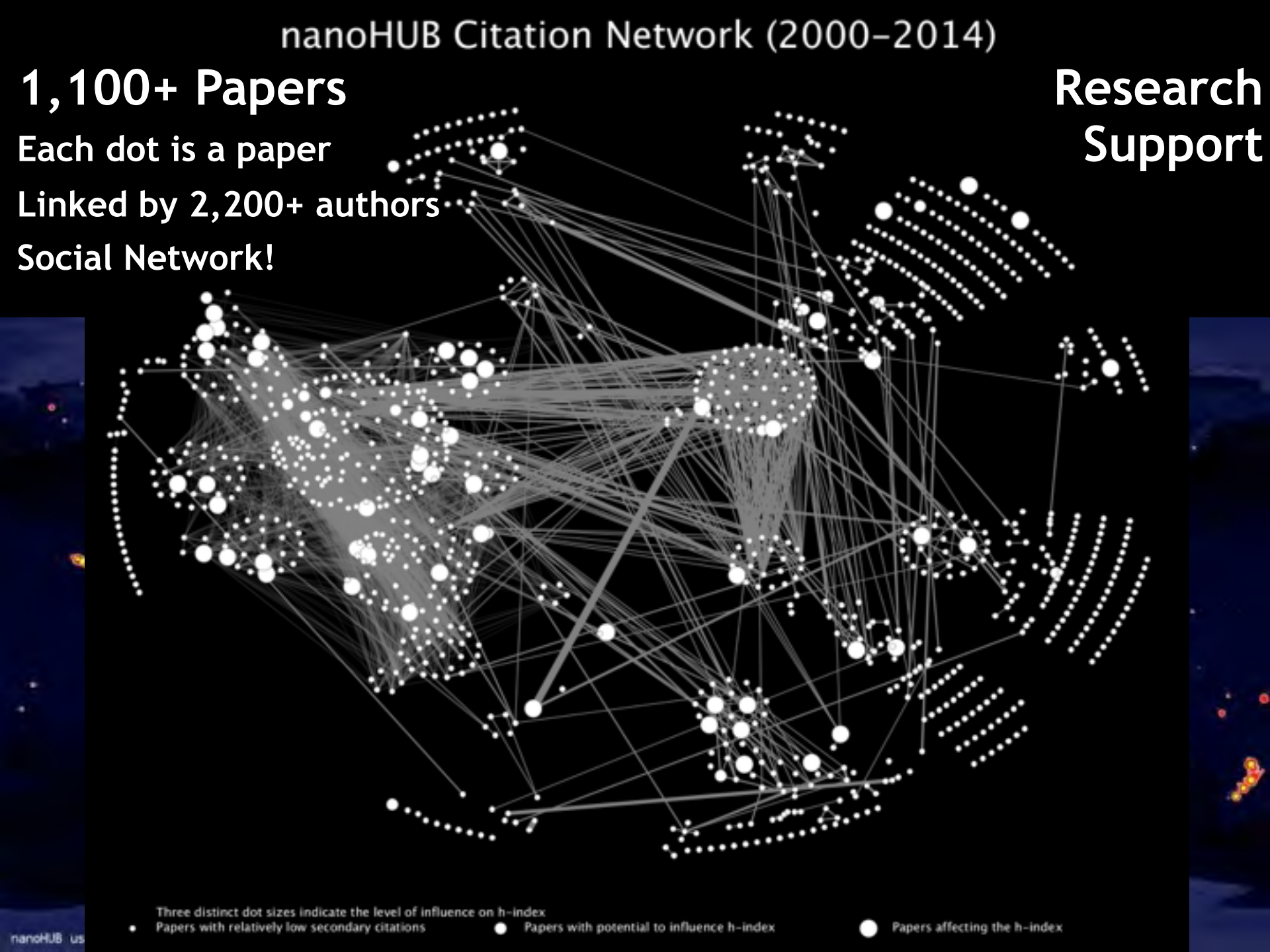


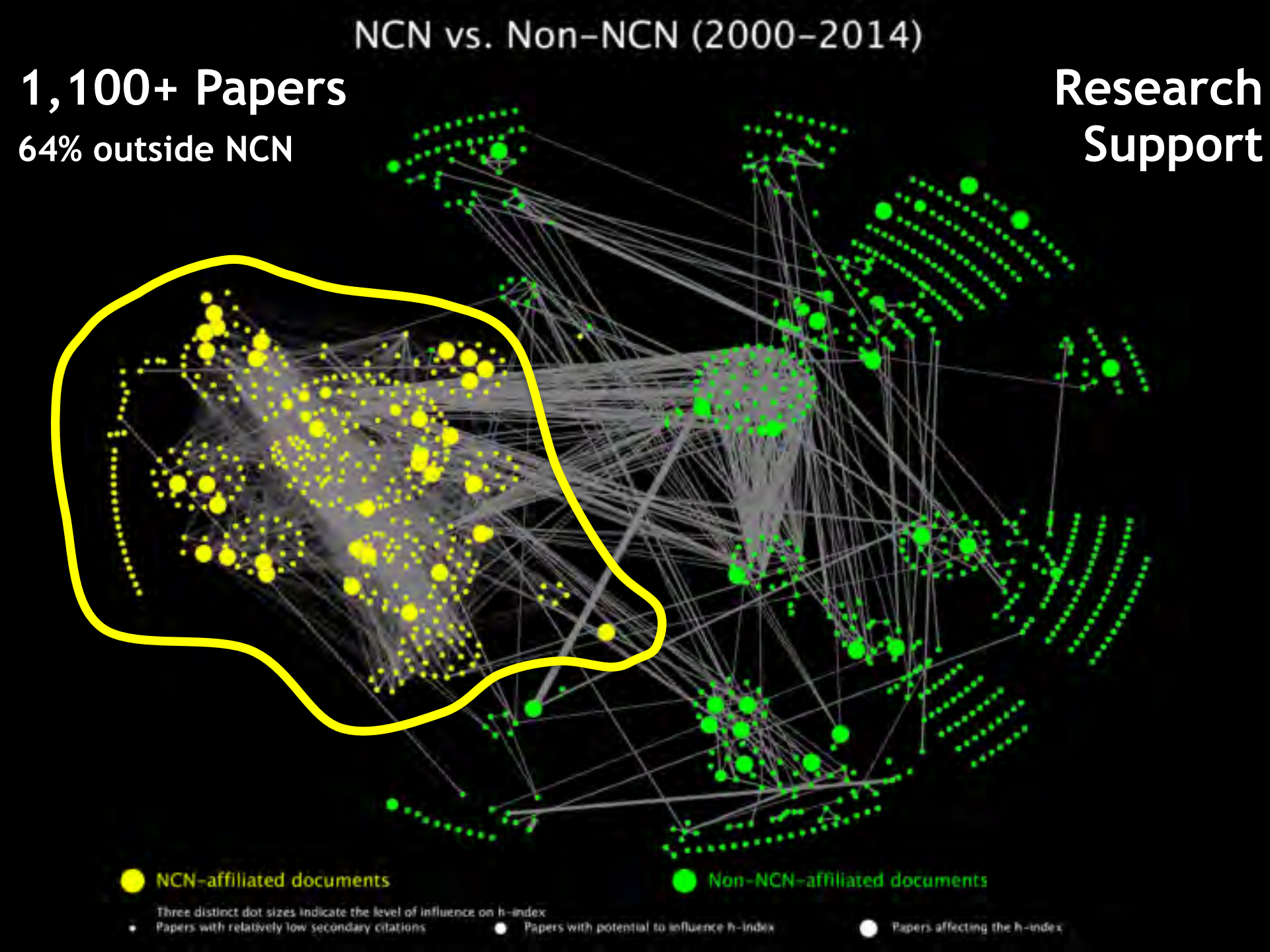
Voluntary / Viral Use

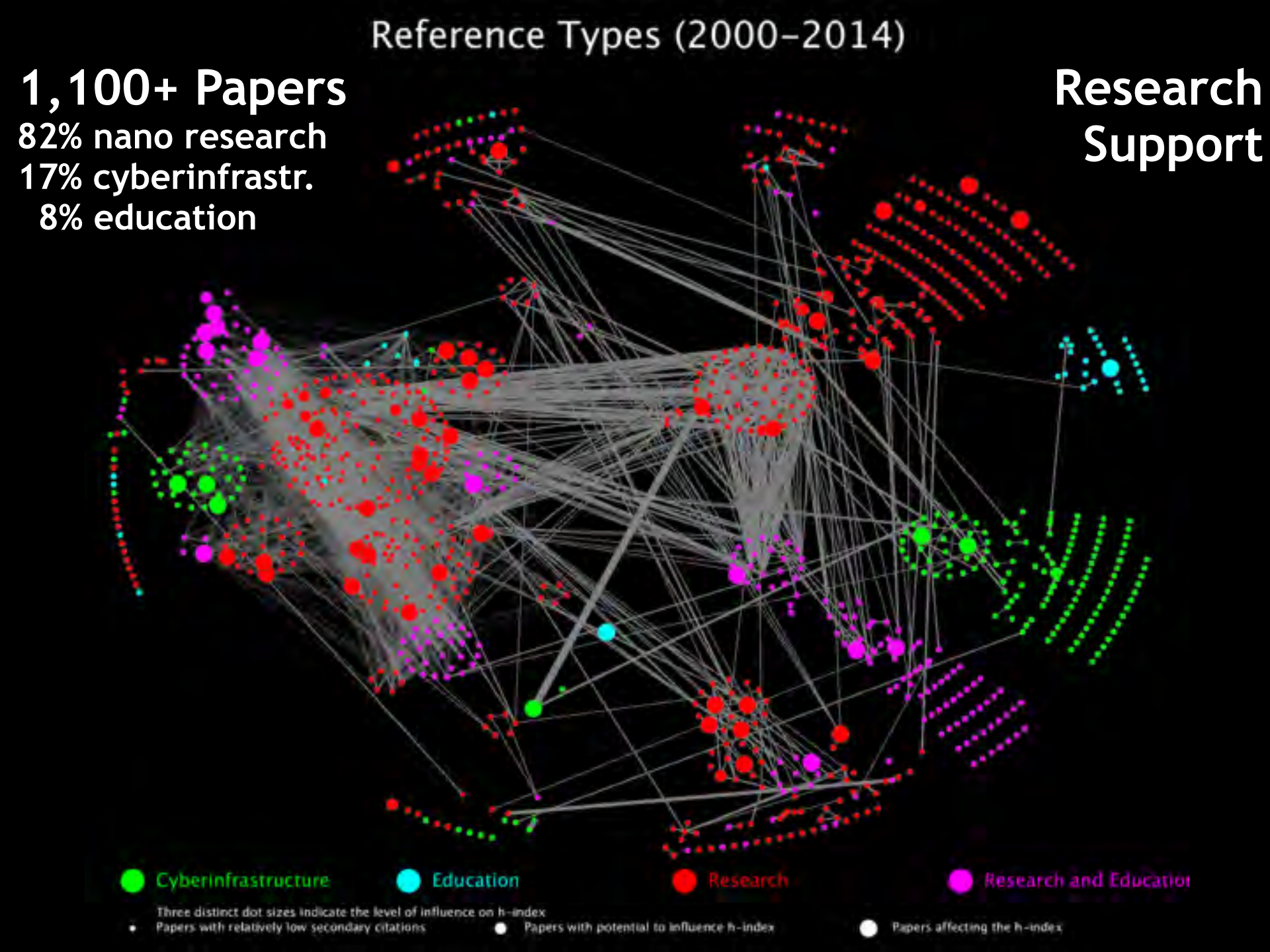
Myth Busted:
Proof of use in EDUCATION!
Knowledge Transfer out of Research
22,649 students,
1,164 courses,
185 institutions

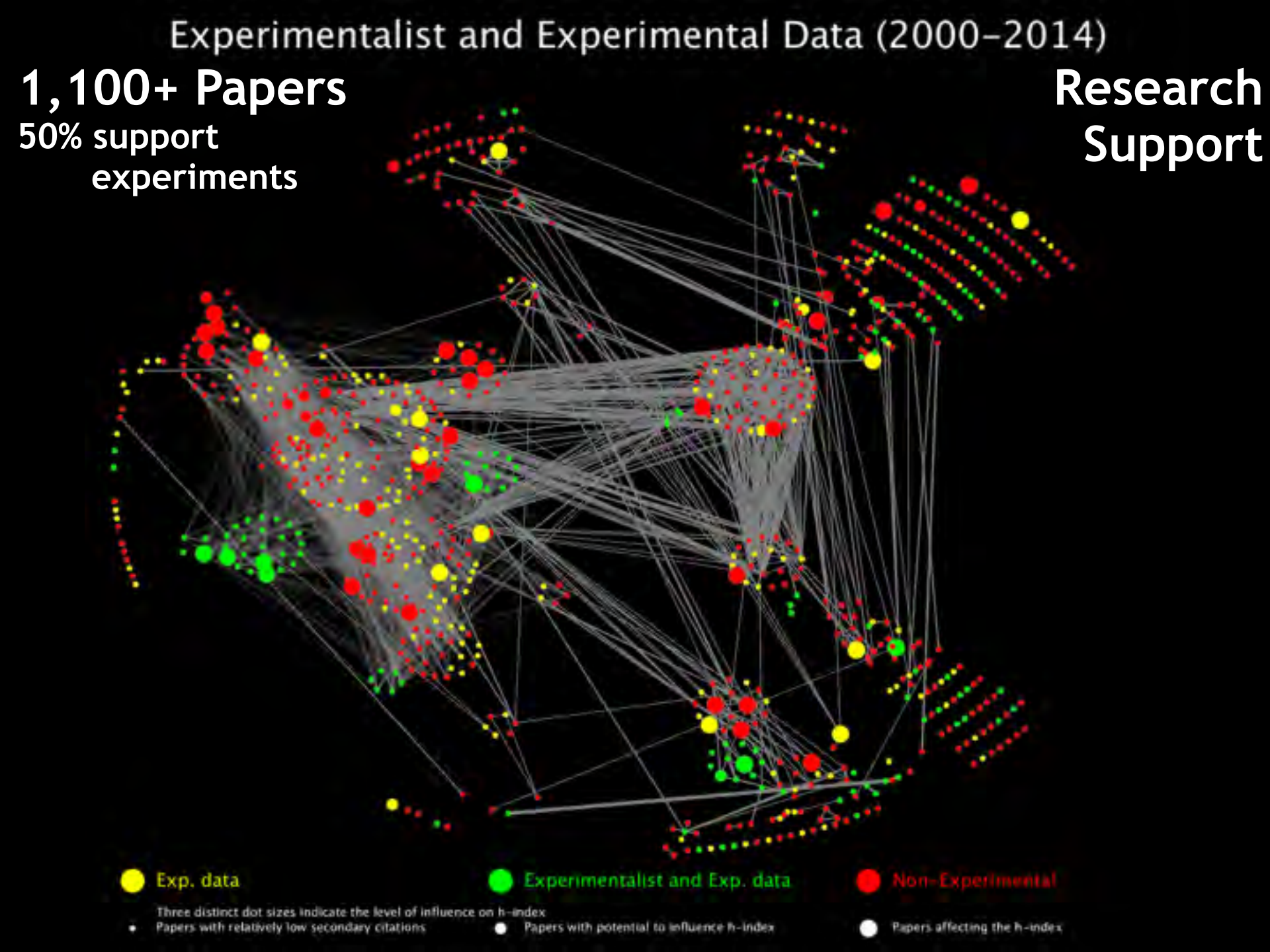
User Behavior Analysis
=> Is Research Possible?

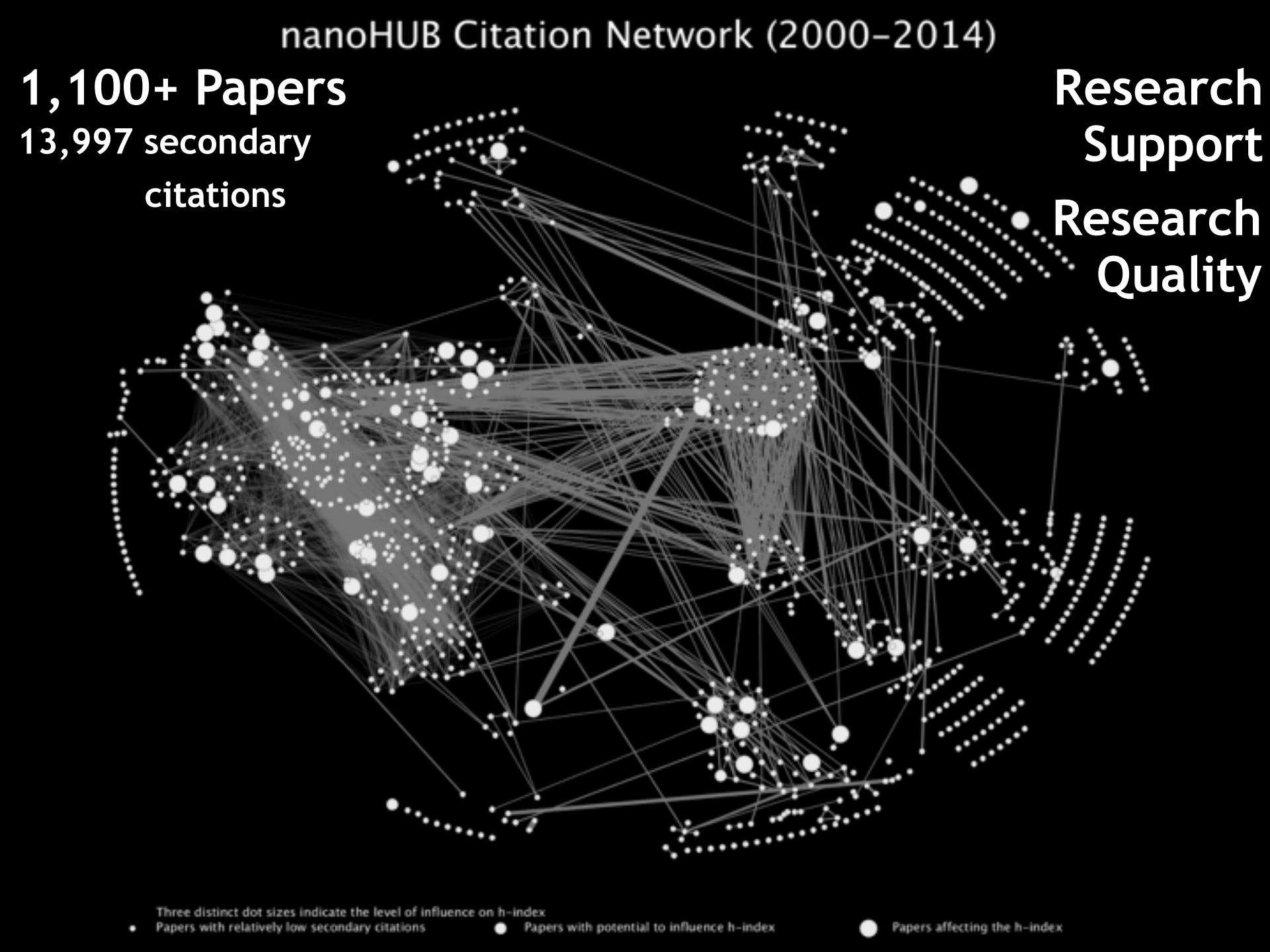



nanoHUB Citation Network (2000–2014)
1,100+ Papers
Each dot is a paper
Linked by 2,200+ authors
Social Network!
Research Support
Three distinct dot sizes indicate the level of influence on h-index
Papers with relatively low secondary citations
Papers with potential to influence h-index
Papers affecting the h-index


NCN vs. Non-NCN (2000-2014)
1,100+ Papers
64% outside NCN
Research Support
NCN-affiliated documents
Non-NCN-affiliated documents
Three distinct dot sizes indicate the level of influence on h-index
Papers with relatively low secondary citations
Papers with potential to influence h-index
Papers affecting the h-index


Reference Types (2000–2014)
1,100+ Papers
82% nano research
17% cyberinfrastr.
8% education
Research Support
Cyberinfrastructure
Education
Research
Research and Educatio
Three distinct dot sizes indicate the level of influence on h-index
Papers with relatively low secondary citations
Papers with potential to influence h-index
Papers affecting the h-index

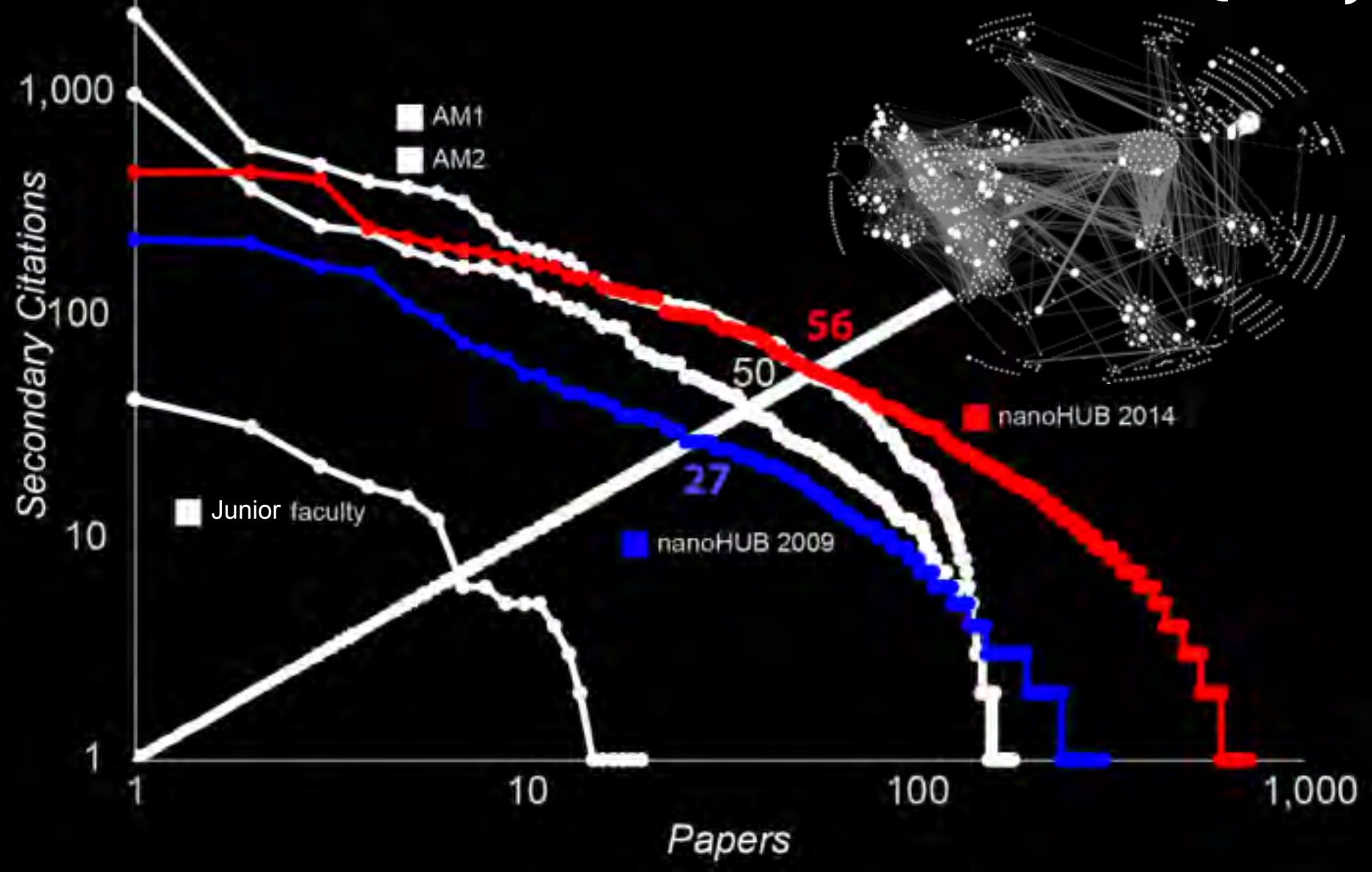

Experimentalist and Experimental Data (2000–2014)
1,100+ Papers
50% support experiments
Research Support
Exp. data
Experimentalist and Exp. data
Non-Experimental
Three distinct dot sizes indicate the level of influence on h-index
Papers with relatively low secondary citations
Papers with potential to influence h-index
Papers affecting the h-index


nanoHUB Citation Network (2000–2014)
1,100+ Papers
13,997 secondary citations
Research Support
Research Quality
Three distinct dot sizes indicate the level of influence on h-index
Papers with relatively low secondary citations
Papers with potential to influence h-index
Papers affecting the h-index

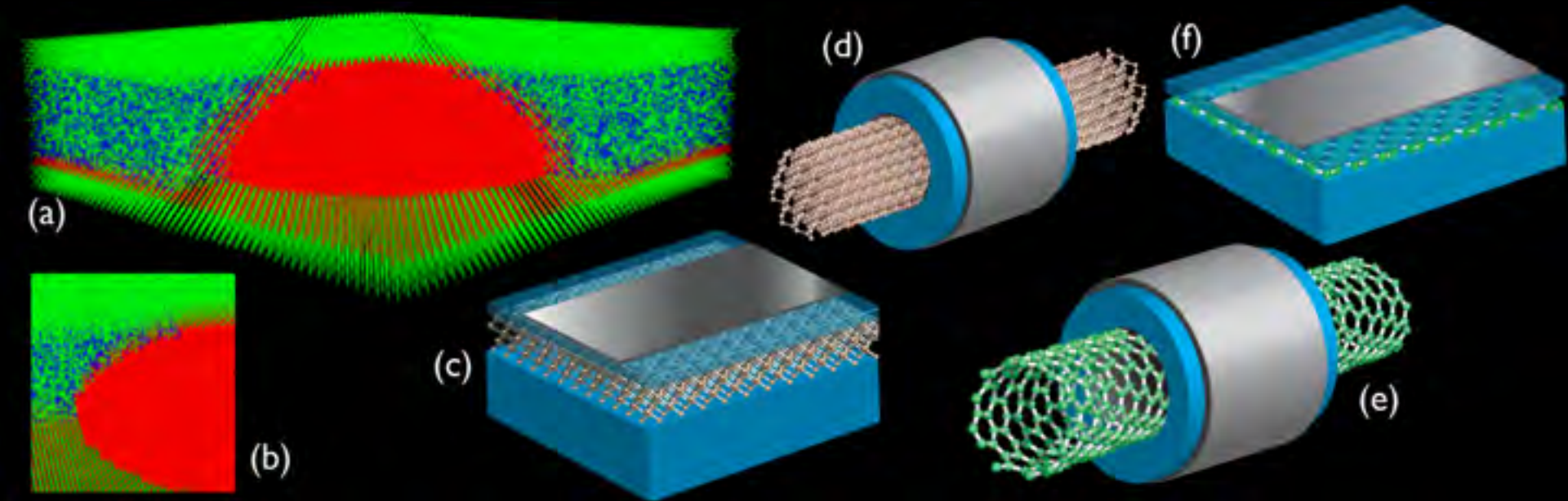
nanoHUB 2014: 1,108 Papers

13,997 secondary citations h-index 56

Research Quality



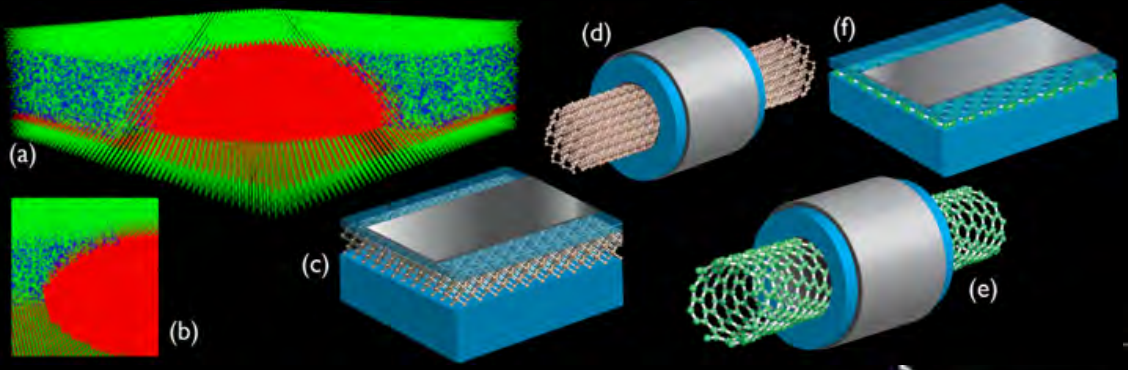
Compute Intensive: NEMO/OMEN



20 years development

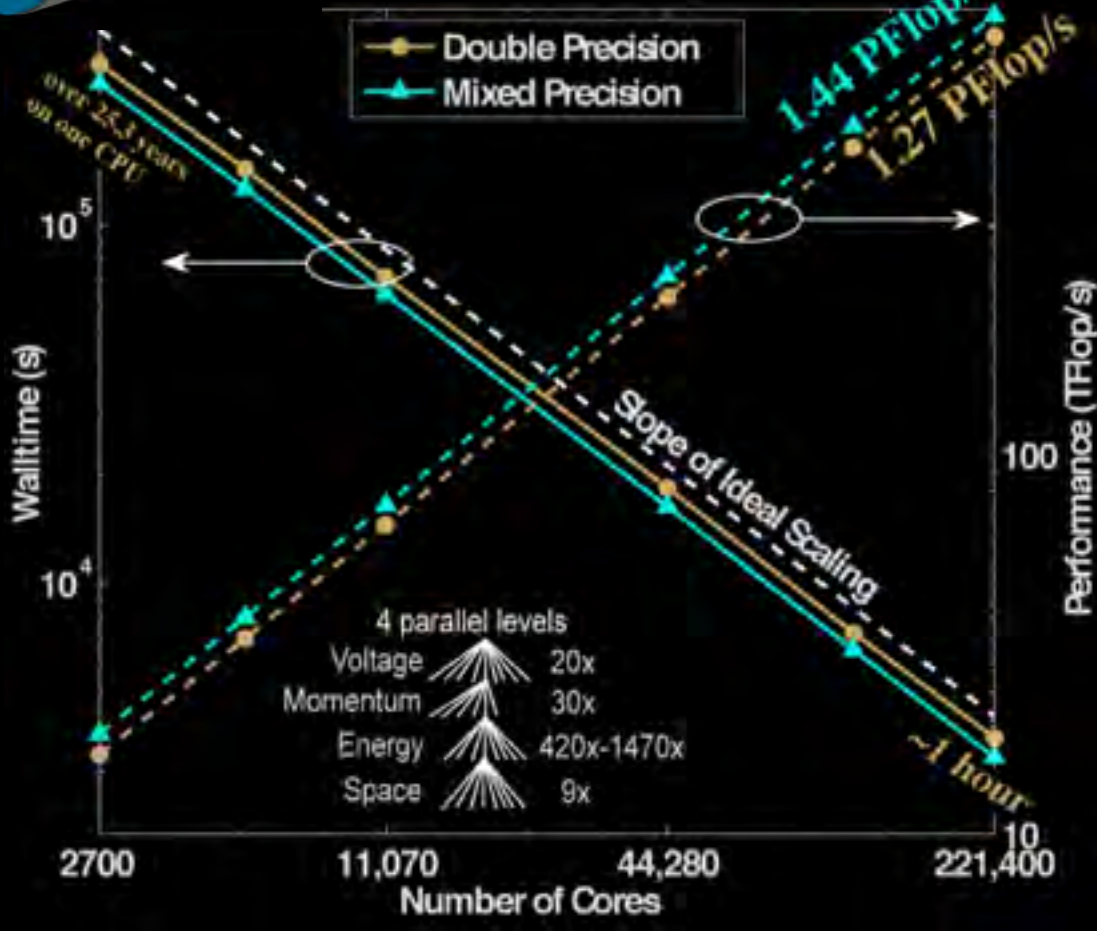
- Texas Instruments
- NASA JPL
- Purdue

Compute Intensive: NEMO/OMEN

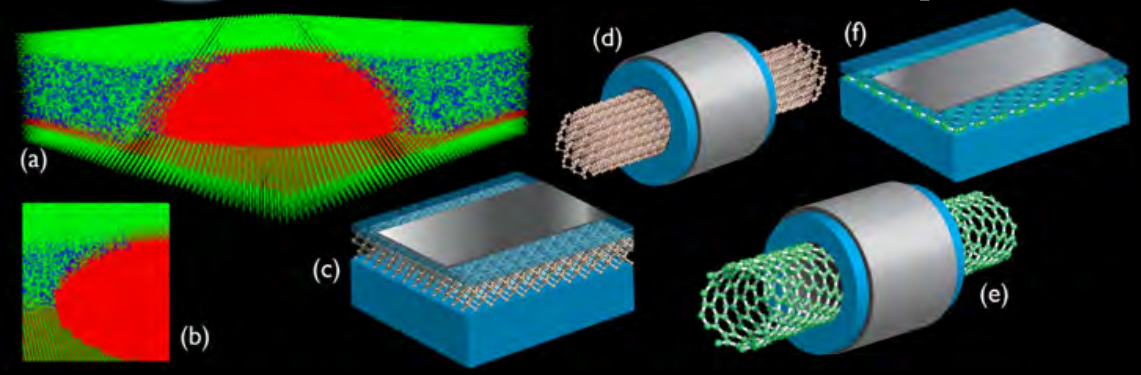


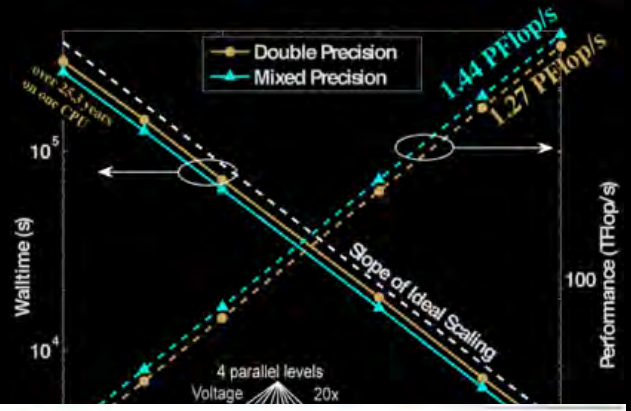
20 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering



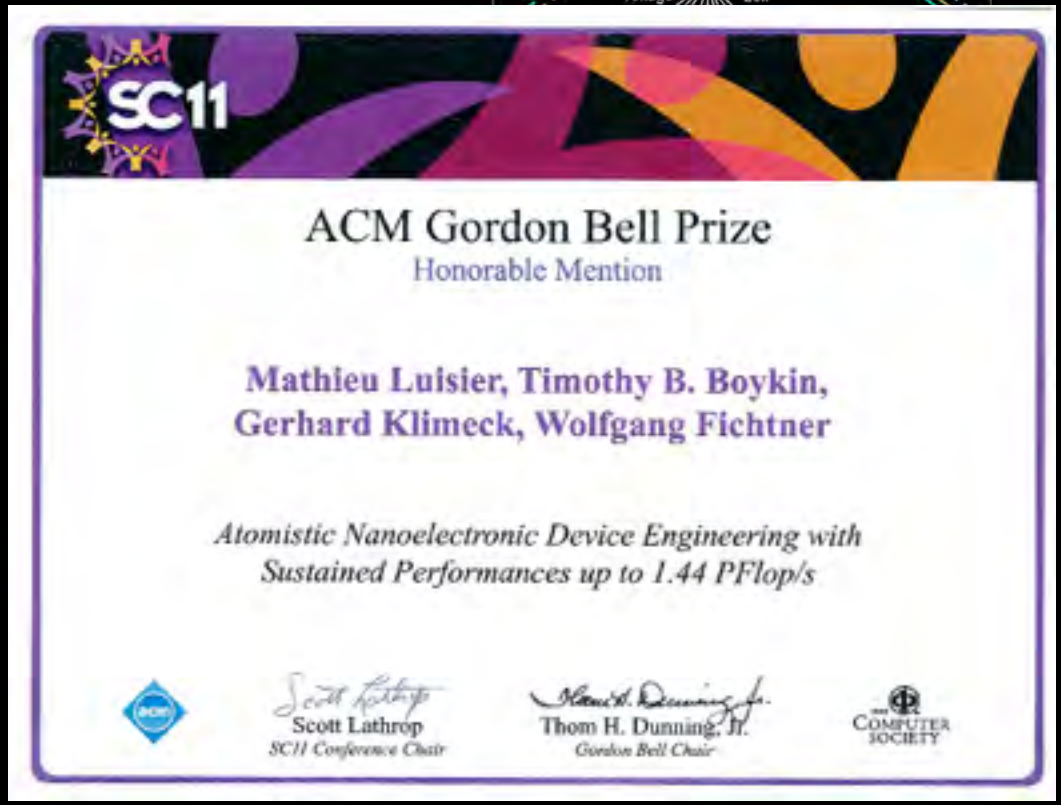
Compute Intensive: NEMO/OMEN



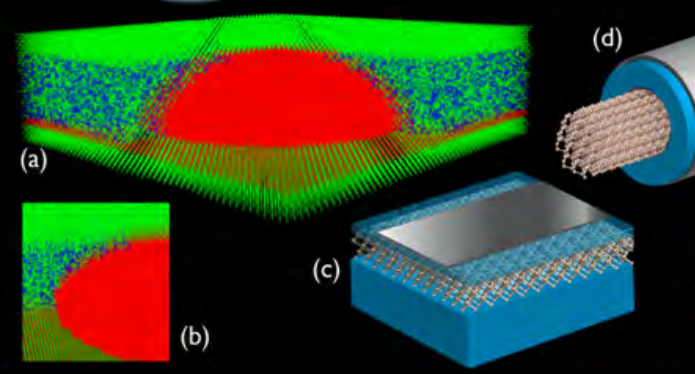


20 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell



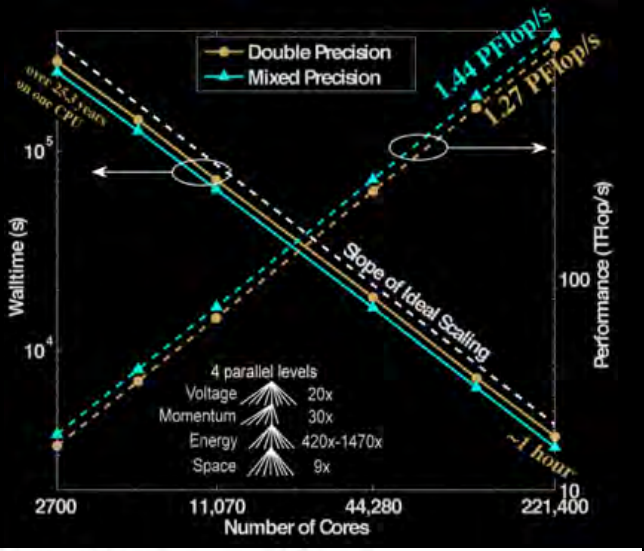
Compute Intensive: NEMO/OMEN

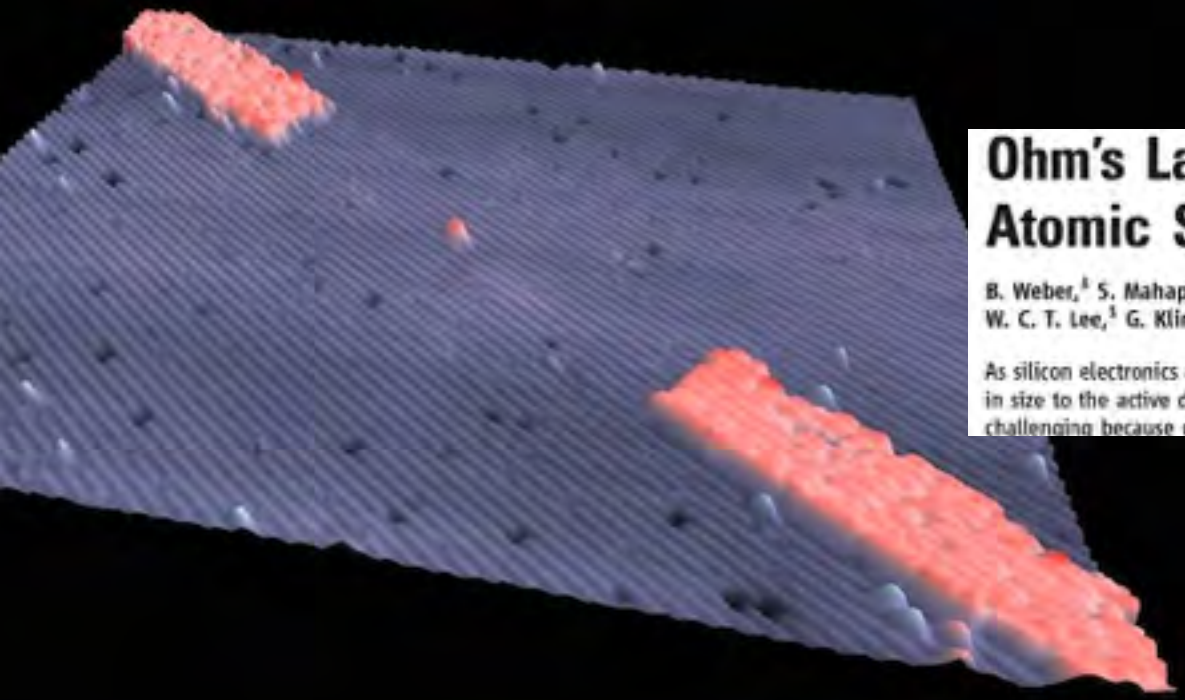


SC11

ACM Gordon Bell Prize
Honorable Mention

Mathieu Luisier, Timothy B. Boykin,
Gerhard Klimeck, Wolfgang Fichtner





Ohm's Law Survives to the Atomic Scale

B. Weber,[1] S. Mahapatra,[1] H. Ryu,[2*] S. Lee,[2] L. Thompson,[1]
W. C. T. Lee,[1] G. Klimeck,[2] L. C. L. Hollenben

Science
AAAS

As silicon electronics approaches the atomic sc ome comparable in size to the active device components. Maint is scale is challenging because of the presence of confining surfaces and interfaces. We report on the

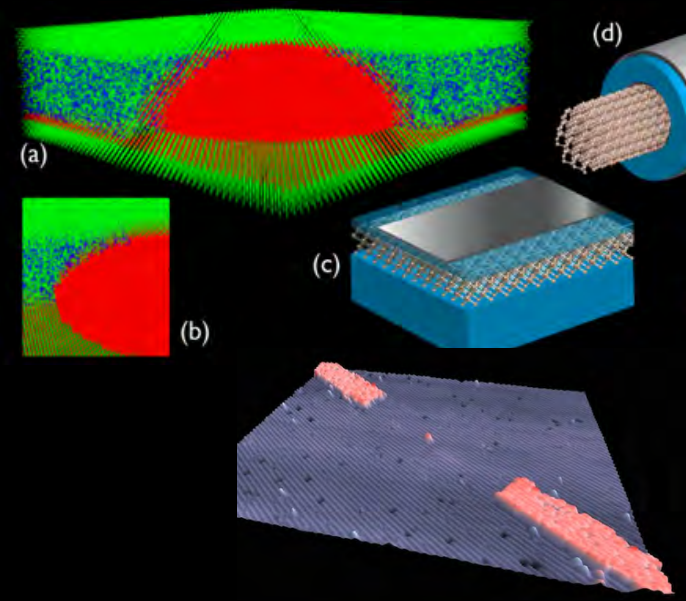
nature nanotechnology

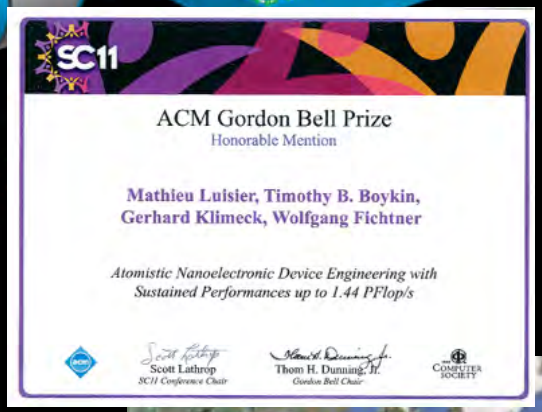
A single-atom transistor

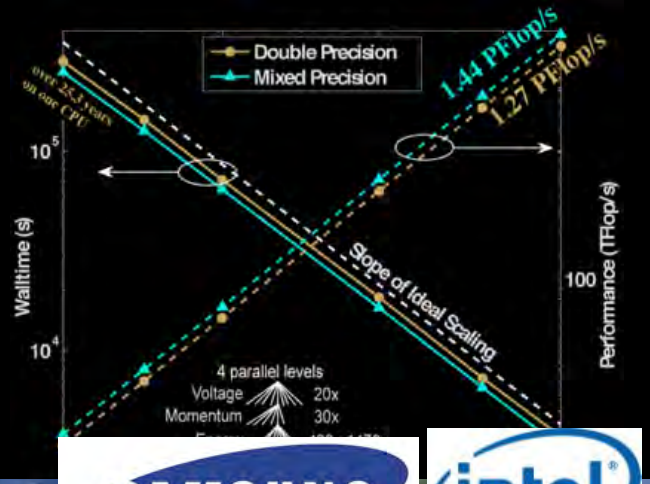
Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard

- Science, Nature Nano

Compute Intensive: NEMO/OMEN



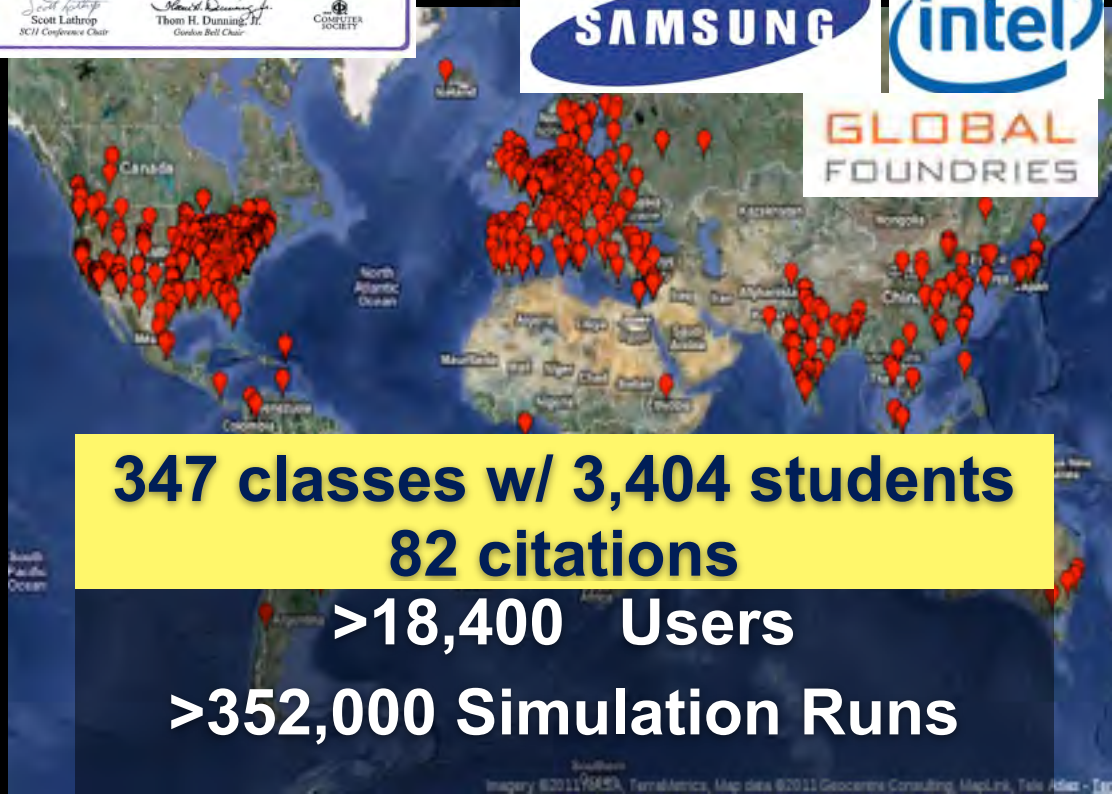




SAMSUNG intel GLOBAL FOUNDRIES

20 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell
- Science, Nature Nano



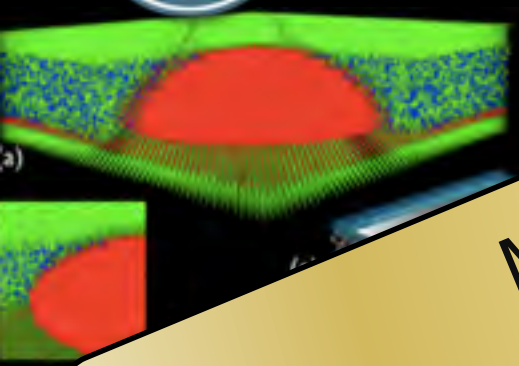
347 classes w/ 3,404 students
82 citations

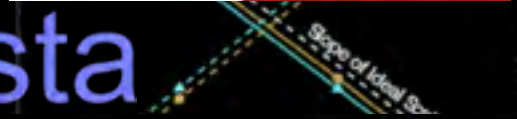
>18,400 Users

>352,000 Simulation Runs

Myth Busted! Prove Computational Extensive Work

pute Intensive





18 years development

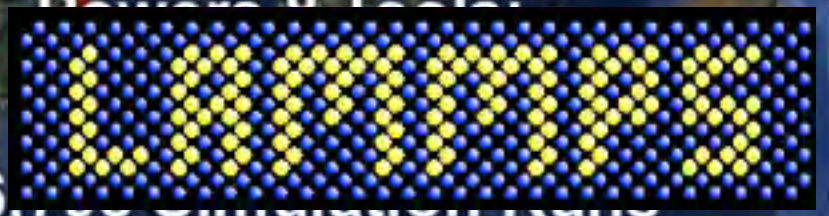
- 267,362 Simulation Runs
- 10,786 Users
- 3,874 Users in 100 classes

SeqQuest

qwalk

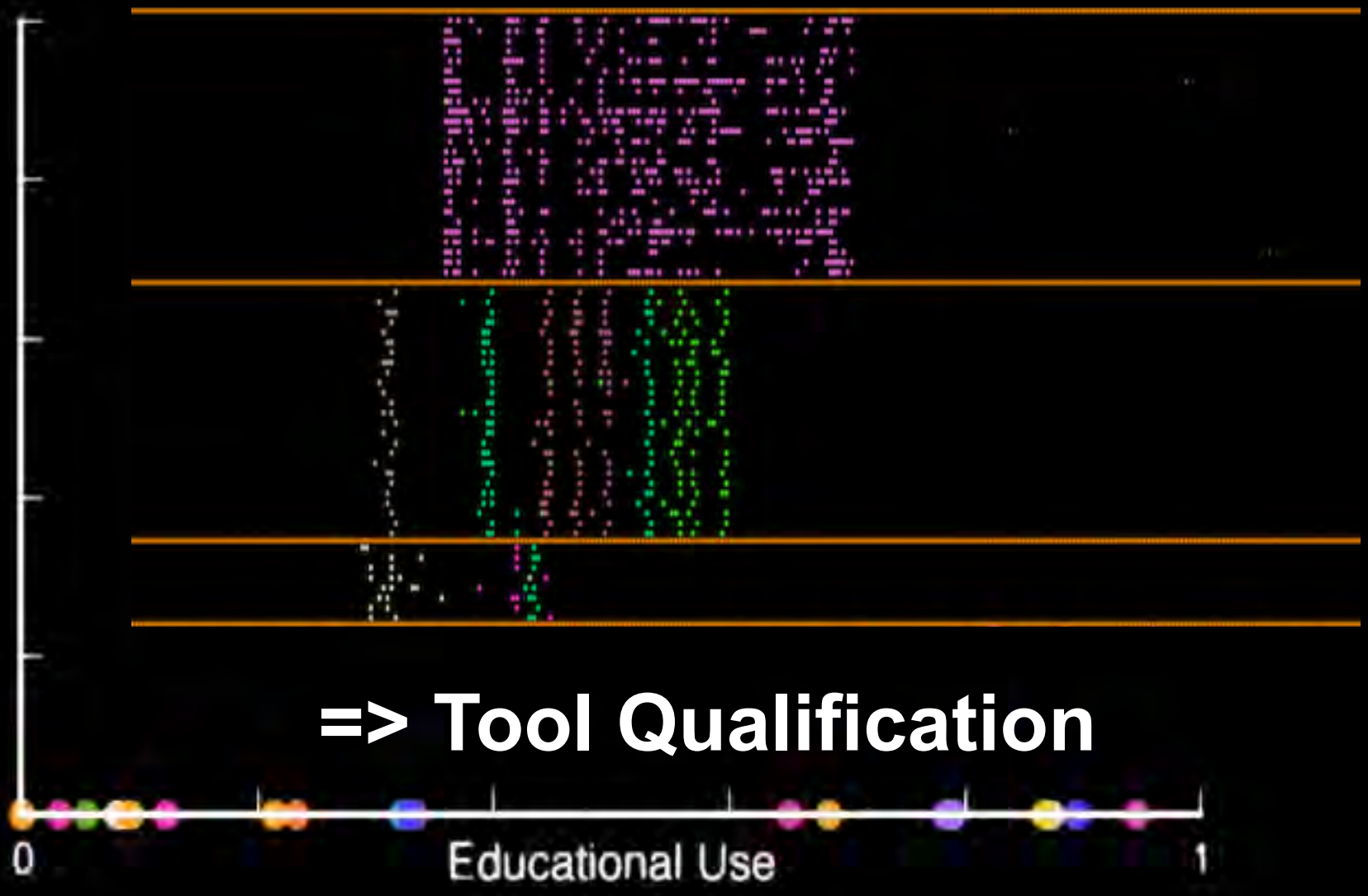
QWalk: Continuum electronic structure quantum Monte C

- Peta
- Gord
- Scie



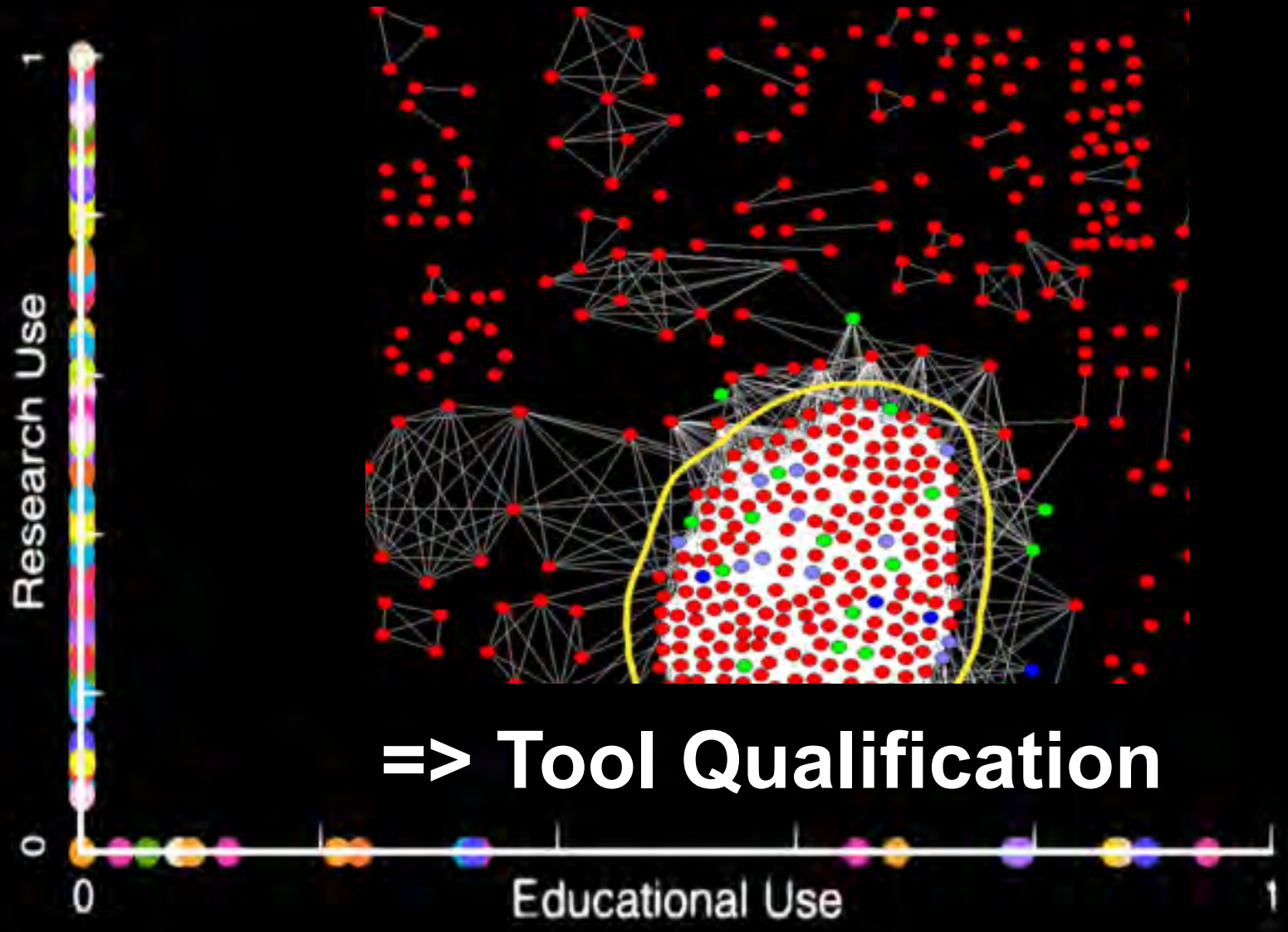
166,

Usage Patterns

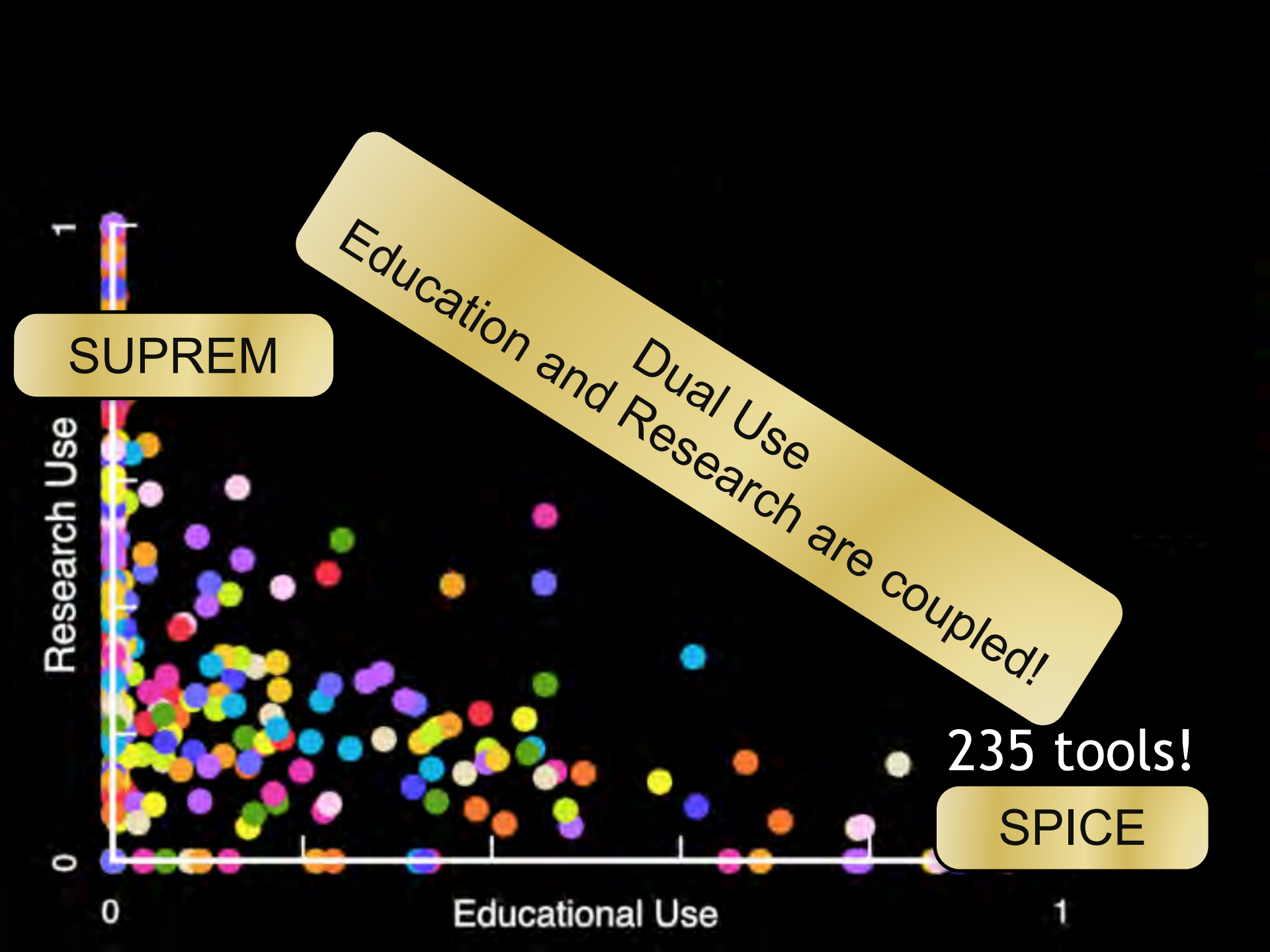


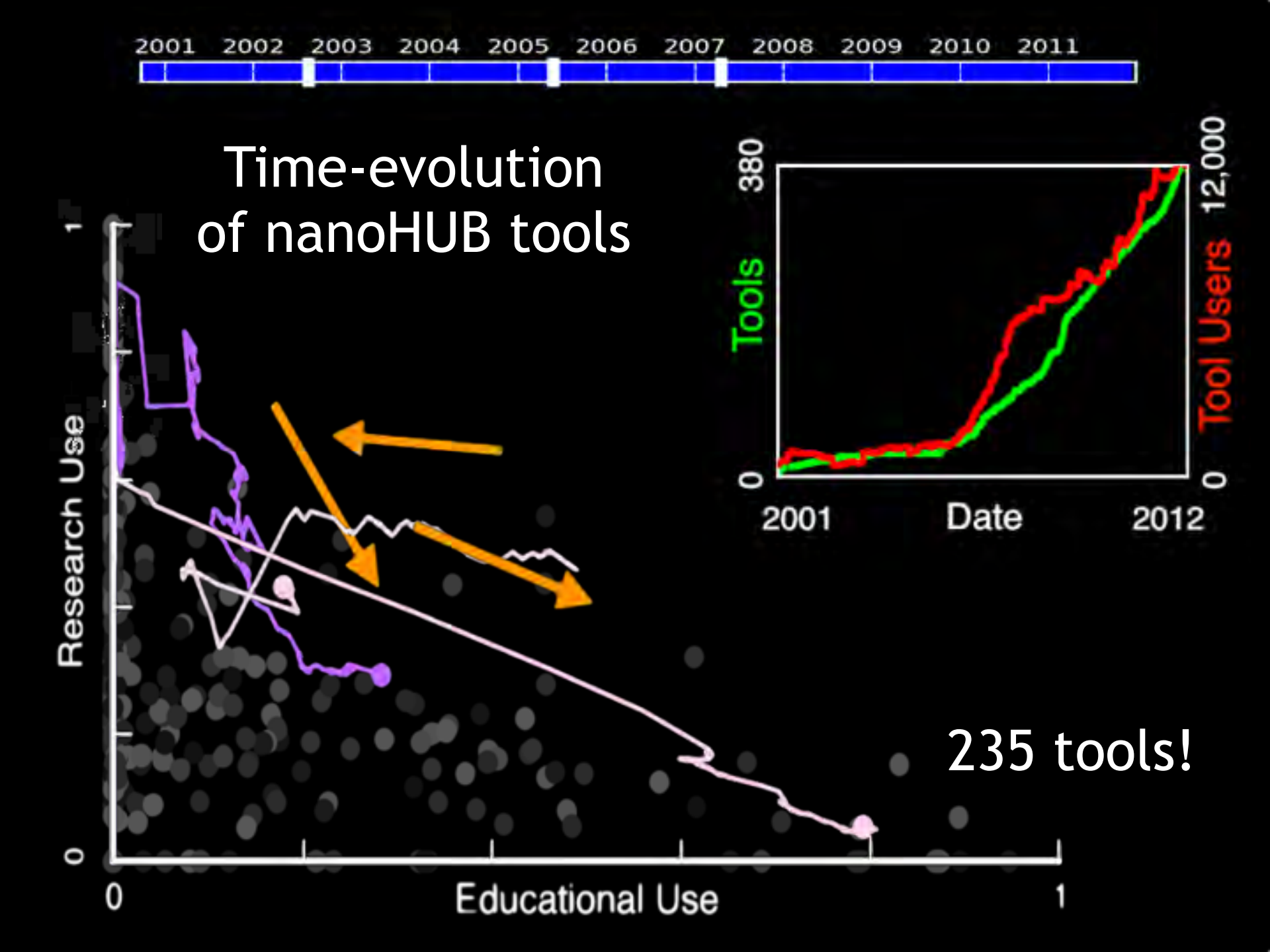
=> Tool Qualification

Literature Citations

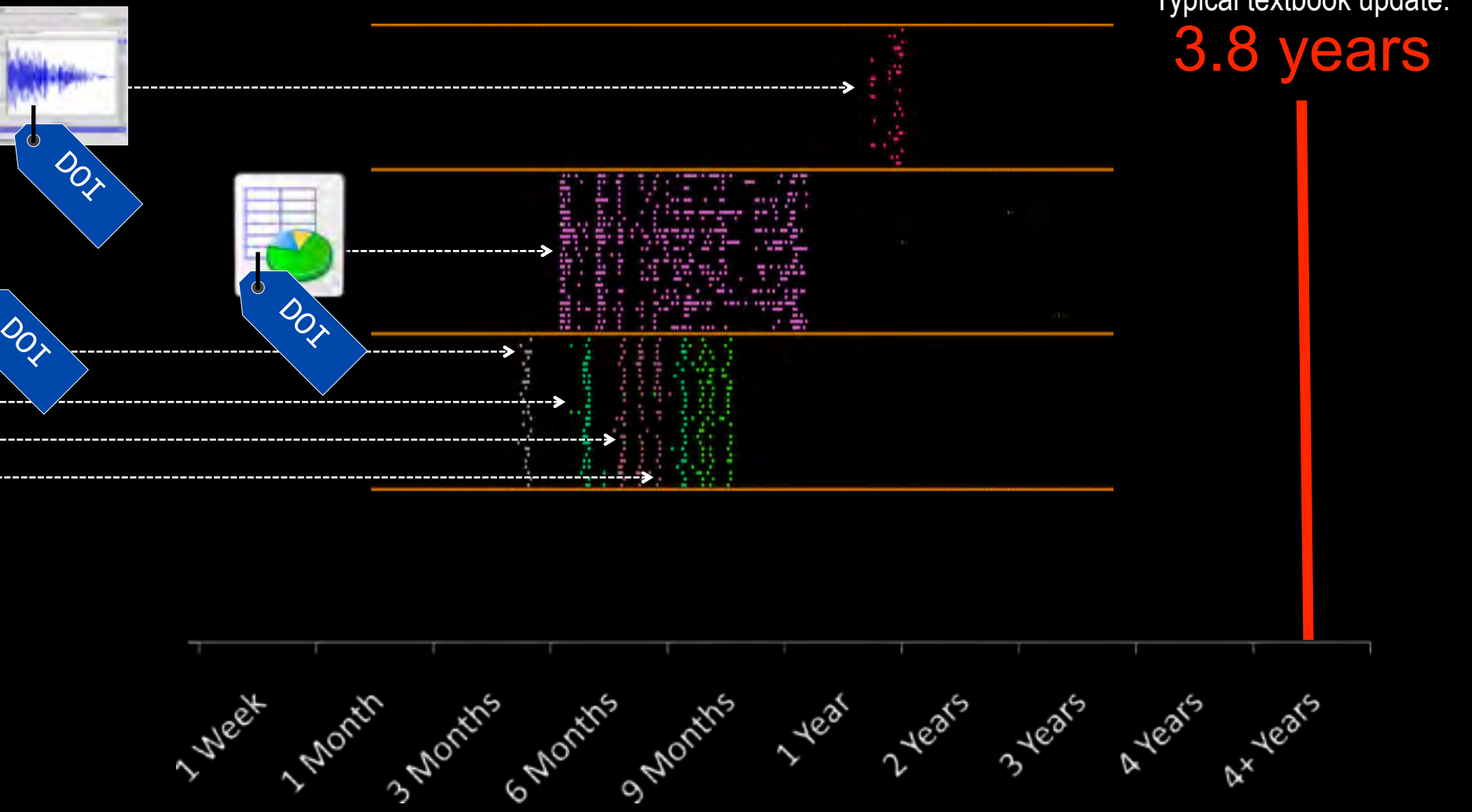


=> Tool Qualification


Dual Use
Education and Research are coupled!
SUPREM
235 tools!
SPICE
Research Use
Educational Use
0
1
0
1

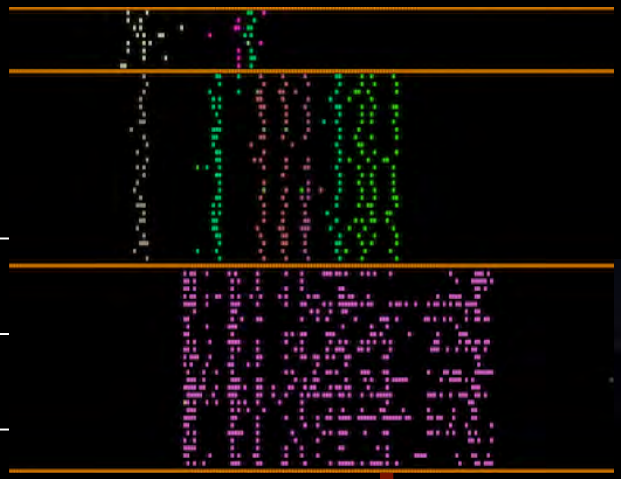

2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011
Time-evolution
of nanoHUB tools
Tools
380
0
Tool Users
12,000
0
2001
Date
2012
Research Use
1
0
0
Educational Use
1
235 tools!

Time to First Adoption



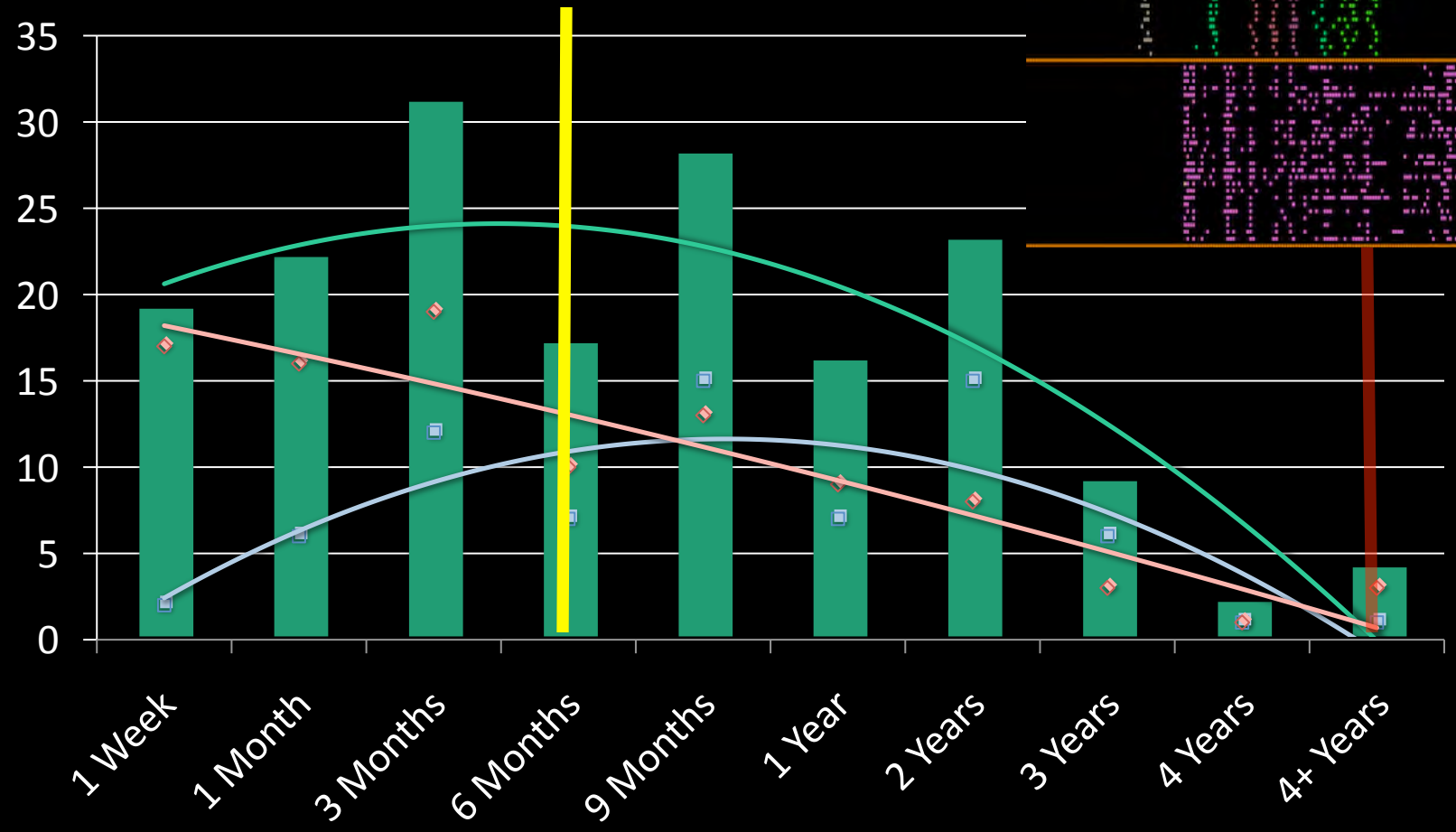
Time Between Tool Publications and First Use in Classroom

Revolutionizing Research → Classroom



Median adoption time:

174 days (5.7 months)



Time Between Tool Publications and First Use in Classroom

Imagine

Simulation Tools

- Used by researchers
- Used by experimentalists
- Used in education

In a scientific cloud

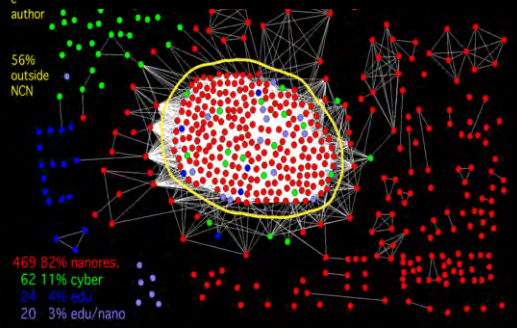
Without any installation

Fully operational 24/7

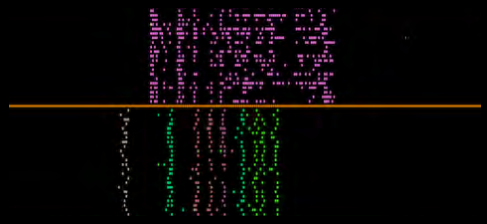
With assessed IMPACT

Over 329,000 Users Annually

1100 papers



22,000 students



Imagine

Simulation Tools and Experimental Data

- Used by researchers
- Used by experimentalists
- Used in education

In a scientific cloud

Without any installation

Fully operational 24/7

With assessed IMPACT

Reproducible

Nano Engineering

In all areas of Nano Engineering and Science

Personalized Learning at all workforce levels

Become Part of the Day-to-Day Workflow

We WON the next 5+5 Years

- *NSF Reconfigures NCN/nanoHUB*
- *2 types of awards:*
  - *$2.9M/yr Central CI development – 5+5 years*
  - $0.7M/yr 3 content creation awards – 5 years
  - **$50M total – 56% increase**

Transferrable?

New perspectives:

- $500M Presidential Initiative – Manufacturing
- $1,000M Presidential Initiative – Materials Genome Initiative

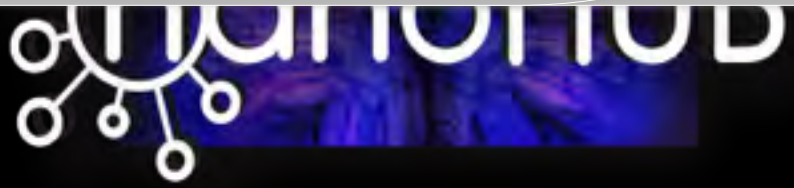
PURDUE UNIVERSITY

CEINT, National Registry & nanoHUB

CEINT Center for the Environmental Implications of NanoTechnology

NANOMATERIALREGISTRY

Have:	Experimental Data	erimental Data
	Hypothesis Driven Data Structure	ess
Need:	Broad Exposure	community
	Data integration with Registry	ith supporting data
	Data analysis tools to answer questions	tion capability



Analytics - Established User Community - Simulation Tools

nanoHUB
THE PROFESSIONAL nano SOCIETY

Good Nano Guide

GoodNanoGuide

Have: Rich nano content
Need: Broad Exposure
Flexible site hosting Infrastructure
Customizations for content development and management

nanoHUB

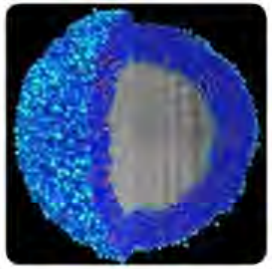
Established User Community - Flexible Content Hosting

their data, nanoHUB.org supports the use of computational tools in nanotechnology research. Researchers can access state-of-the-art modeling algorithms and collaborate with colleagues via the website. To rapidly increase knowledge of first principles and advance

Co
Maj
beh
use
New
mat
For
disc
con
Furt
ana
con
and

The

to industry's limited confidence in accepting non-empirically-based conclusions. Materials scientists have developed powerful computational tools to predict materials behavior, but these tools have fundamental deficiencies that limit their usefulness. The primary problem is that current predictive algorithms do not have the ability to model behavior and properties across multiple spatial and temporal scales; for example, researchers can measure the atomic vibrations of a material in picoseconds, but from that information they cannot predict how the material will wear down over the course of years. In addition, software tools that utilize the algorithms are typically written by academics for academic purposes in separate universities, and therefore lack user-friendly interfaces, documentation, robustness, and the capacity to scale to industrial-sized problems.



algorithms of materials behavior into existing product design tools. For example, the crystal structure and physical properties of the materials in a product may change during the product's processing, due to varying conditions. It could be disastrous to the performance of a product if, for instance, the tensile strength of its bolts changed during manufacture. The ability to model these morphology and property changes will enable faster and better design.

Achieving these objectives will require a focus in three necessary areas: (1) creating accurate models of materials performance and validating model predictions from theories and empirical data; (2) implementing an open-platform framework to ensure that all code is easily used and maintained by all those involved in materials innovation and deployment, from academia to industry;

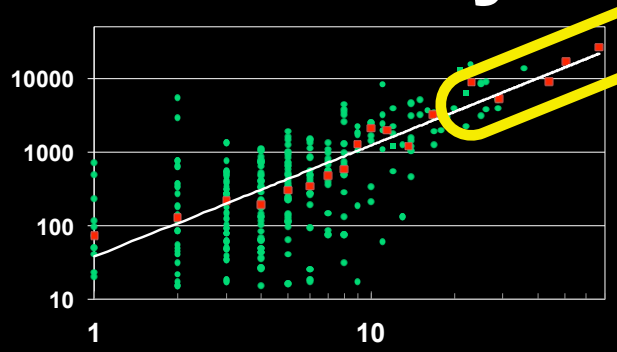
the pace of innovation, which currently occurs in isolated academic settings. An existing system that is a good example of a first step toward open innovation is the nanoHUB, a National Science Foundation program

is the nanoHUB, a National Science Foundation program run through the Network for Computational Nanotechnology.[8] By providing modeling and simulation applications that researchers can download and use on data on materials properties. Experimental data is required to create models as well as to validate their key results. Where computations based on theoretical frameworks fall short, empirical testing will fill in the

The Essence of a Research University

Global

Growing



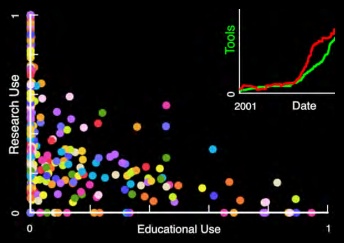
Collaboration Focused

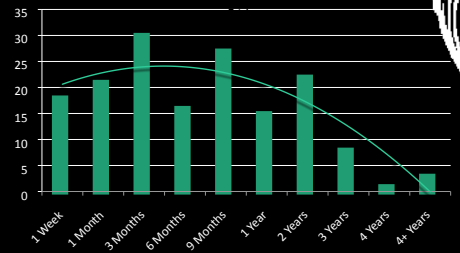
Recognized

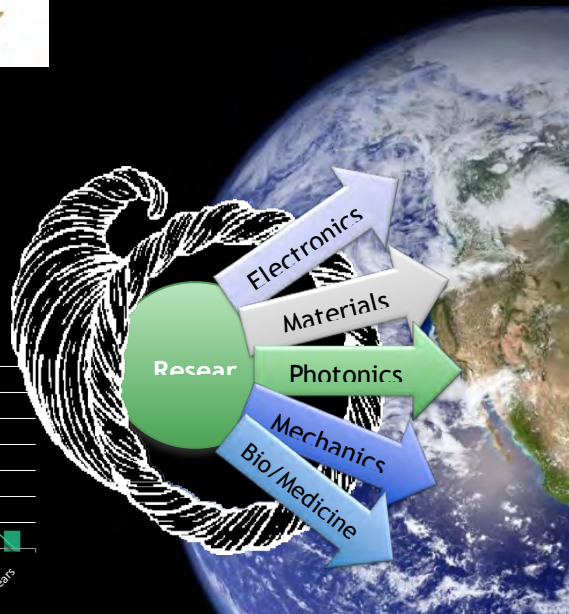
PURDUE
UNIVERSITY

Creative

Transformative







Thank You!