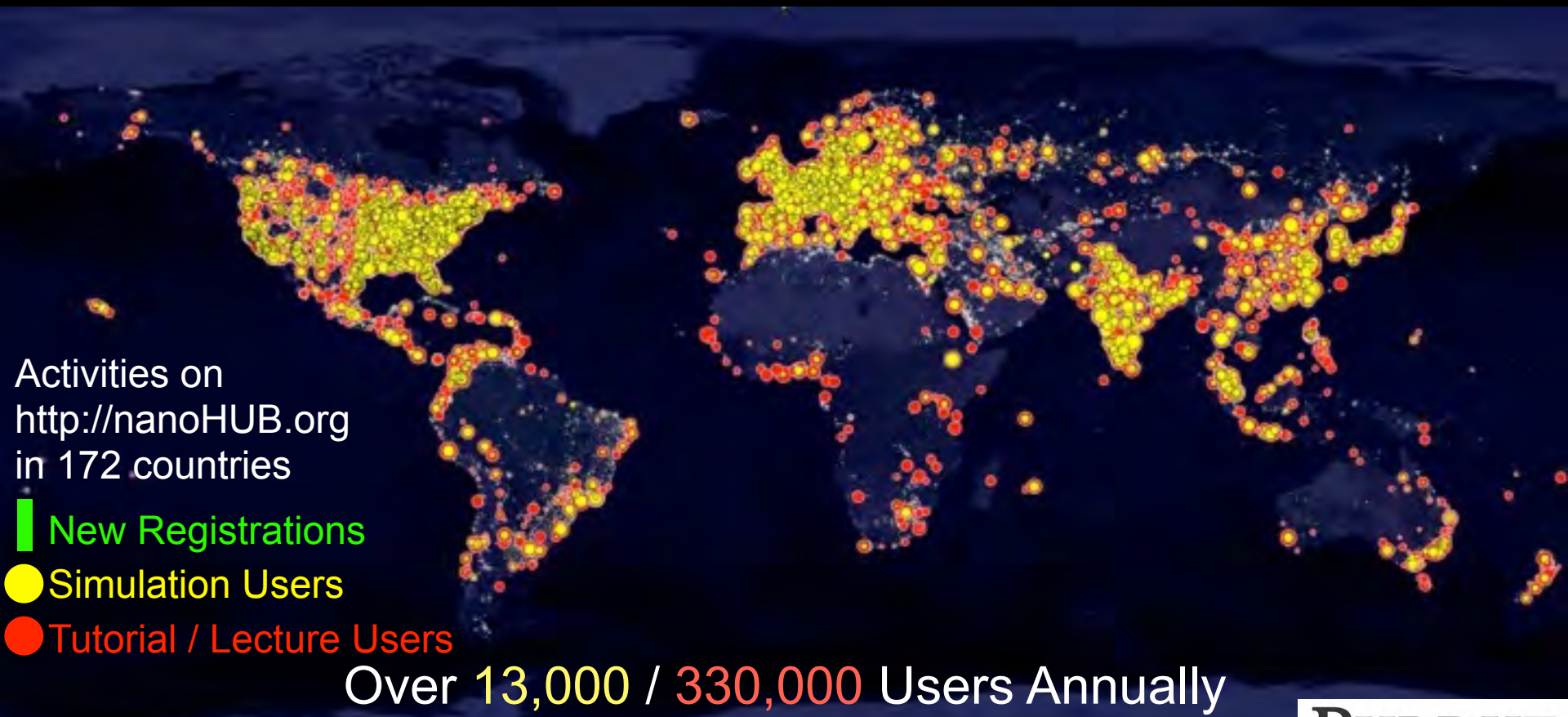




Mythbusting Scientific Knowledge Transfer with nanoHUB.org

Gerhard Klimeck, Purdue University, gekco@purdue.edu



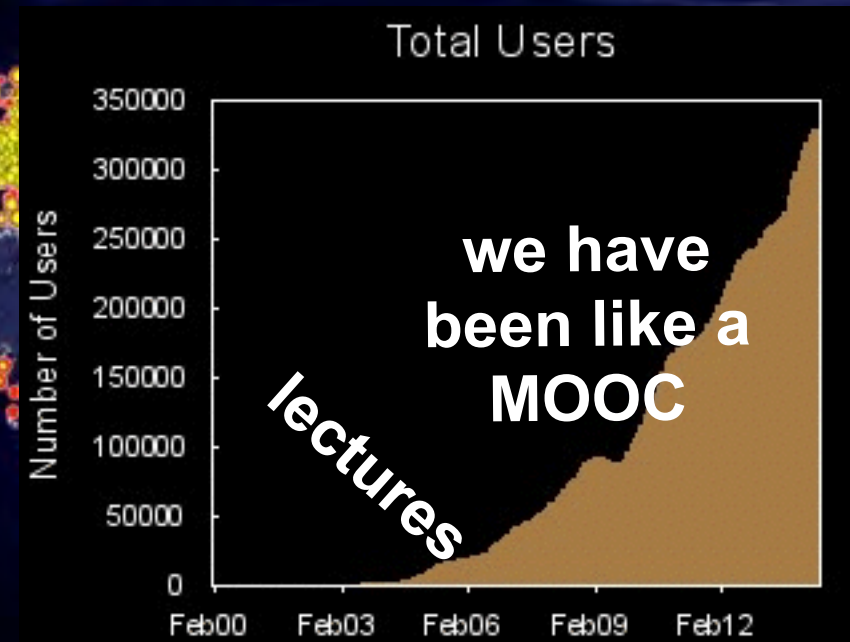
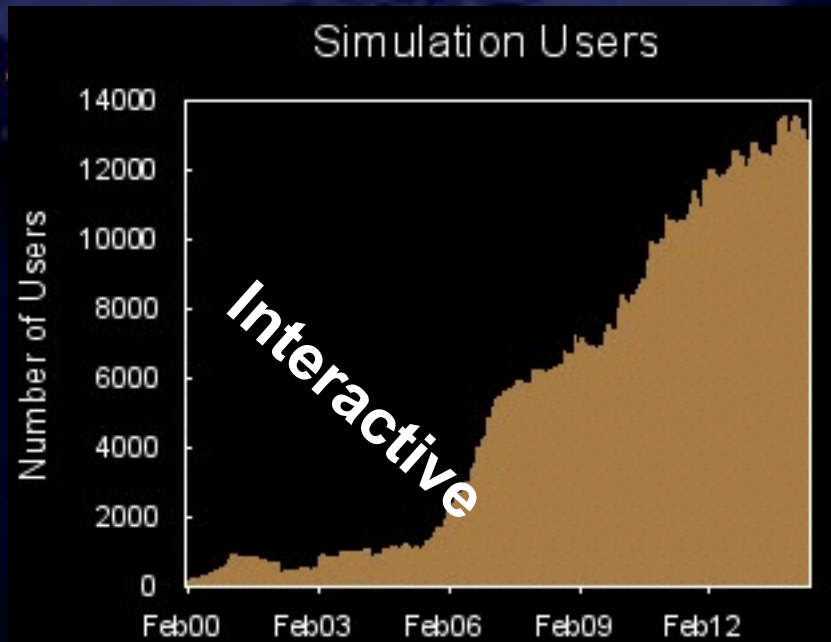


Documenting with Real Data

Research \rightleftharpoons Education, Collaborative, Global Impact

The Essence of a Research University

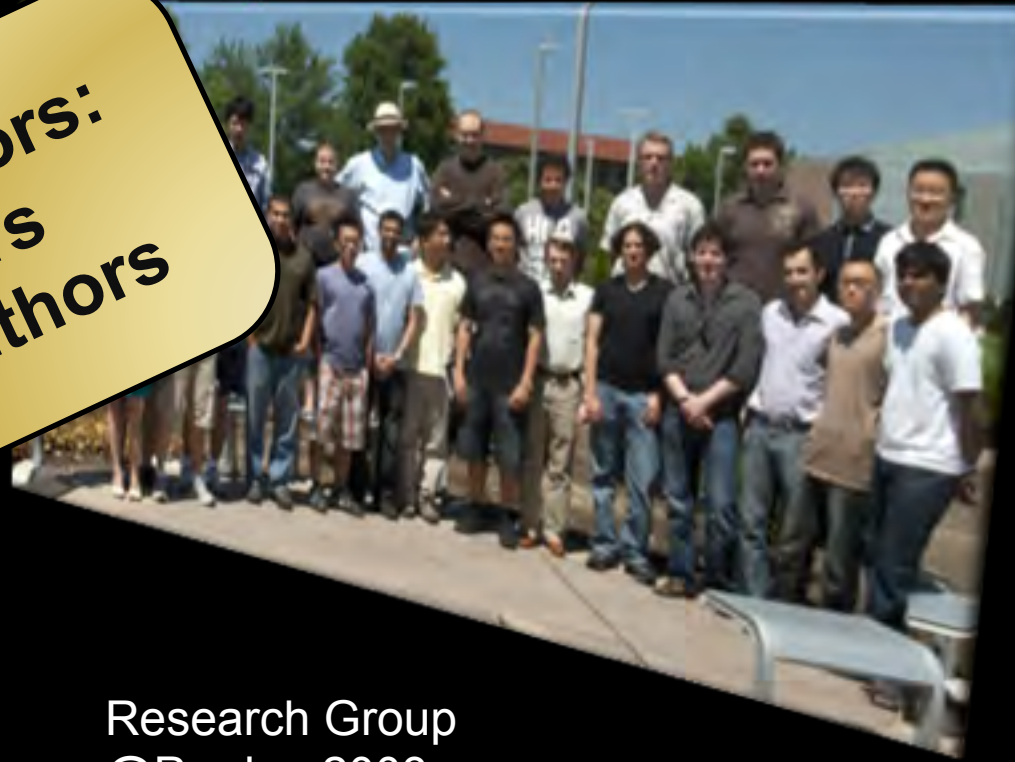
Gerhard Klimeck, Purdue University, gekco@purdue.edu



Over 13,000 / 330,000 Users Annually

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



ONLINE SIMULATION AND MORE
FOR NANOTECHNOLOGY

New Messages

Kishna Madhavan (on)


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nanoHUB-U offers
FREE courses

Self-paced nanotechnology
courses for working professionals
and students.

<http://nanohub.org/group/u>

SIMULATE with over 320 tools for nanoelectronics,
nanophotonics and more >

RESEARCH & COLLABORATE via groups, question board
and more >

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

SHARE & PUBLISH tools and research through our easy
upload process

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

Over 280,000 users annually

29 Live Simulation Sessions

Detailed statistics | Who's online?

RESOURCES

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Series, Teaching Materials, Tools, Workshops... All Categories >

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FEATURED




nanoHUB-U : New course starting Nov 7 - Register now! Principles of
Electronic Nanobiosensors




Active Media FDTD Nanophotonic Device Simulator : Modeling and
analysis of solid state, molecular or atomic semiconductor photonic
media. - In Tools




Introduction of MEMS Activity at Nano/Micro System Engineering Lab,
Kyoto ... - In Online Presentations



MSE 376 Lecture 15: Nanomagnetism, part 1 - In Online Presentations



ECE 606 Lecture 27: Introduction to Bipolar Transistors - Featured on
iTunes U



About - asked by Sharmali Islam, in Answers

NOTABLE QUOTE

*nanoHUB.org shows that there are more potential solutions than
there are problems.*

Jack Uldrich, Futurist and author (2013) - In Notable Quotes

NEW IN RESOURCES

nanoHUB-U, Principles of Nanoelectronic Biosensors Week One Scripts
in Online Presentations, Nov 10, 2013

MVS 1.0.1 Nanotransistor Model (Silicon)
in Compact Models, Nov 06, 2013

ECE 695S Lecture 12: The Exciting Science of Light with Metamaterials II
in Online Presentations, Nov 05, 2013

ECE 695S Lecture 11: The Exciting Science of Light with Metamaterials II
in Online Presentations, Nov 05, 2013

ECE 695S Lecture 10: The Exciting Science of Light with Metamaterials I
in Online Presentations, Nov 05, 2013

Does "http://nanohub.org/" is a new tab

It's FREE !!!

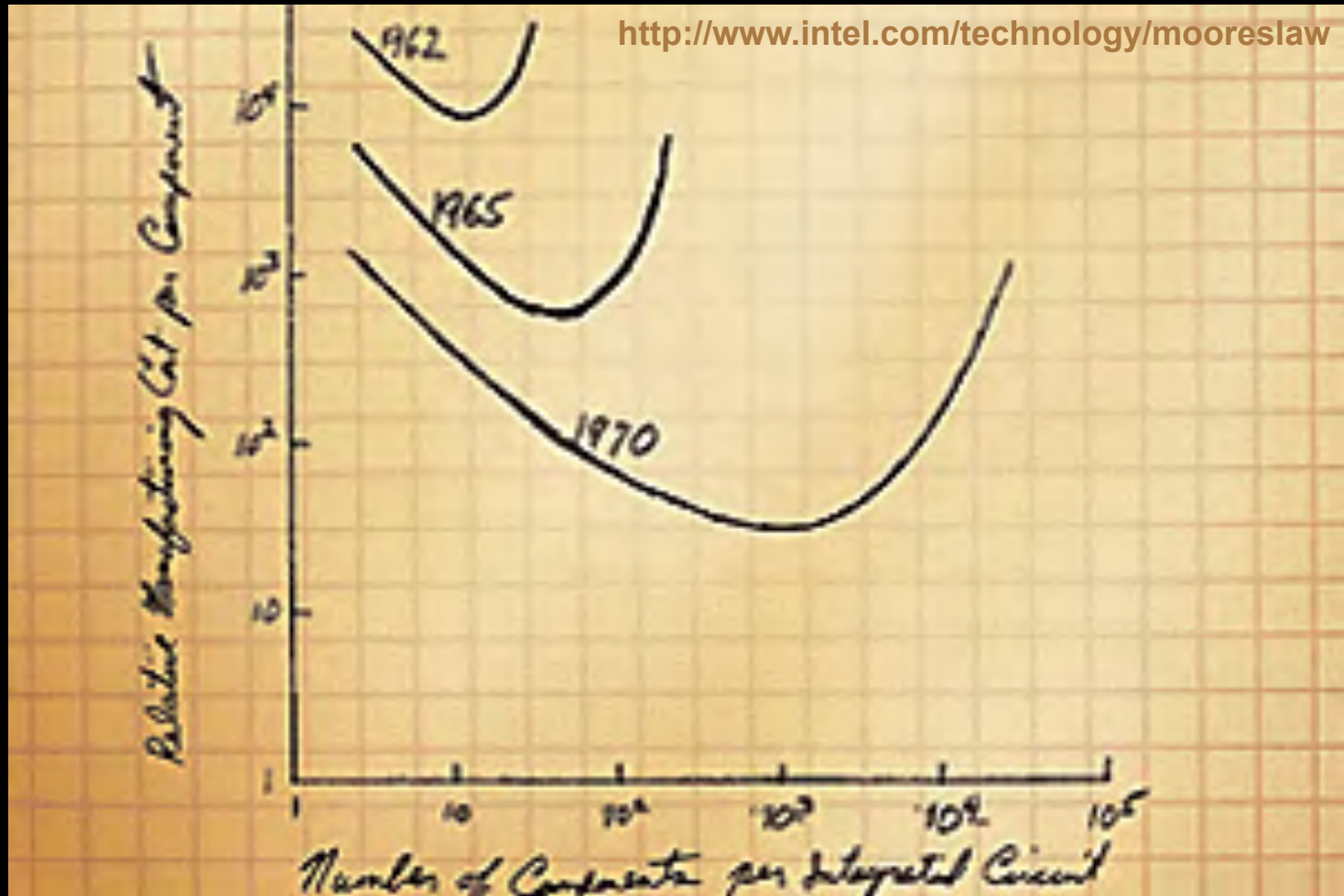
Yes, really !!!

Users do not pay anything!

1965

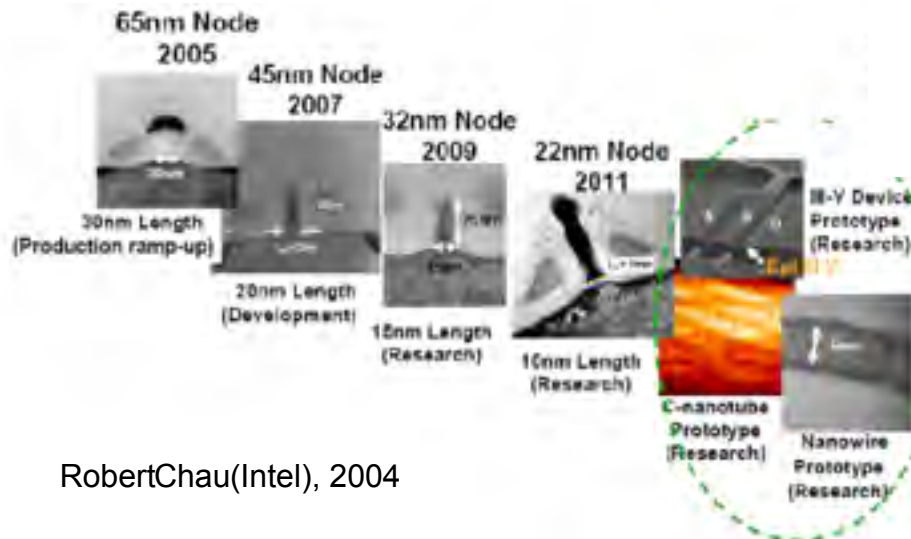
Gordon Moore

Relative Manufacturing Cost per Component



Number of Components per Integrated Circuit

Moore's Law

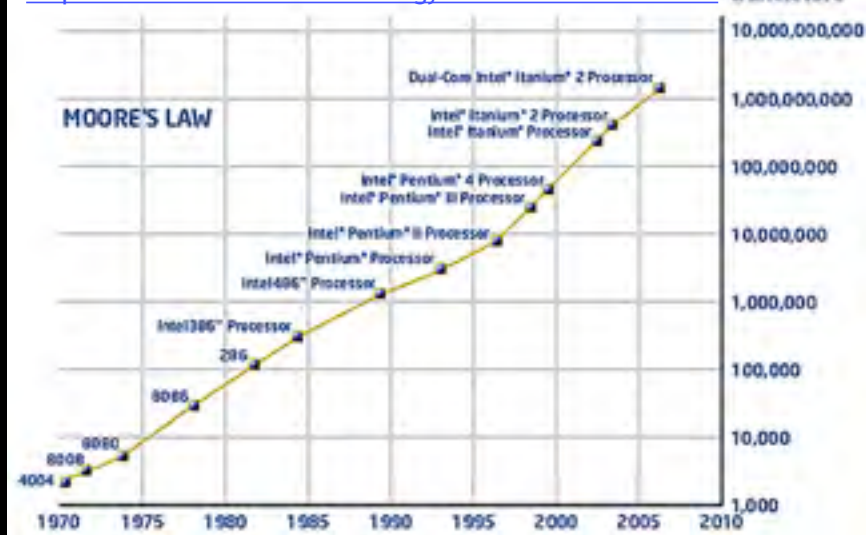


RobertChau(Intel), 2004

Device Size:
Tens of nanometers

Stanford SUPREM

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



Device Integration:
>2 Billion

Berkeley SPICE

Berkeley

Simulation Program with Integrated Circuit Emphasis.



Ronald
A. Rohrer



Laurence
W. Nagel



Donald O.
Pederson

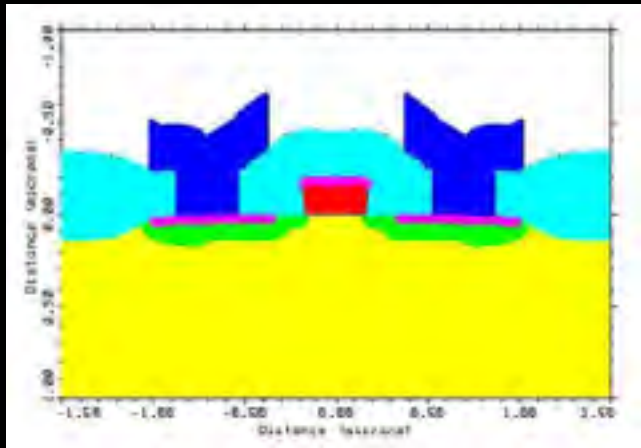
<http://www.omega-enterprises.net/>

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

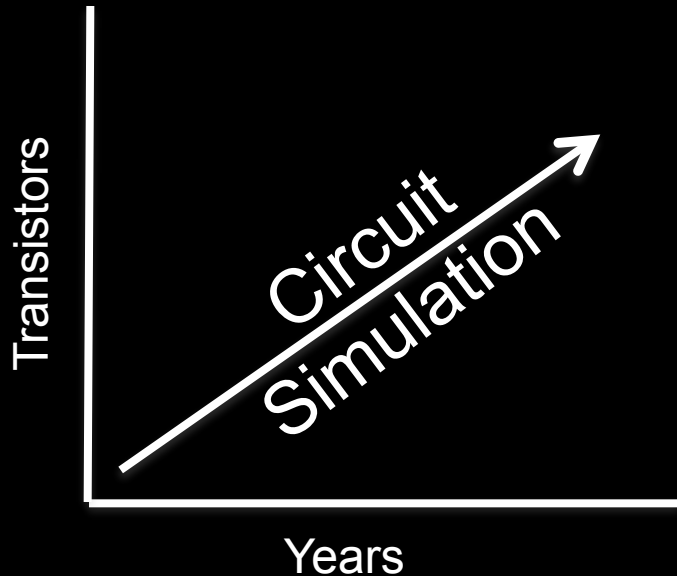
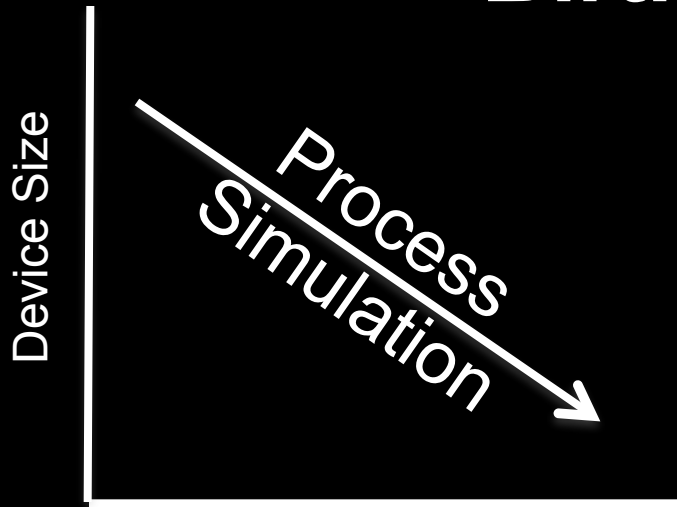
Stanford

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 Industry



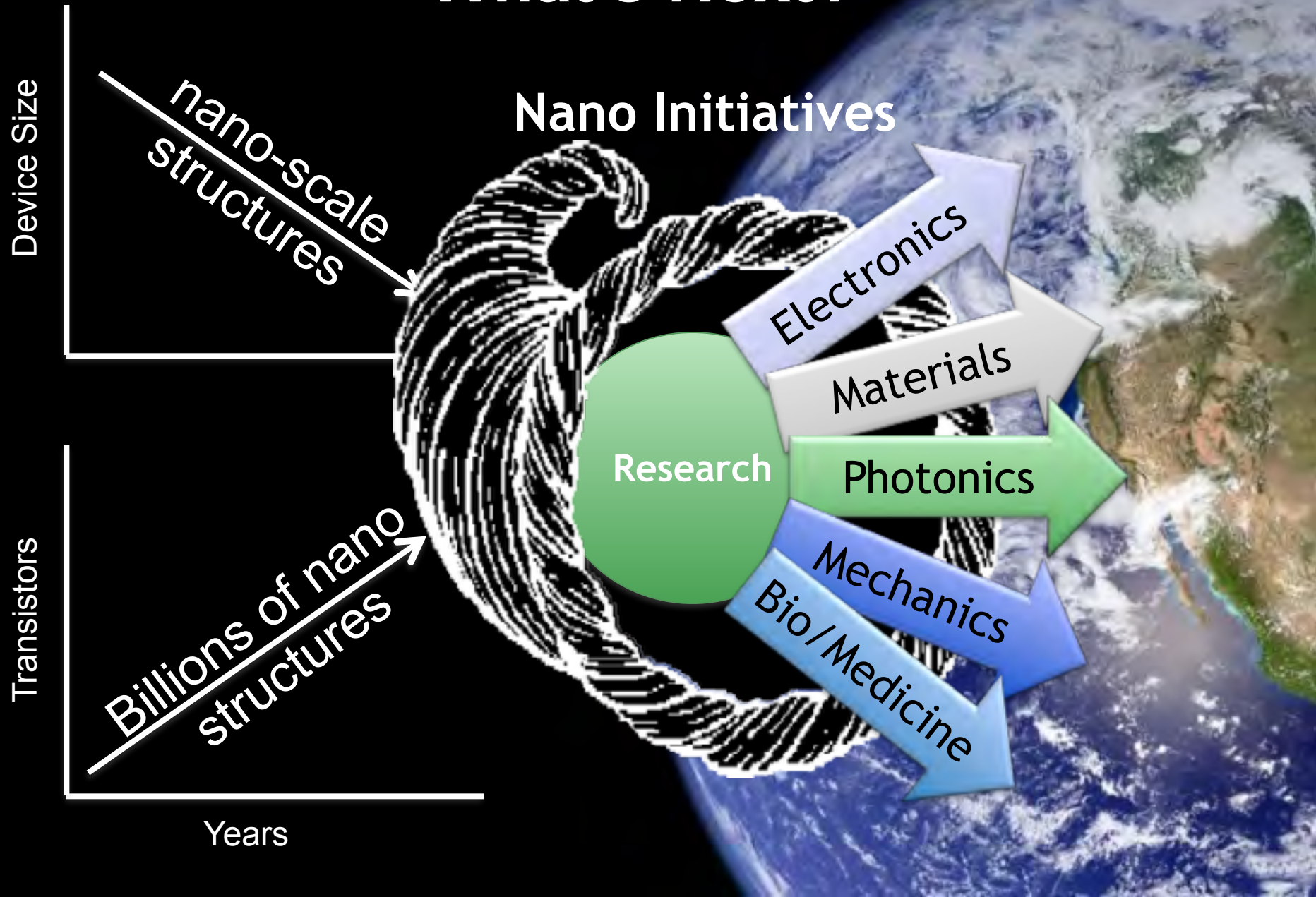
Intel Capitalization:

\$85B

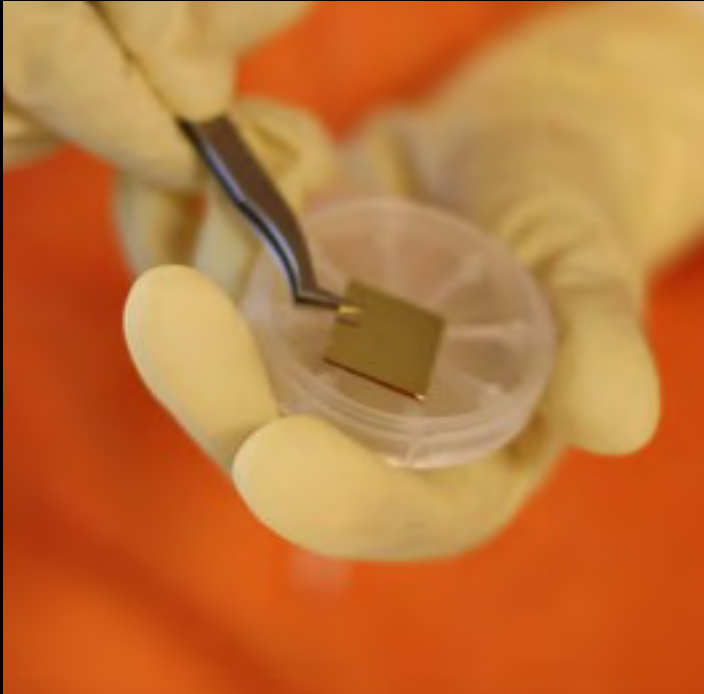
Total Industry:

\$280B

What's Next?



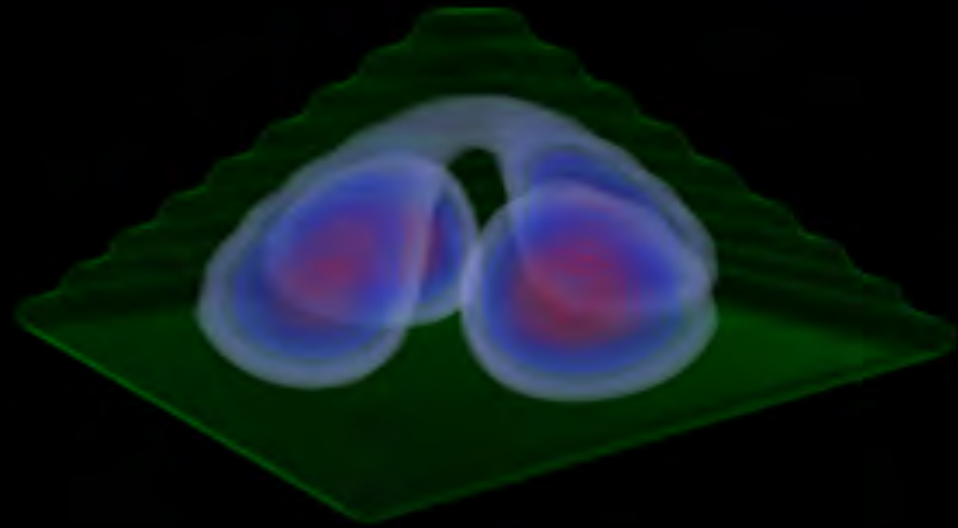
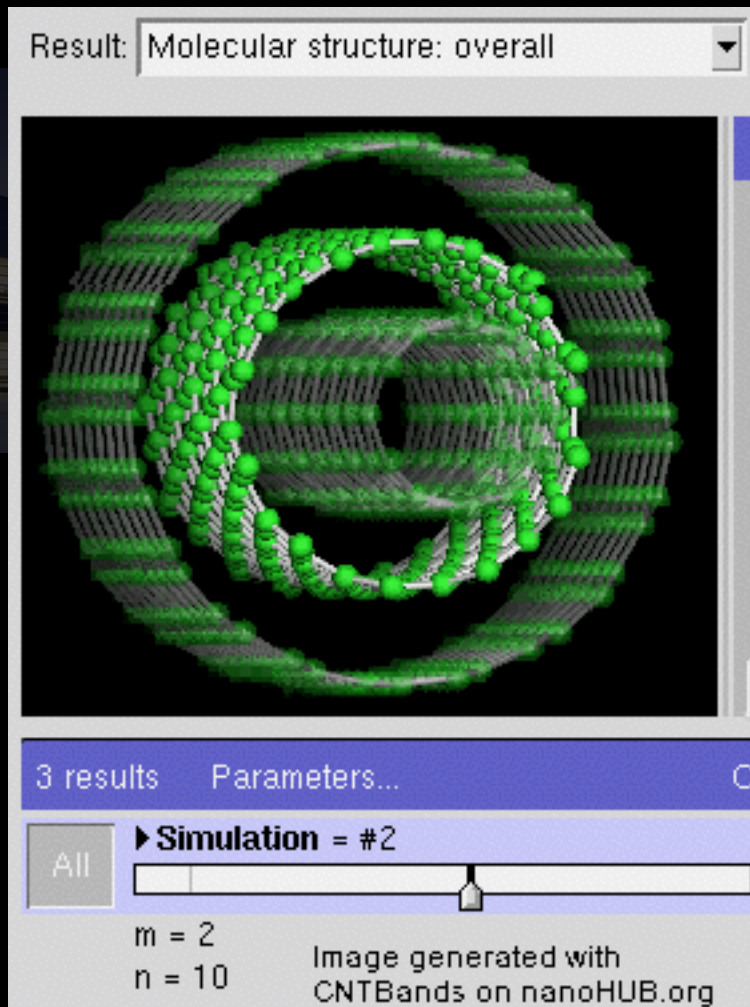
Nanotechnology



Extensive Facilities



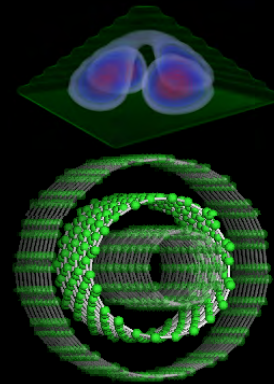
Nano Models



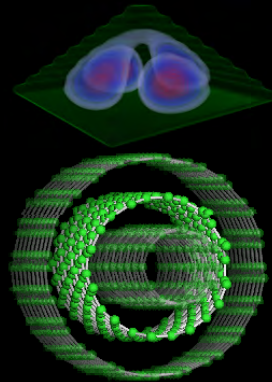
Quantum Dots
Artificial Atoms

Carbon Nanotubes

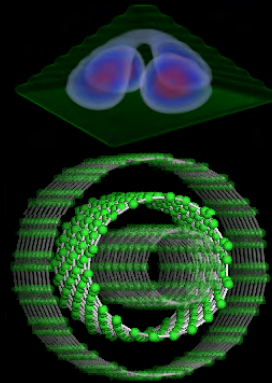
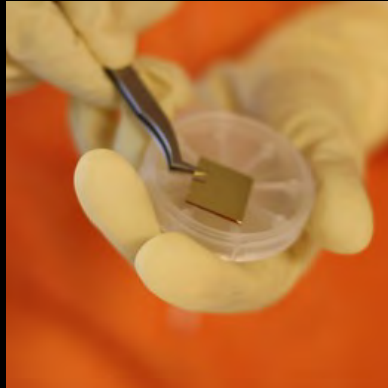
Computational Nano



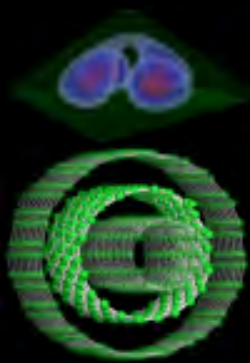
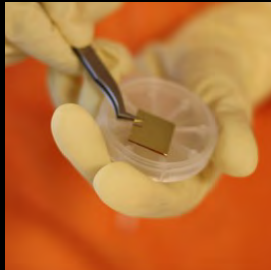
Computational Nano



Different Worlds



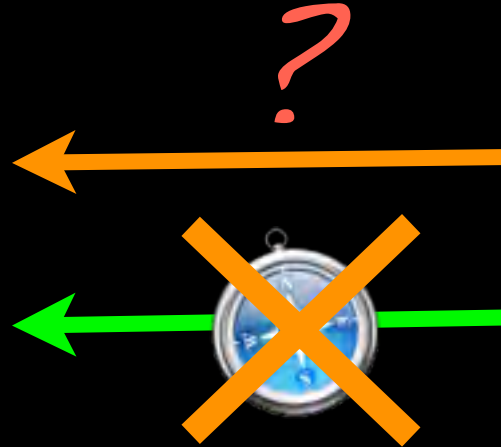
Imagine Breaking Barriers



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:potential = 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

Number of States: 7

Surface passivation: ☒ yes

Device Structure

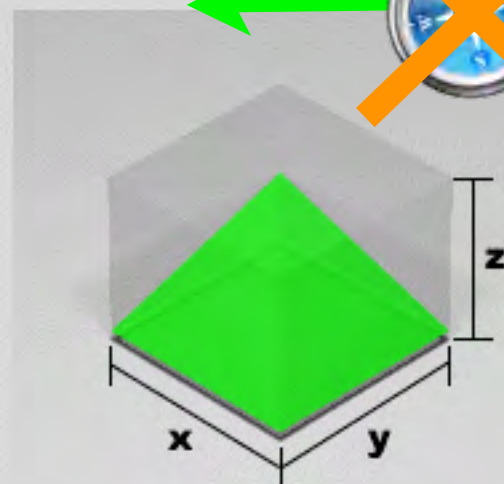
Light Source

Geometry: Pyramid

X dimensions: 10nm

Y dimensions: 10.5nm

Z dimensions: 5nm

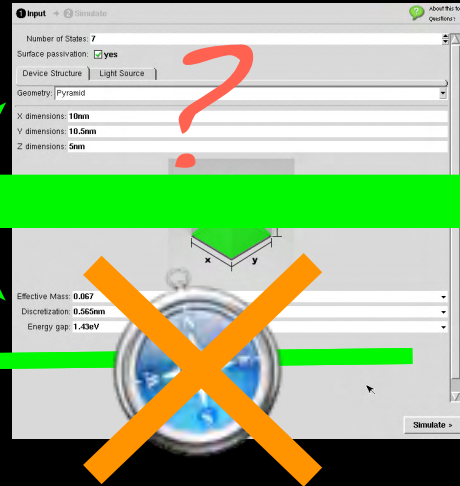


Effective Mass: 0.067

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

User Friendly

HUBzero

Rappture

Emerging Myths

User Friendly

Cannot use research codes for education

Must write own code to do research

Experimentalists cannot use research codes

Customers

Accessible (no installation)

NO End-to-end Science Cloud Possible

Market

Developer Friendly

Building User Interfaces too Difficult

Must rewrite code for web deployment

There is no incentive to share codes

Suppliers

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

```
Files: Double Gate MOSCap

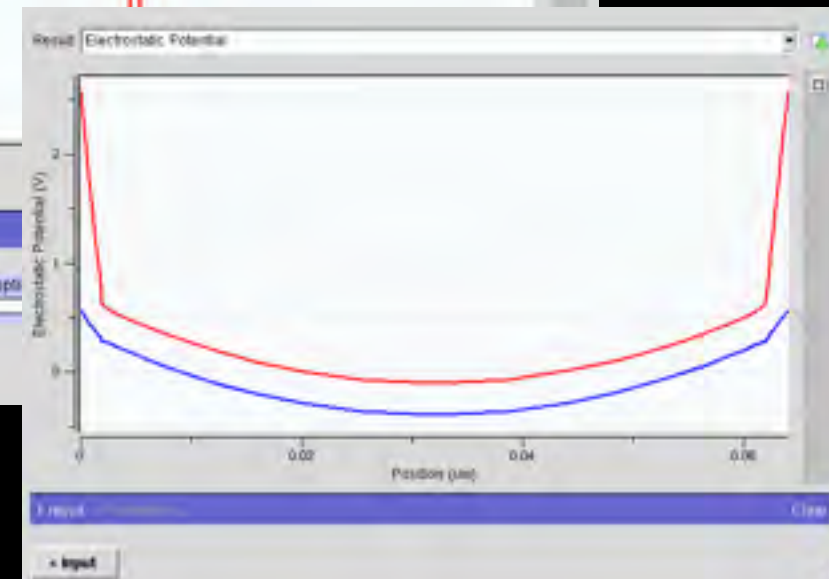
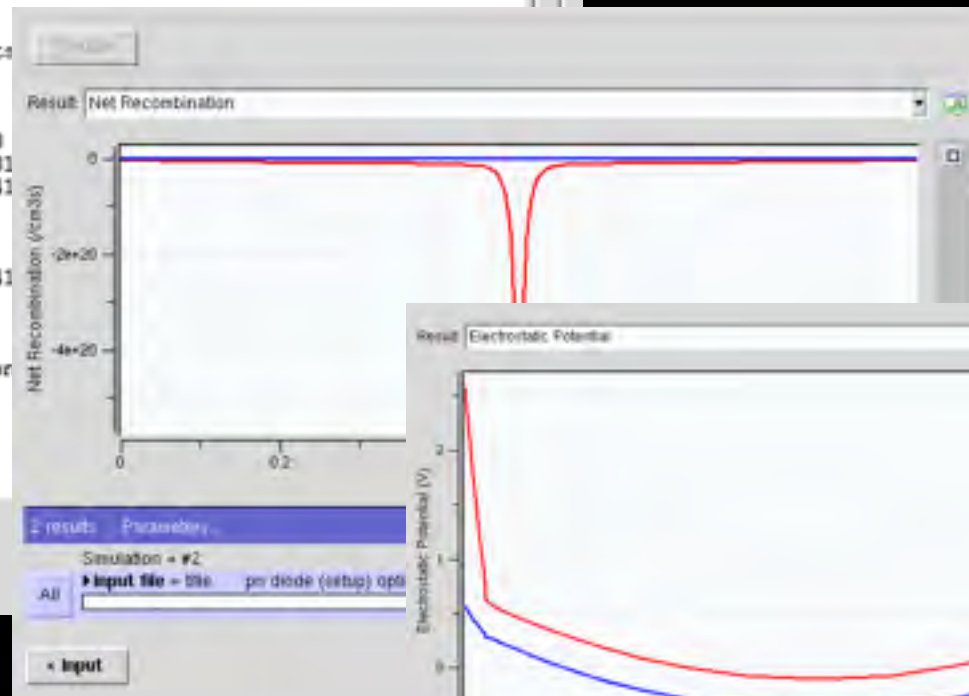
Input file: $ Mesh Specification
mesh      rect rox=3 ny=41
y.m       n=1  l=0 r=1
y.m       n=10 l=0.002 r=0.8
y.m       n=21 l=0.032 r=1.25
y.m       n=31 l=0.062 r=0.8
y.m       n=41 l=0.064 r=1.25
x.m       n=1 l=0 r=1
x.m       n=3 l=1 r=1
$ The y.m nodepoints and distance are inputs
$ The x.m parameters are static

$ Regions specification
region    num=1 ix.l=1 ix.h=3 iy.l=1 iy.h=10
region    num=2 ix.l=1 ix.h=3 iy.l=10 iy.h=31
region    num=3 ix.l=1 ix.h=3 iy.l=31 iy.h=41

$ Electrodes specification
elec      num=1 ix.l=1 ix.h=3 iy.l=1 iy.h=1
elec      num=2 ix.l=1 ix.h=3 iy.l=41 iy.h=41

$ Doping specification
dop reg=2 p.type conc=1e+18 uniform
$ doping can be p.type or n.type (two options)

$ Contact specification
contact   all neutral
contact   num=1 n.polysilicon
contact   num=2 n.polysilicon
```



MOSFET: Running PADRE Simply

Structural Properties | Model | Voltage Sweep

Simulate new input parameters

About this tool

Device Type: MOSFET n-type

Doping Profile: Uniform Doping Density

Source/Drain Length: 50nm

Source/Drain Nodes: 15

Channel Length: 100nm

Channel Nodes: 20

Oxide Thickness: 2nm

Oxide Nodes: 5

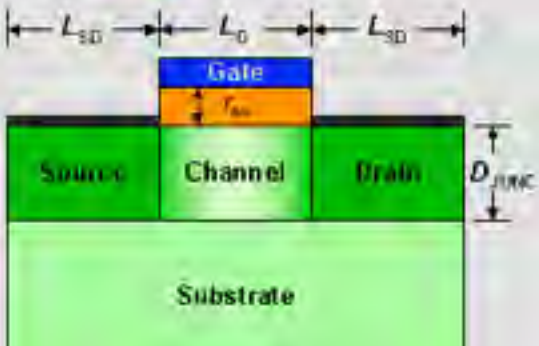
Junction Depth: 21nm

Junction Nodes: 20

Substrate Thickness: 68nm

Substrate Nodes: 25

Device Width: 1000nm



MOSFET tool (v. 1.0padre)

Learn about Metal Oxide Semiconductor Field Effect Transistors (MOSFET) as you explore the devices in this simulator.

Input values for the various parameters on the left and click "Simulate" at the top to run the simulation. (Note: After the simulation has finished, 3D plots may still take some more time to load.)

Parameters:

- Structural Properties
General properties of the materials used, such as physical dimensions and doping.
- Model
Toggle simulation parameters to take certain physical phenomena into account, such as impact ionization, at the sacrifice of computation speed. Also define the effects the surroundings have on the device, including temperature.
- Voltage Sweep
Define the effects the surroundings have on the device, including applied voltage.

MOSFET model notes:

- V_substrate, the voltage applied to the substrate is tied to the source and is always grounded. The user can vary the gate and drain voltage, with respect to ground, in this simulation model.
- The entire device, except the oxide layer, is simulated as silicon.

Impact of Simplified GUI Tools

945 Users,
41,285 jobs

6,649 Users,
104,282 jobs

```
Files: Double Gate MOSCap
Input file:
$ Mesh Specification
mesh rect x0=0 x1=41
y.m n=1 l=0 r=1
y.m n=10 l=0.002 r=0.8
y.m n=21 l=0.032 r=1.25
y.m n=31 l=0.062 r=0.8
y.m n=41 l=0.064 r=1.25
x.m n=1 l=0 r=1
x.m n=3 l=1 r=1
$ The y.m nodepoints and distance are inputs
$ The x.m parameters are static

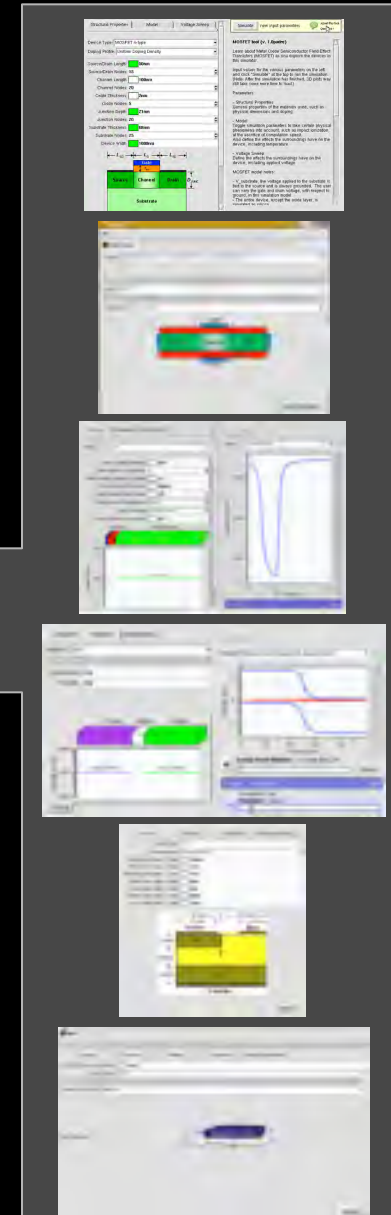
$ Regions specification
region num=1 ix l=1 ix h=3 iy l=1 iy h=10 name=sio2 INS
region num=2 ix l=1 ix h=3 iy l=10 iy h=31 name=silicon SEMI
region num=3 ix l=1 ix h=3 iy l=31 iy h=41 name=sio2 INS

$ Electrodes specification
elec num=1 ix l=1 ix h=3 iy l=1 iy h=1
elec num=2 ix l=1 ix h=3 iy l=41 iy h=41

$ Doping specification
dop reg=2 p.type conc=1e+18 uniform
$ doping can be p.type or n.type (two options), conc is a parameter too

$ Contact specification
contact all neutral
contact num=1 n.polysilicon
contact num=2 n.polysilicon

Simulate >
```



MOSFET:
2,715 Users,
38,000 jobs

MUGfet:
240 Users,
3,600 jobs

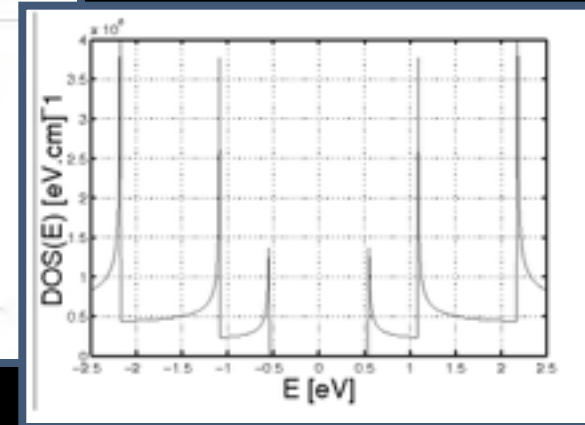
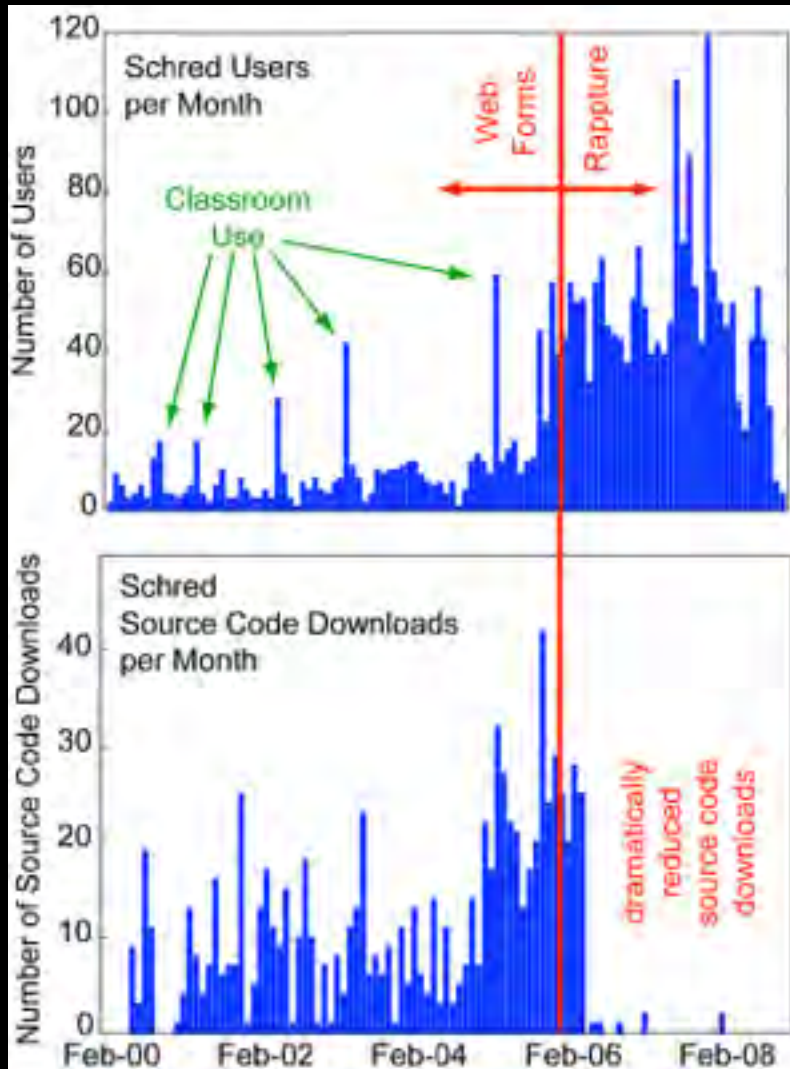
MOSCAP:
1,694 Users,
18,000 jobs

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

BJT:
557 Users,
3,000 jobs

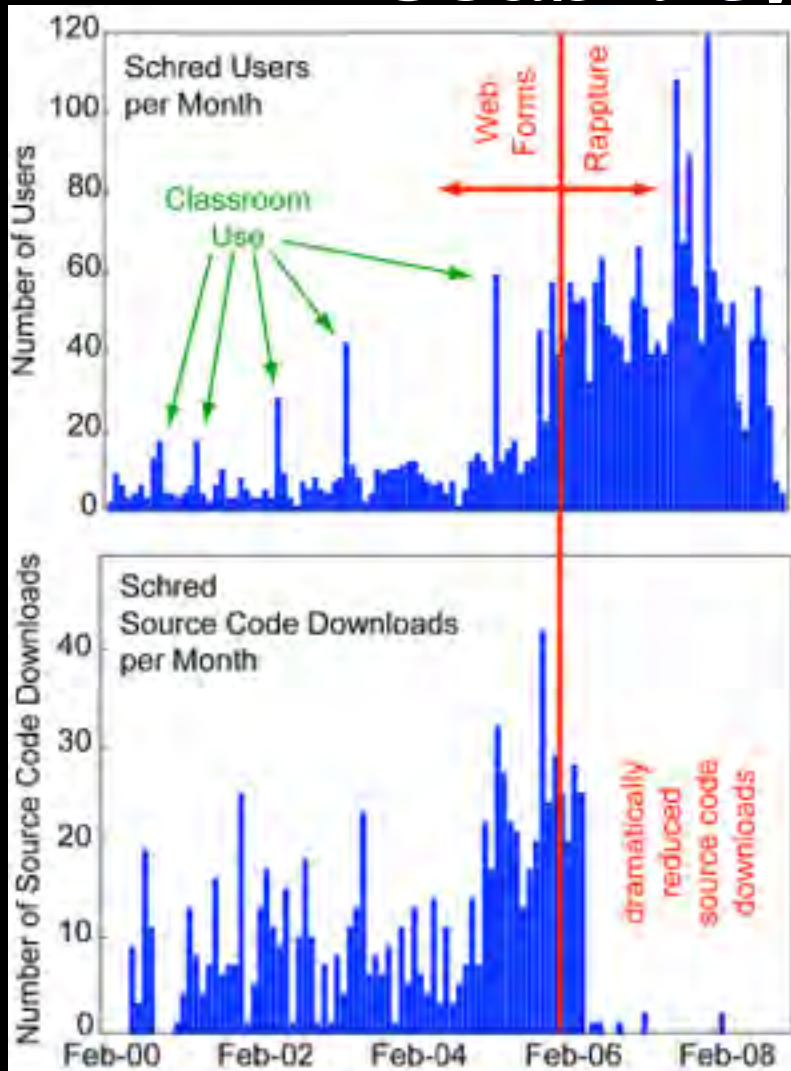
Drift-Diffusion:
721 Users,
7,400 jobs

Importance of a good GUI

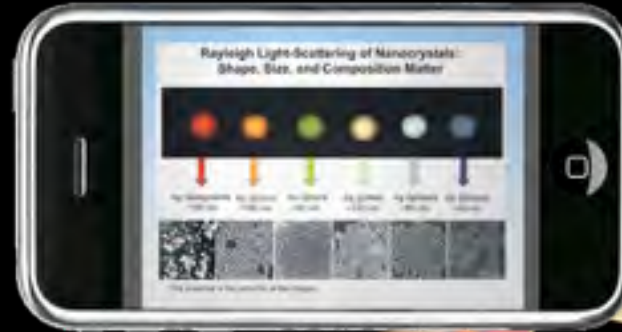


Same behavior across all similar converted tools

Balancing Usability and Capability

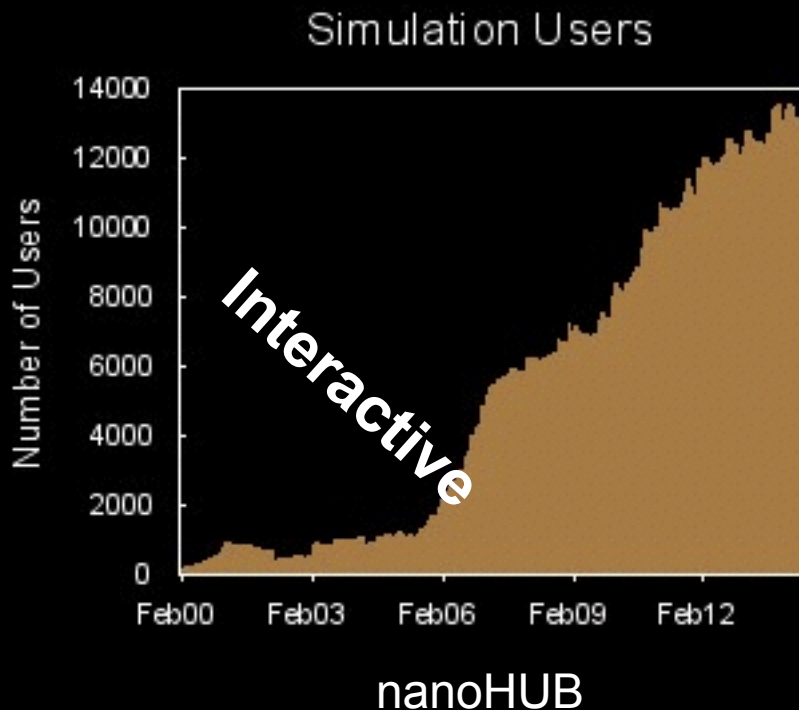
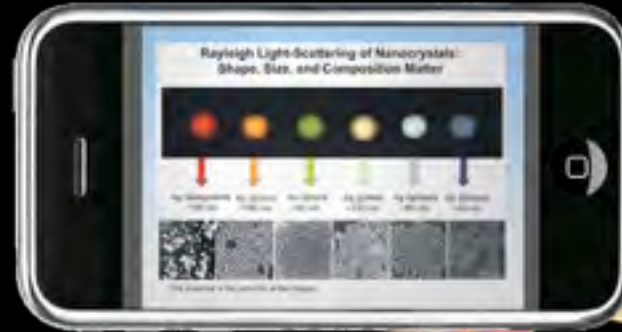


nanoHUB



iPhone / iPad

Balancing Usability and Capability

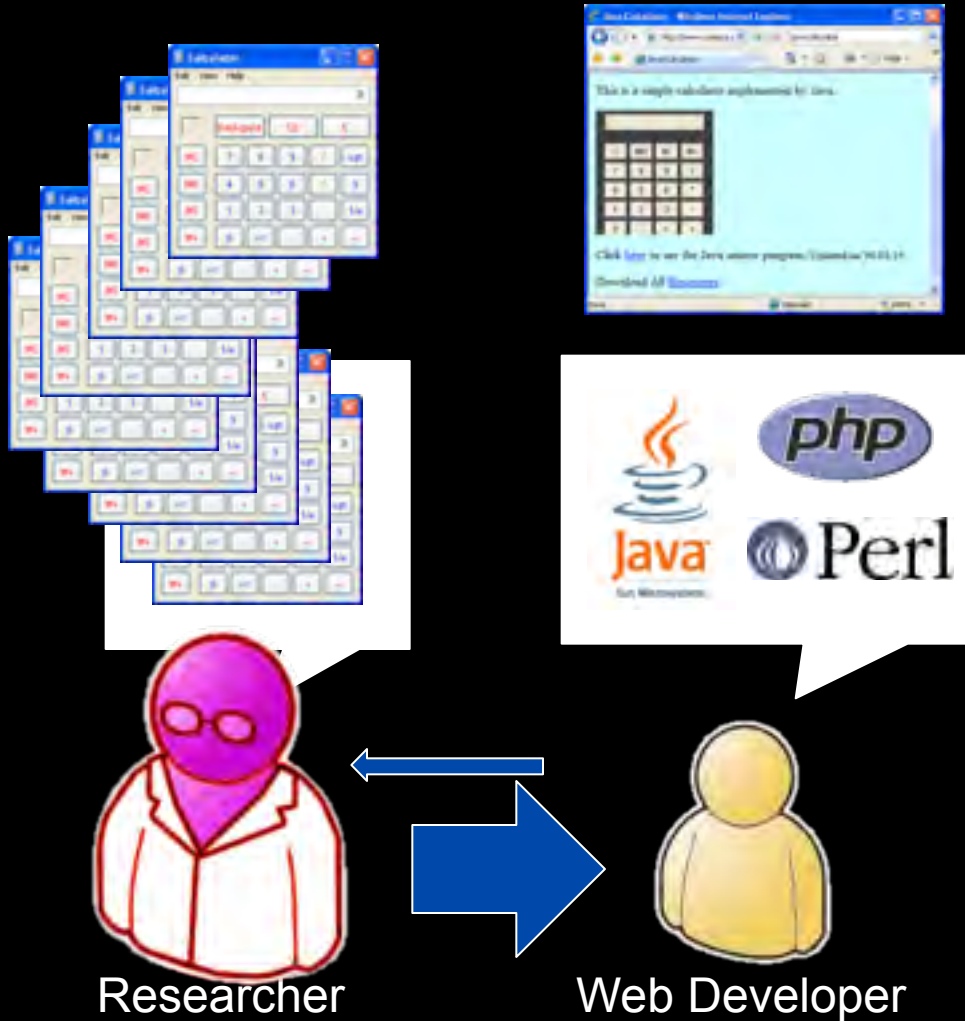


iPhone / iPad

What else is different?
Developer Experience?



Usual Science Gateway Process



• ~~175 tools / 4 years:~~
~~=> \$88M~~

• \$500k/tool



• NO new research!

• Not validated by researcher (disowned)

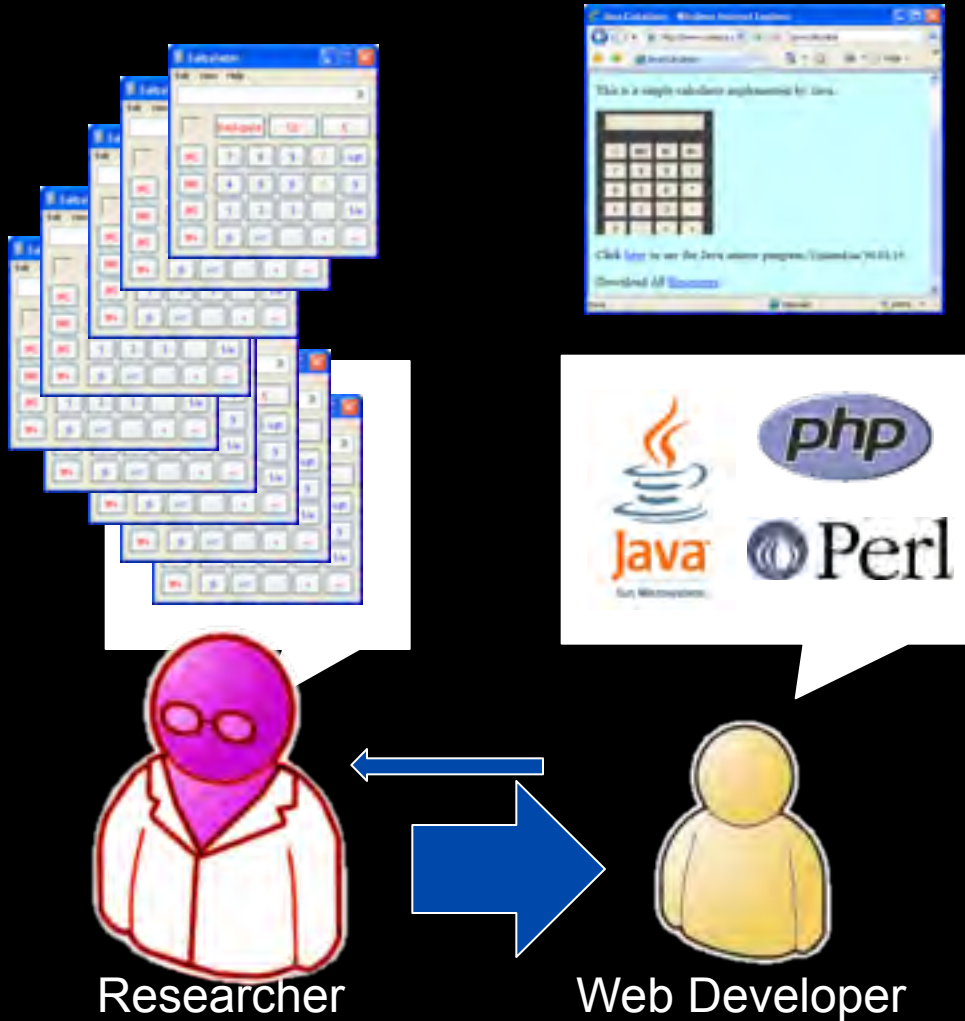
• Researcher has much better version

• Code rewrite takes 2-3 years

Many Proposals read alike



Usual Science Gateway Process



• ~~175 tools / 4 years:~~
~~=> \$88M~~

• \$500k/tool



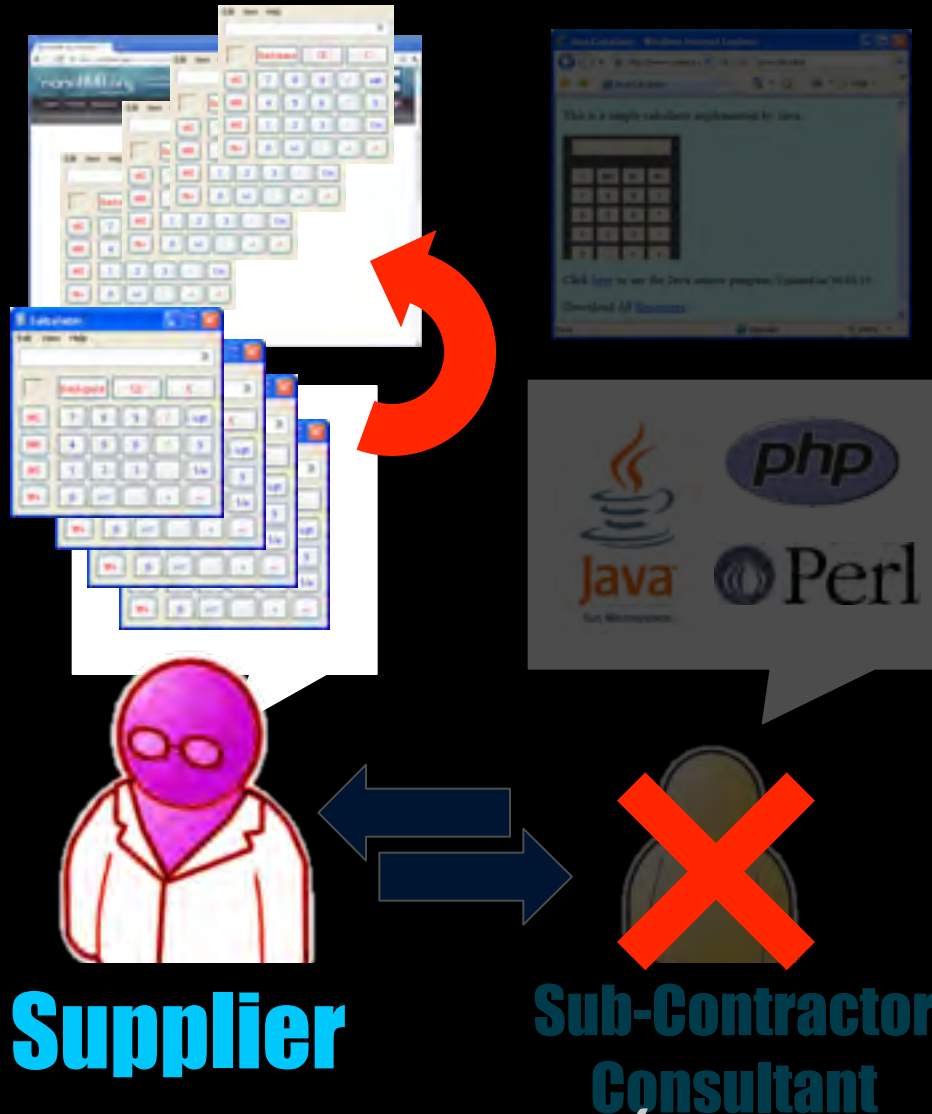
Customers / Users

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

Generating a Bad Reputation

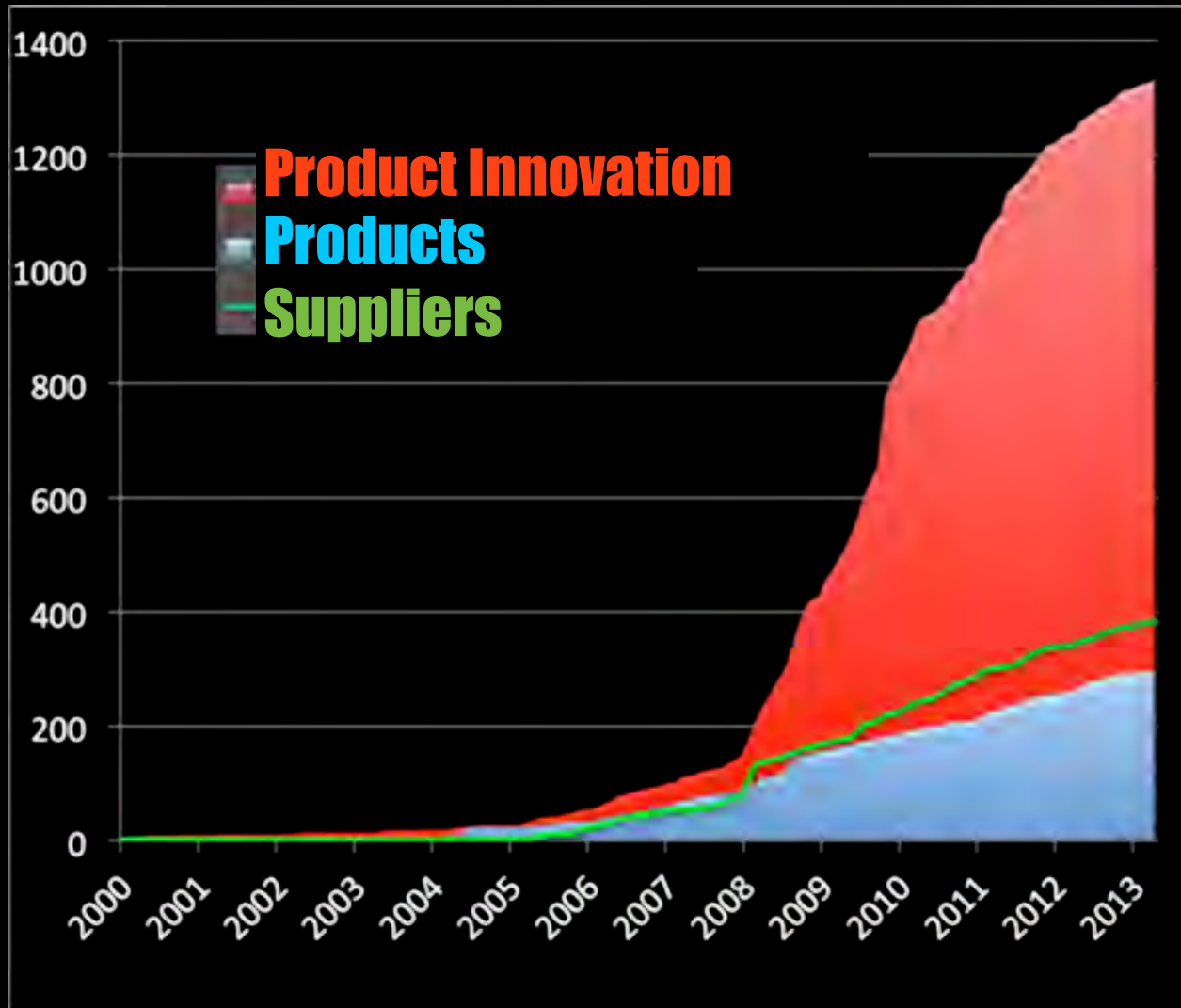


nanoHUB Process



- **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



v3



Continual
Engagement

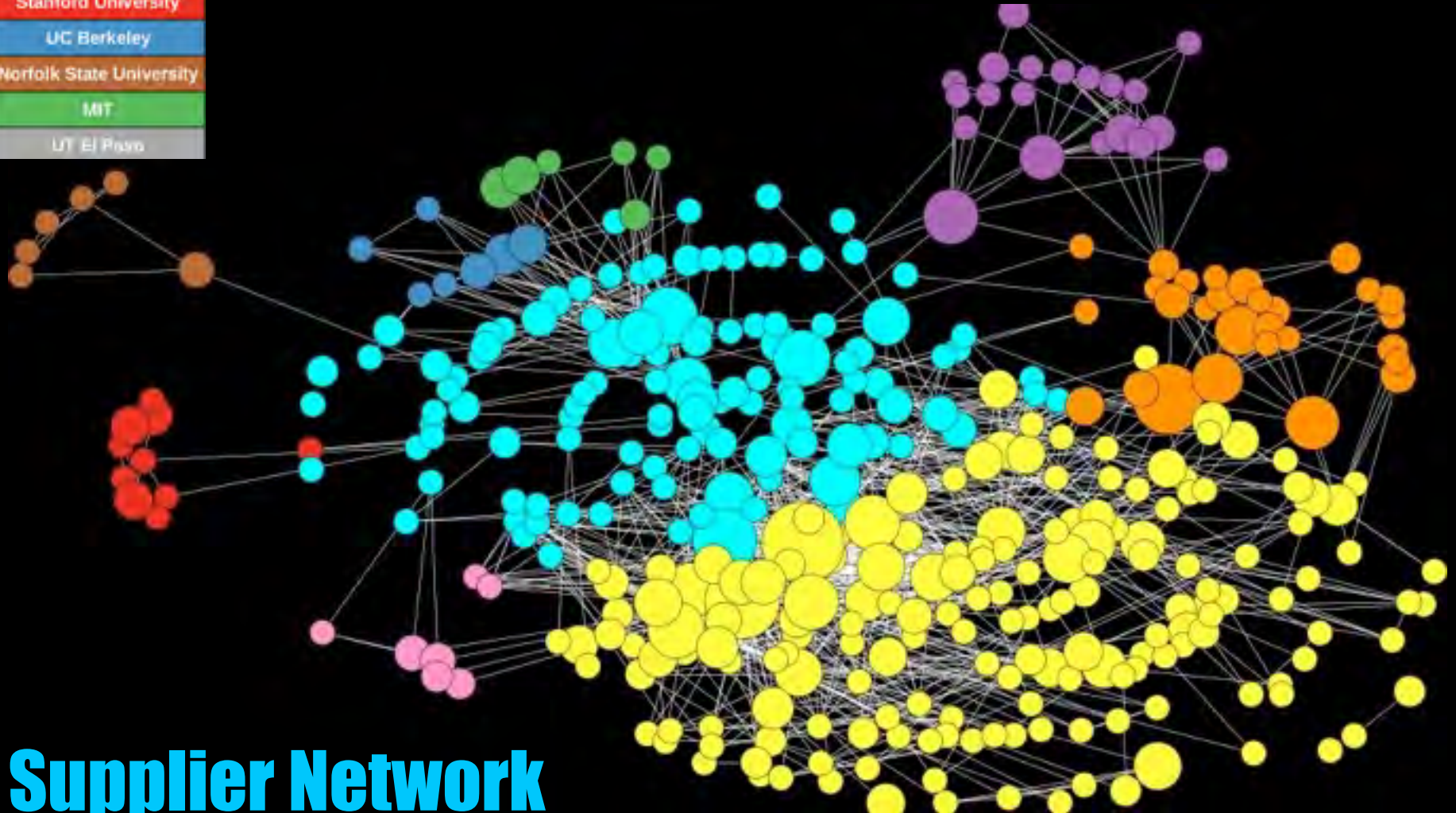
380+ Developers
NOT PAID by NCN

nanoHUB can prove it

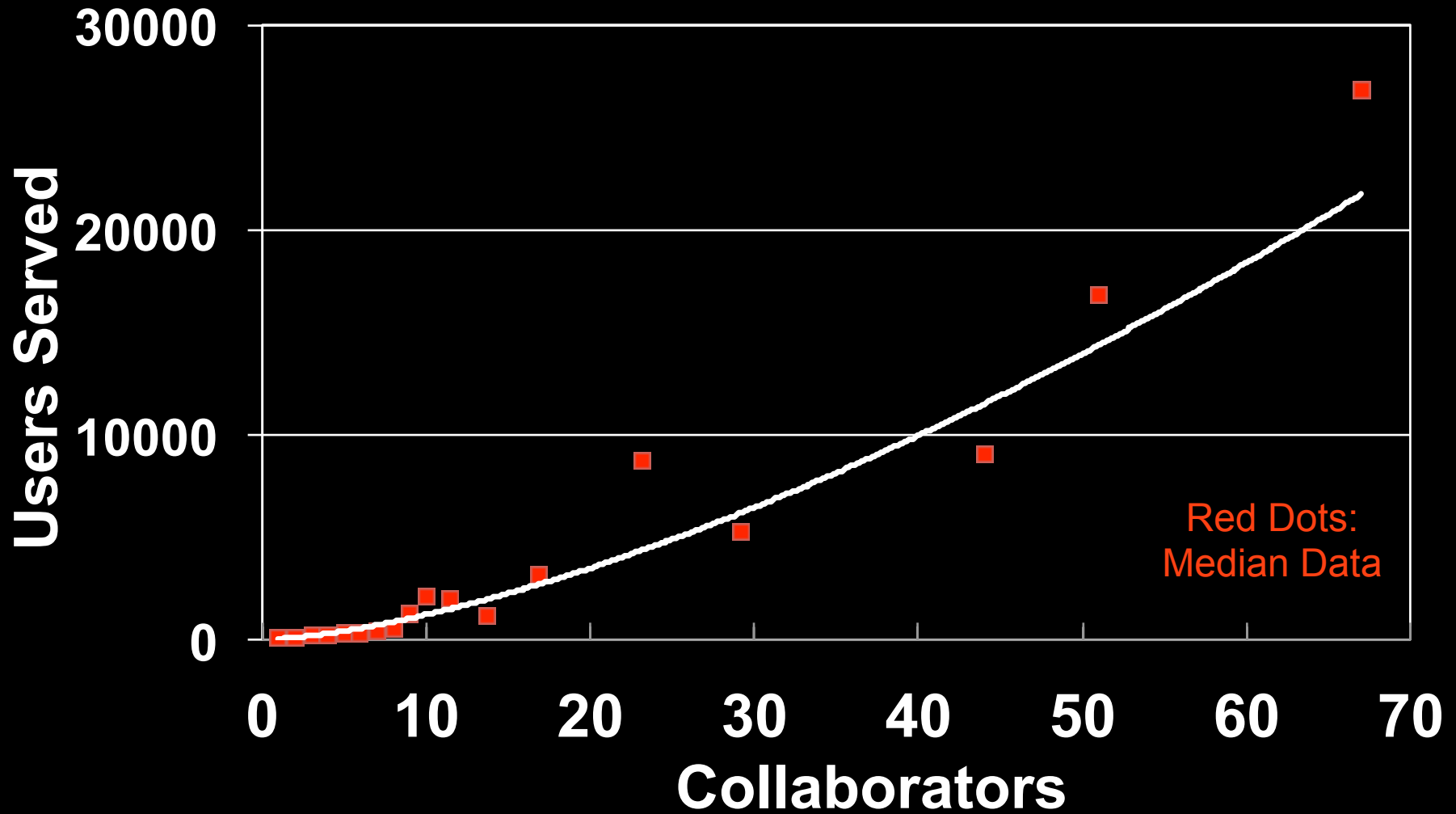
Developer Collaboration Network

Purdue University
Northwestern University
University of Illinois
University of Florida
Stanford University
UC Berkeley
Norfolk State University
MIT
UT El Paso

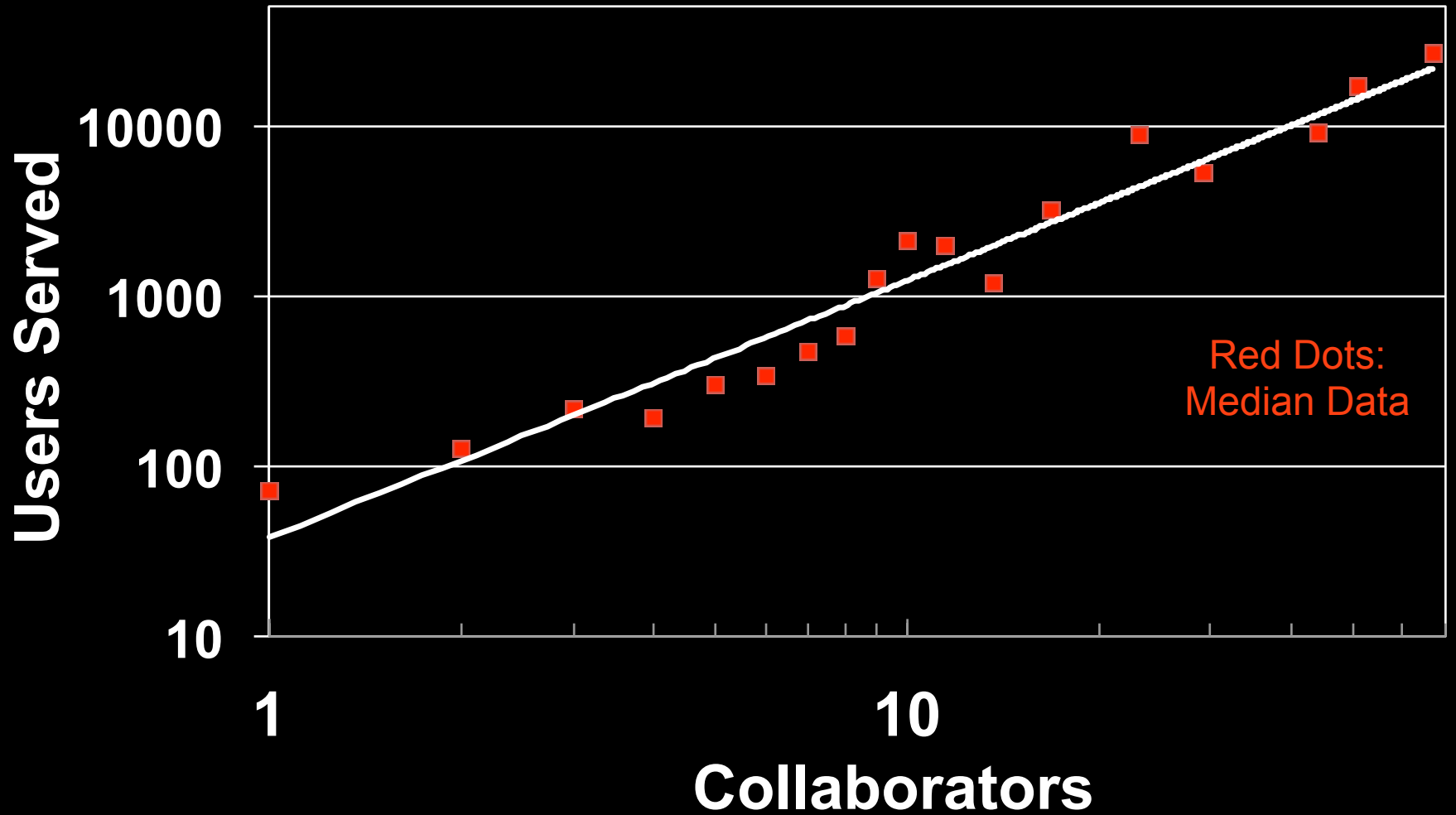
Each dot is a Developer **suppliers**
Links are tools **product**



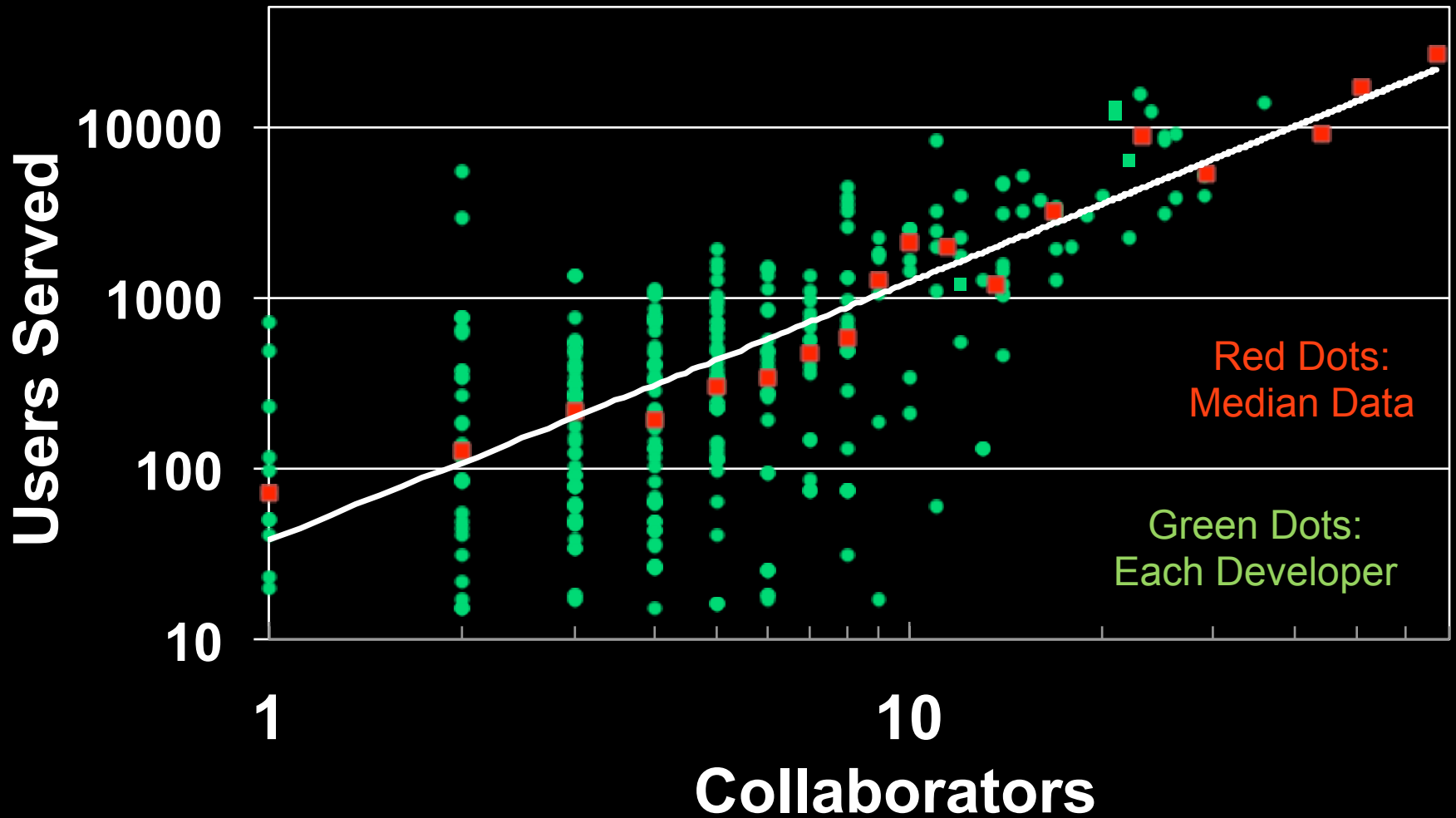
Developer Collaboration Impact



Developer Collaboration Impact

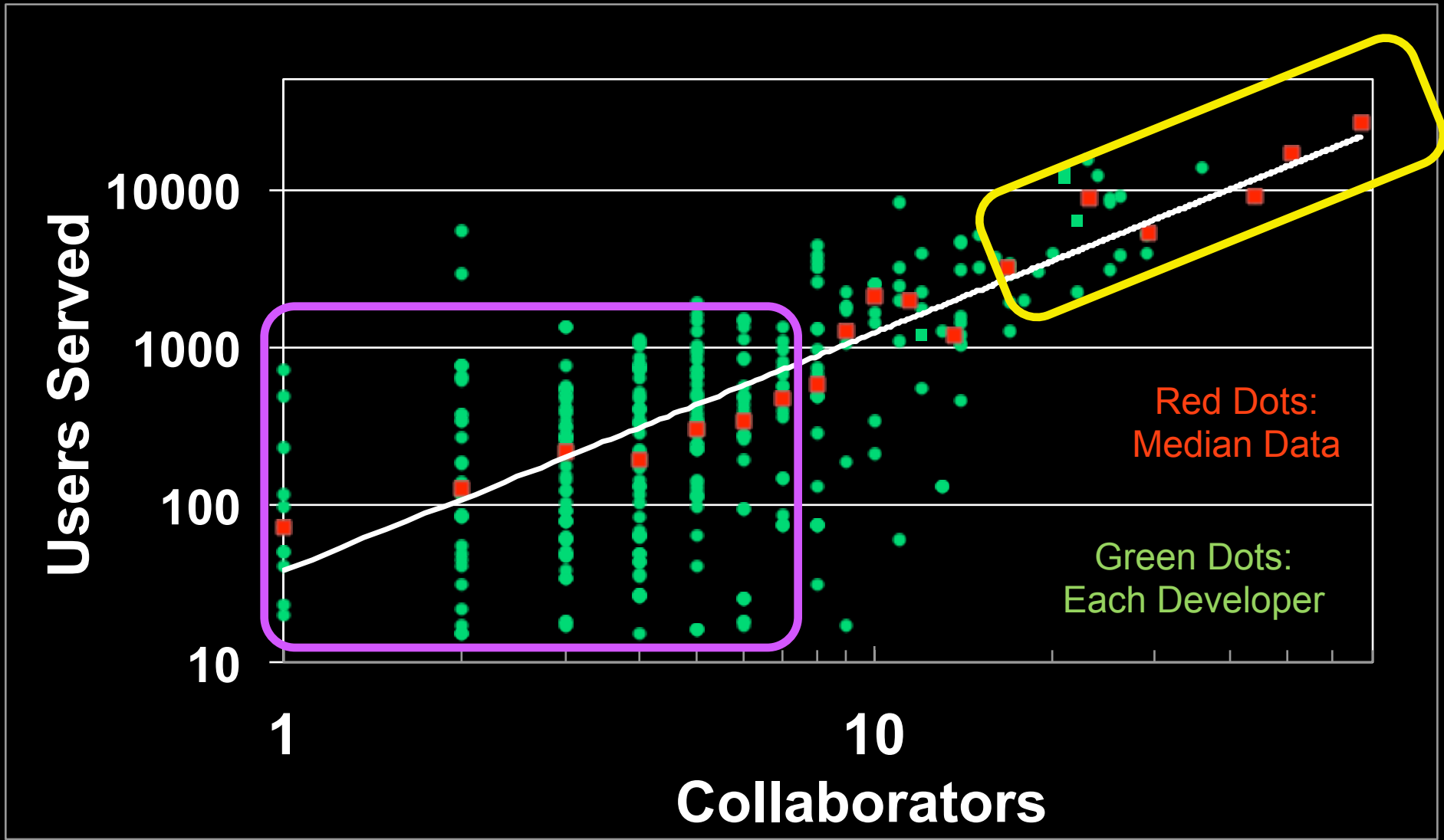


Developer Collaboration Impact



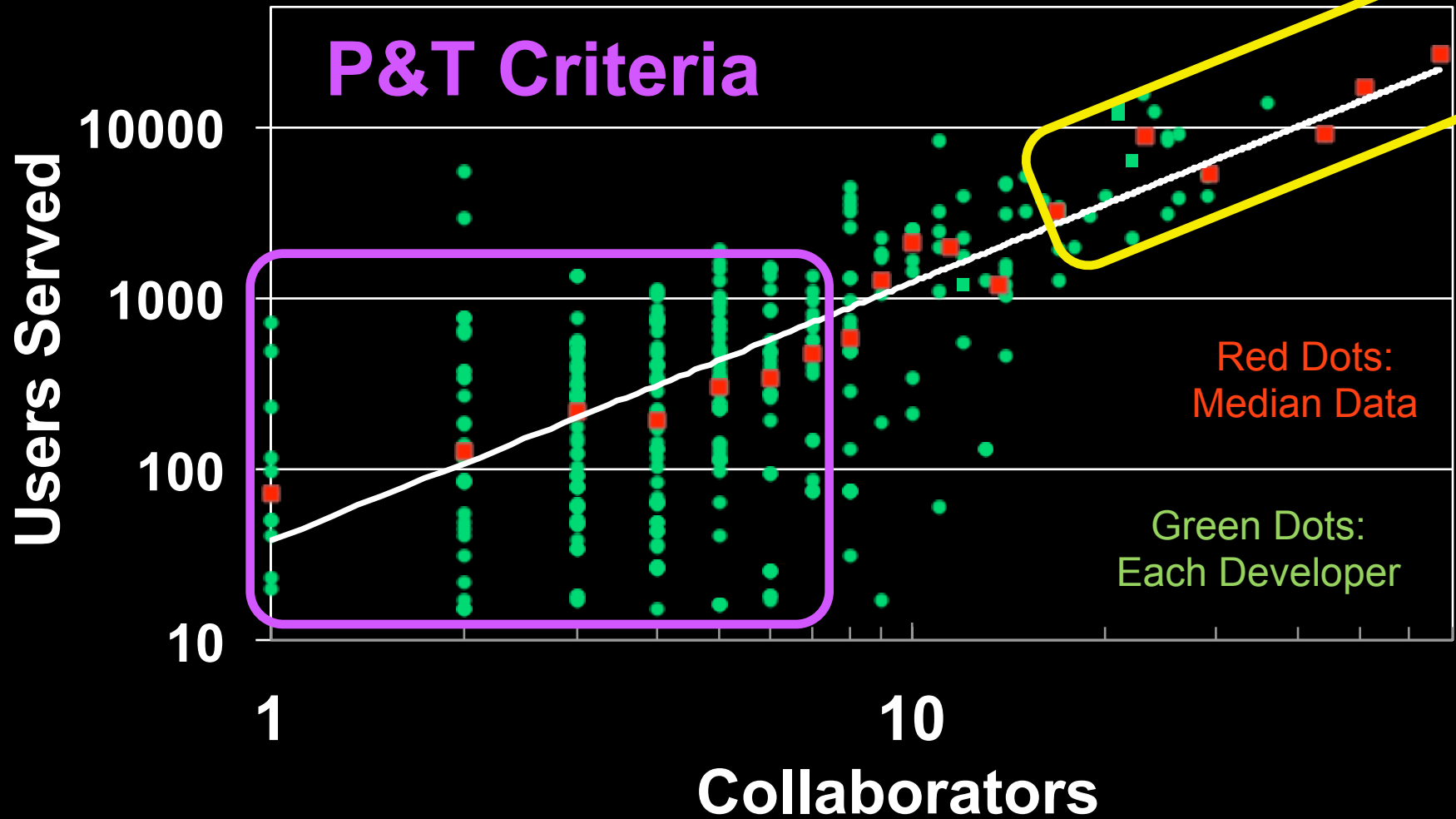
Small Collaborations:
Scattered Success

Large Collaborations:
Predictable Success



Old Approach

Surviving Universities

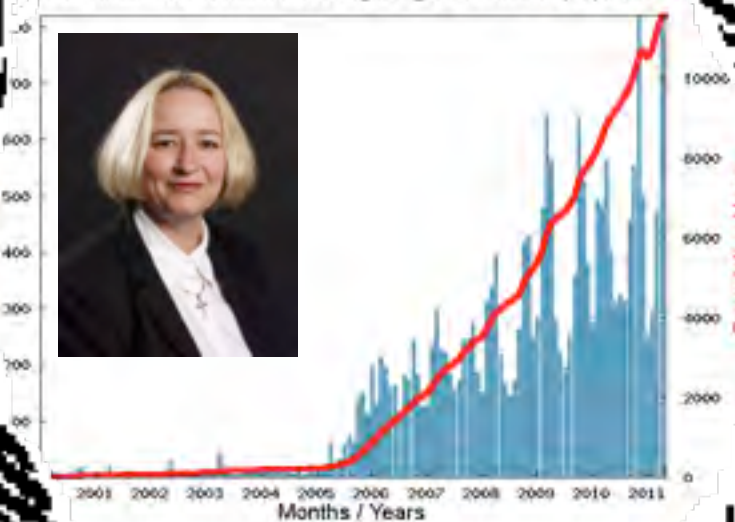


Next Generation Publications Research Incentives

Great for Proposals
=> Proof of outreach

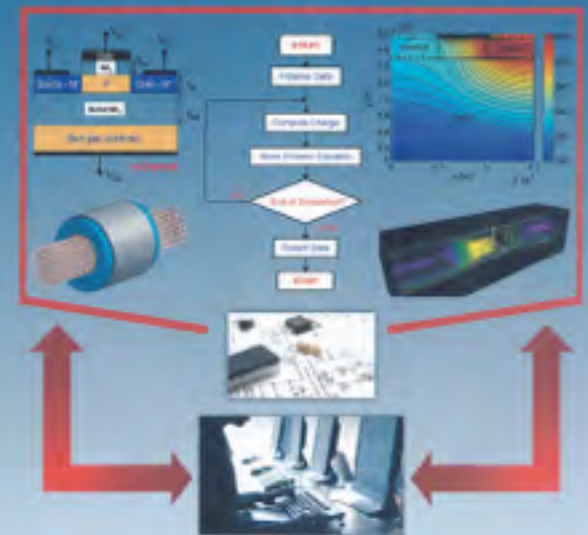
Dragica Vasileska

Years of Simulation Tools Authored by Dragica Vasileska (11,570 Users)



Computational Electronics

Semiclassical and Quantum
Device Modeling and Simulation



Dragica Vasileska • Stephen M. Goodnick • Gerhard Klimeck



CRC Press
Taylor & Francis Group

17 tools
→ 11,570 users
→ 123 citations

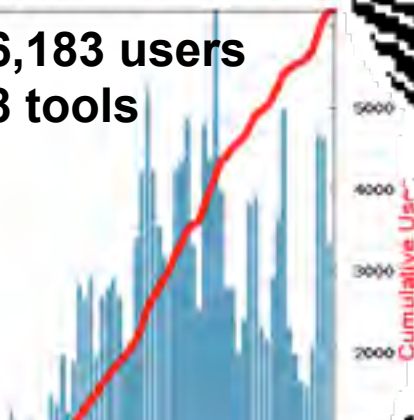
Next Generation Faculty:

Shaikh Ahmed

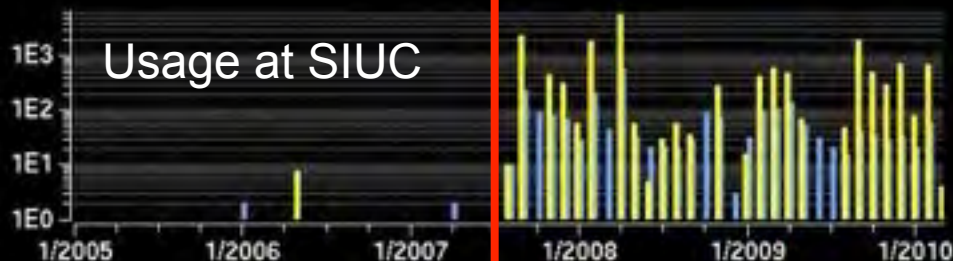
Simulation Tools Authored by Shaikh S. Ahmed (6,183 Users)



6,183 users
8 tools



Usage at SIUC



Post Doc
at Purdue

Faculty at
SIUC

- Infused nanoHUB into existing classes
- Built 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**

Wikipedia Different Advertising

ਨੈਨੋਤਕਨੀਕ

ਨੈਨੋਤਕਨੀਕ ਜਾਂ ਨੈਨੋਪ੍ਰੋਟੈਕਨੀਕ, ਵਿਵਹਾਰਕ ਸੀਮਾ ਦੇ ਅੰਦਰ ਵੈੱਬ ਨੈਨੋਟਕਨੀਕ ਦੇ ਰੂਪ ਵਿੱਚ ਹੈ ਅਣੂਆਂ ਦੇ ਛੋਟੇ ਕੰਟਰੋਲ ਪ੍ਰਭਾਵ ਤੇ ਕੰਟਰੋਲ ਹੈ। ਇਨ੍ਹਾਂ ਵਿਸ਼ੇਸ਼ਤਾਵਾਂ ਵਿੱਚੋਂ ਇੱਕ ਹੈ ਕਿ ਨਤੀਜੇ ਹੇਠਲੇ। C₆₀, ਜਿਨ੍ਹਾਂ ਬਕਿਟਾਲ ਵੀ ਕਹਿੰਦੇ ਹਨ, ਜੋ ਕਾਰ



ਬਕਮਿਨਸਟਰ ਫੁੱਲਰੀਨ C₆₀ ਦਾ ਘੁੰਮਦਾ ਚਿੱਤਰ

Punjabi

Dalla grafite al C₆₀

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

L'adattamento del fullerene nanometrico rimane chimici hanno esplorato che potrebbero essere interstellari dove il carbonio. Smalley (Rice University) ha vaporizzato mediante cluster contenenti spiccioli di 60 atomi. Harry Kroto ha una geometria possibile. Denominati buckminsterfullerene, questi oggetti furono rapidamente



Veduta ruotante di cristallo C₆₀ di Fullerene Buckminster.

Italian

Fullerene

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

German

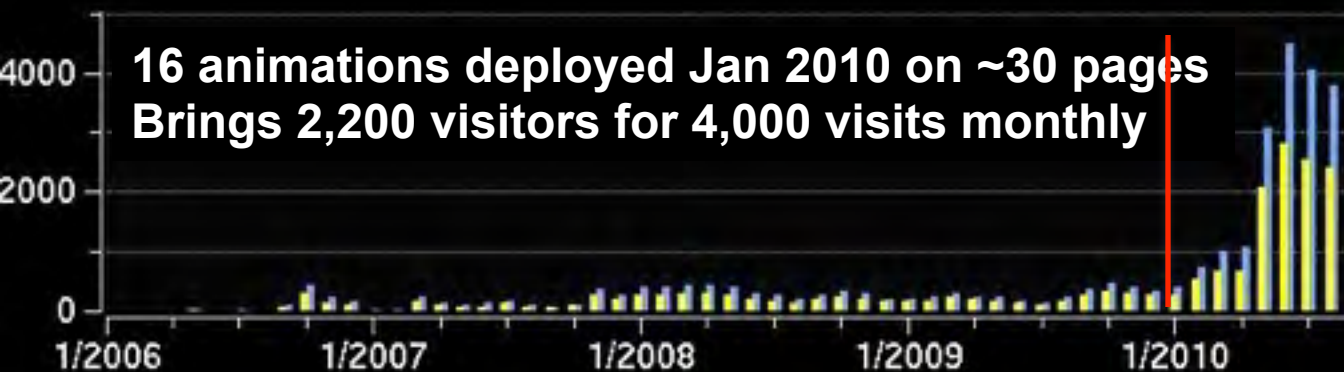


rotierende Struktur von C₆₀



Geschichte

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





360+ Interactive Tools
400+ Developers (mostly volunteers)

Products

Suppliers 'oper Friendly
Myths Busted

User Interfaces too Difficult
rewrite code for web deployment
There is no incentive to share codes

HUBzero
Rapture

Market

Emerged Myths



Activities on
<http://nanoHUB.org>
in 172 countries

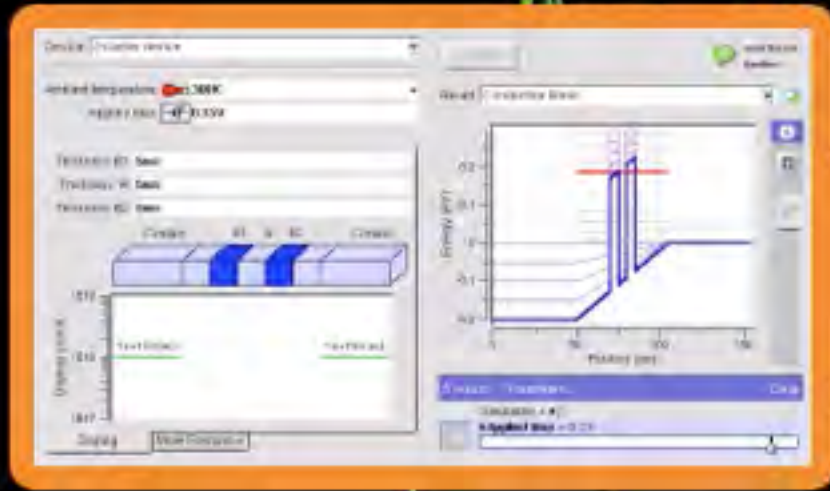
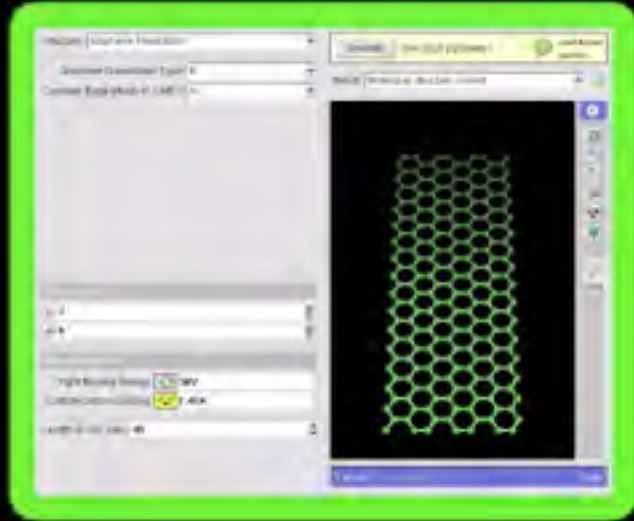
- New Registrations
- Simulation Users
- Tutorial / Lecture Users

Customers

nanoHUB.org usage 2012-02-03 00:00:00

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



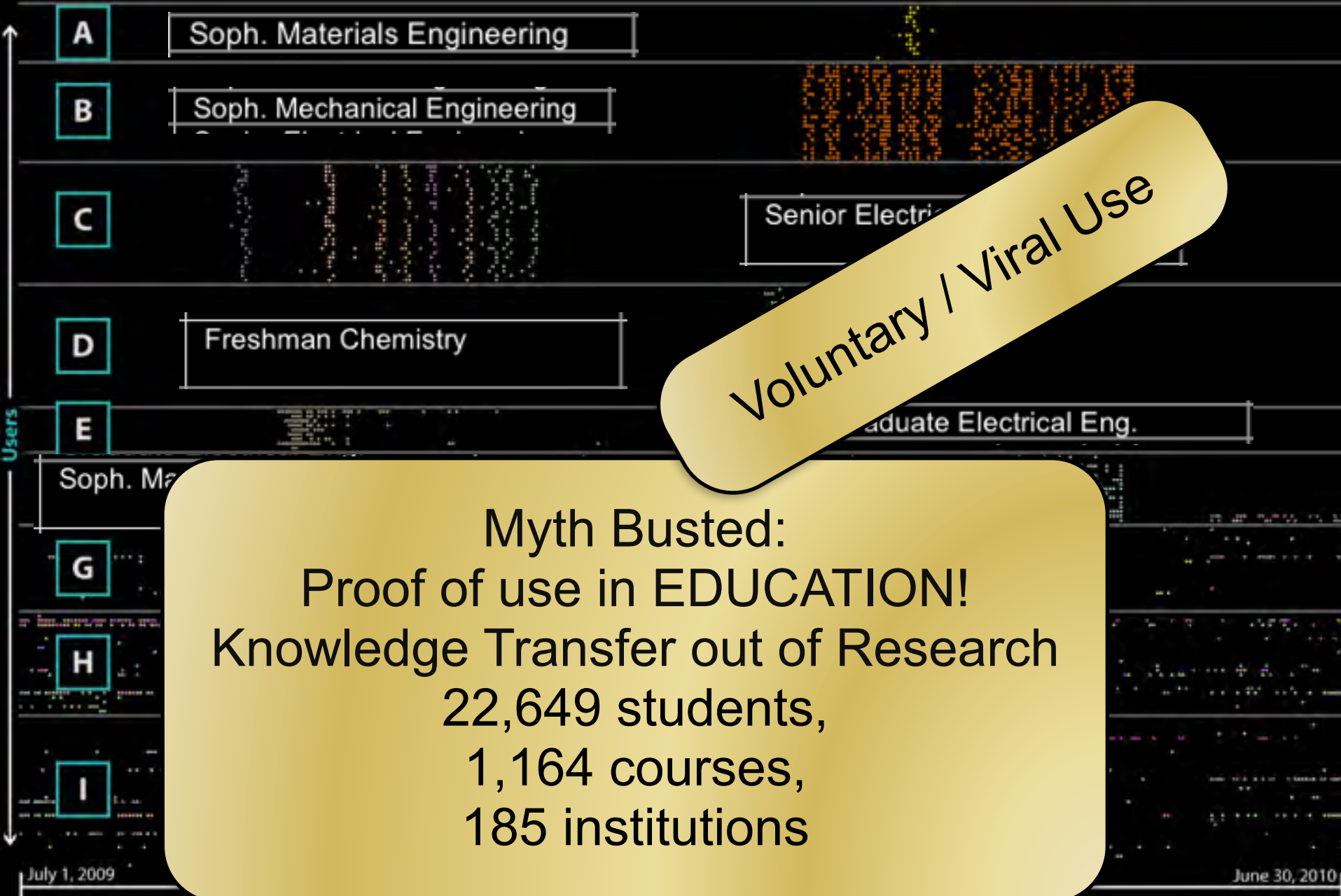
Users



Time (days)

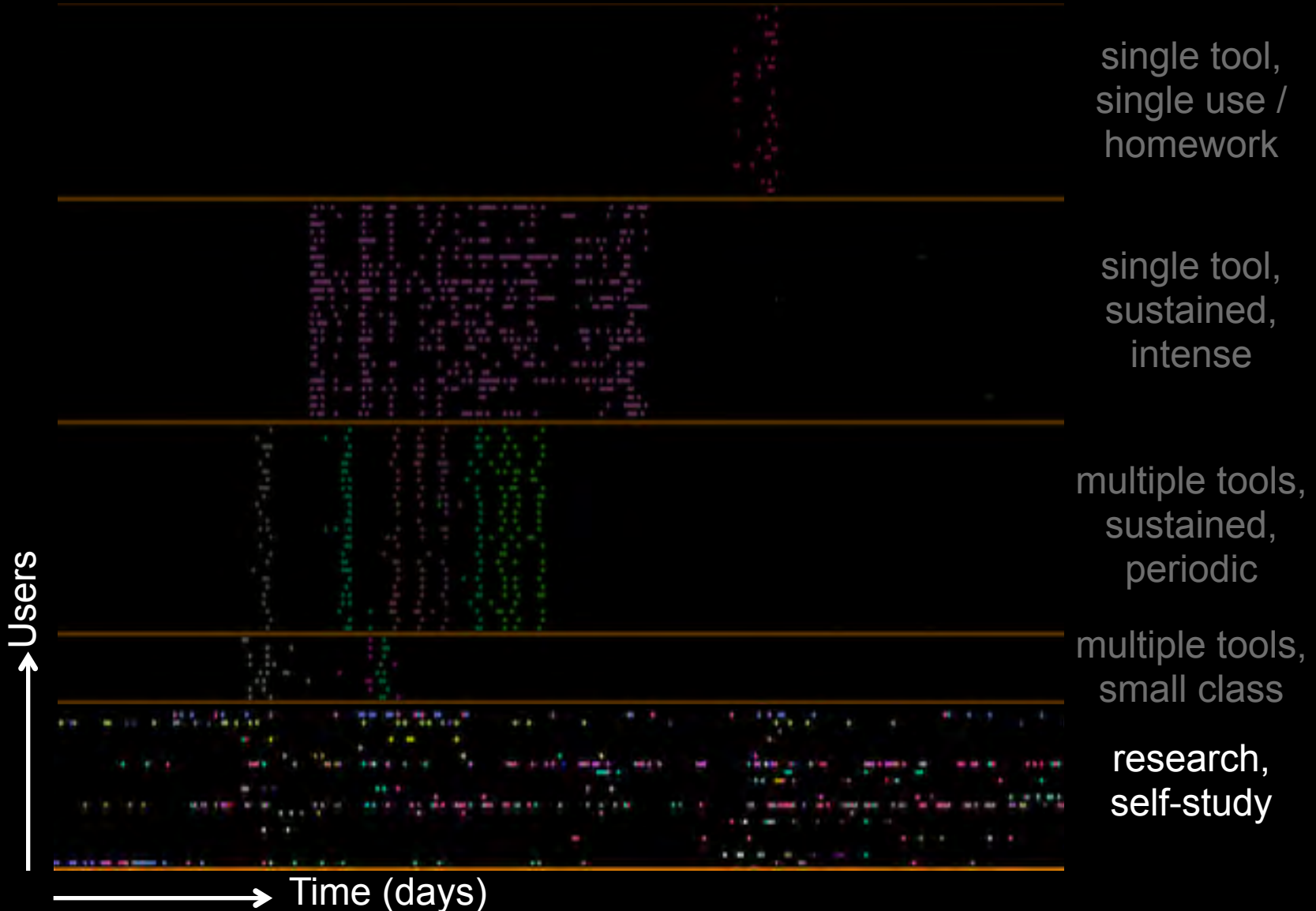


Formal Education vs. Research



User Behavior Analysis

=> Is Research Possible?



nanoHUB Citation Network (2000–2014)

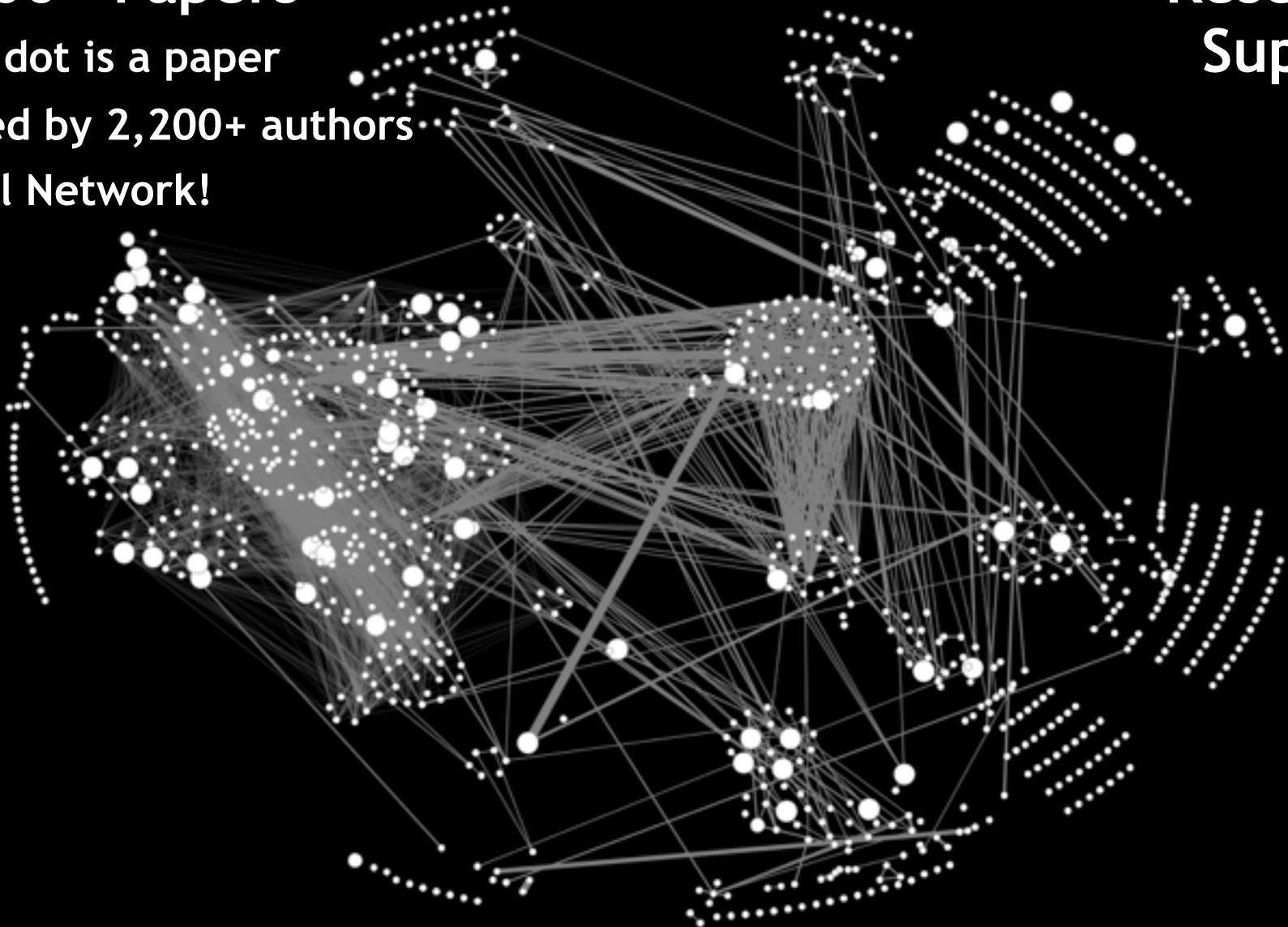
1,100+ Papers

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

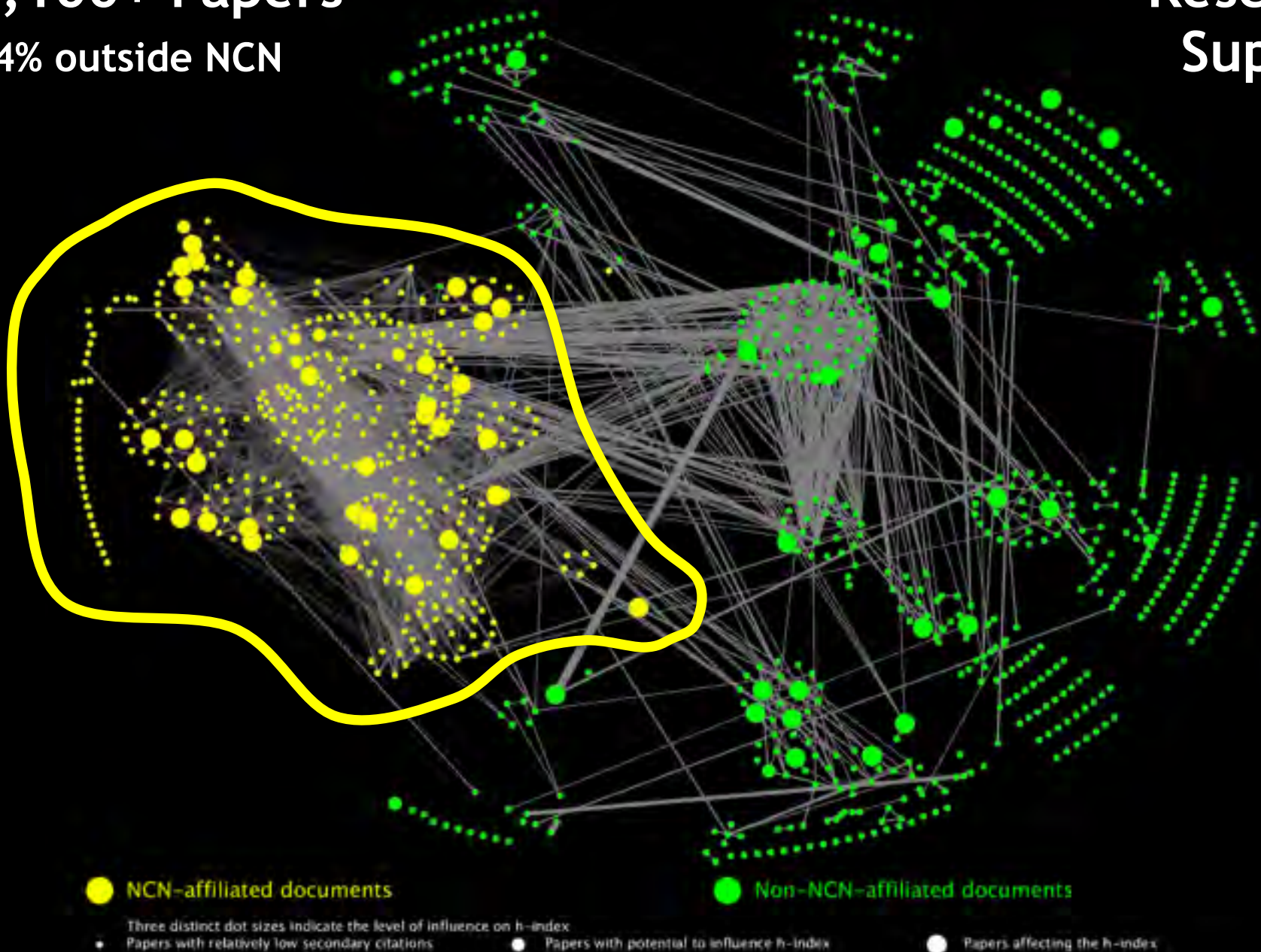
• Papers affecting the h-index

NCN vs. Non-NCN (2000-2014)

1,100+ Papers

64% outside NCN

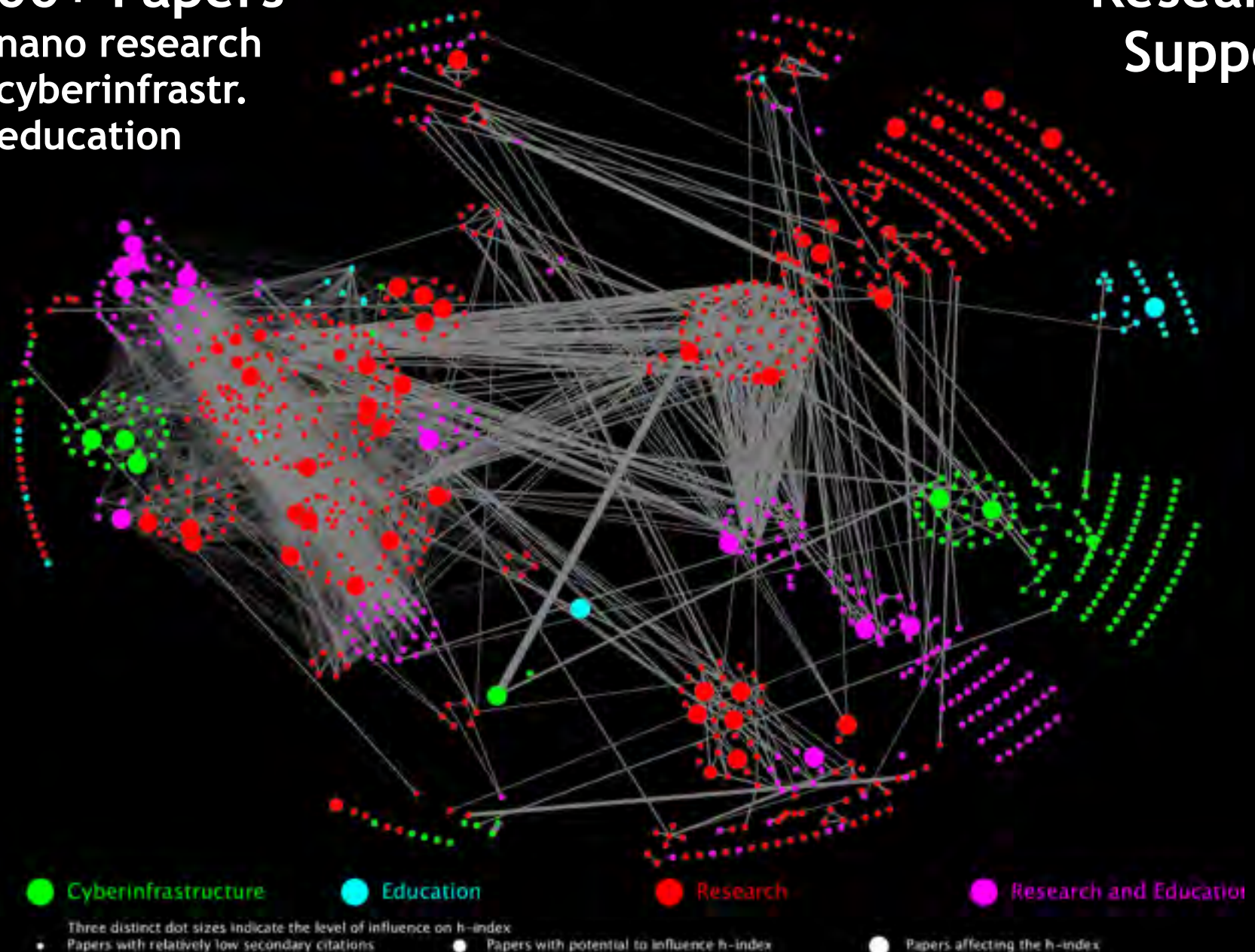
Research
Support



Reference Types (2000–2014)

1,100+ Papers
82% nano research
17% cyberinfrastr.
8% education

**Research
Support**

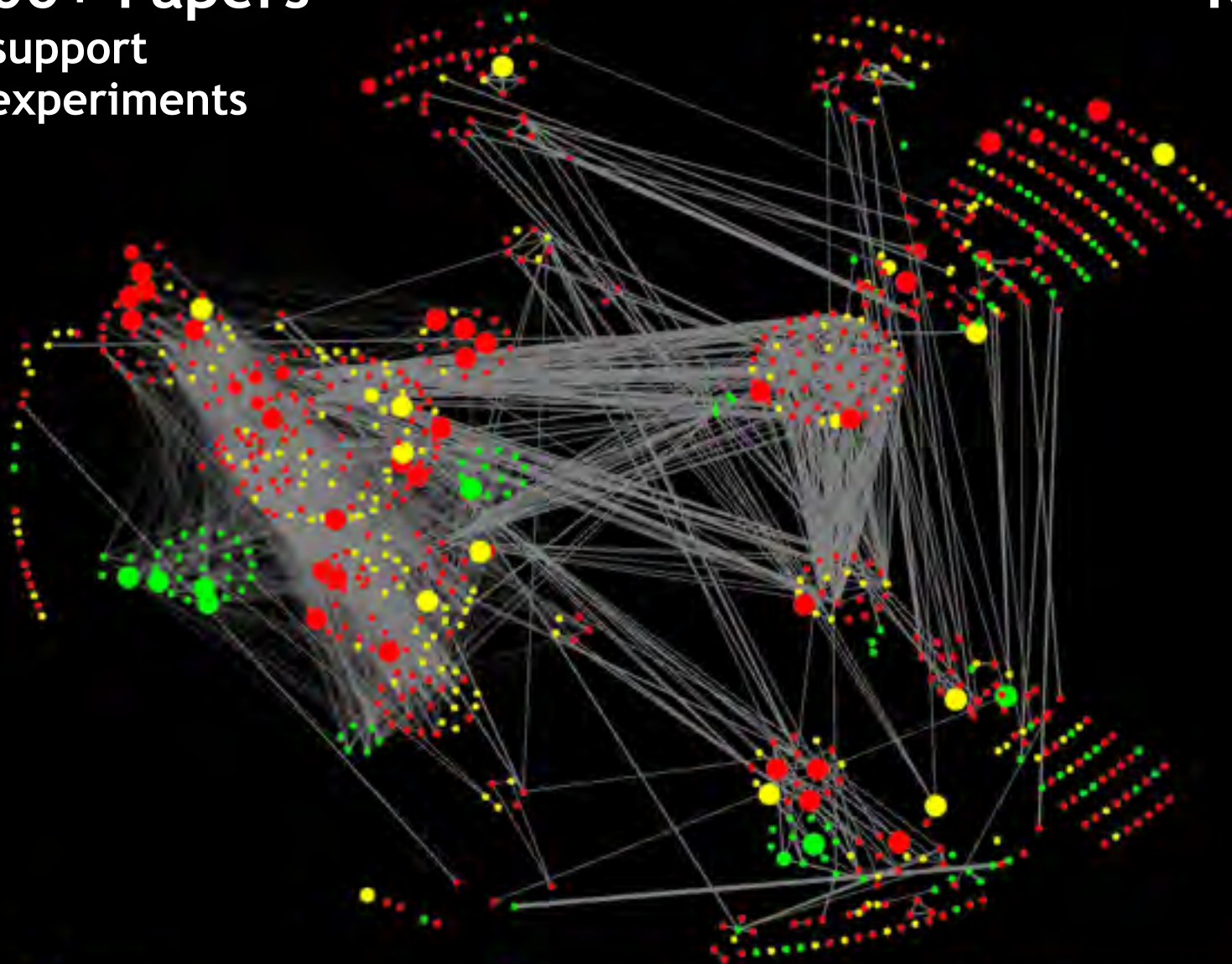


Experimentalist and Experimental Data (2000–2014)

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

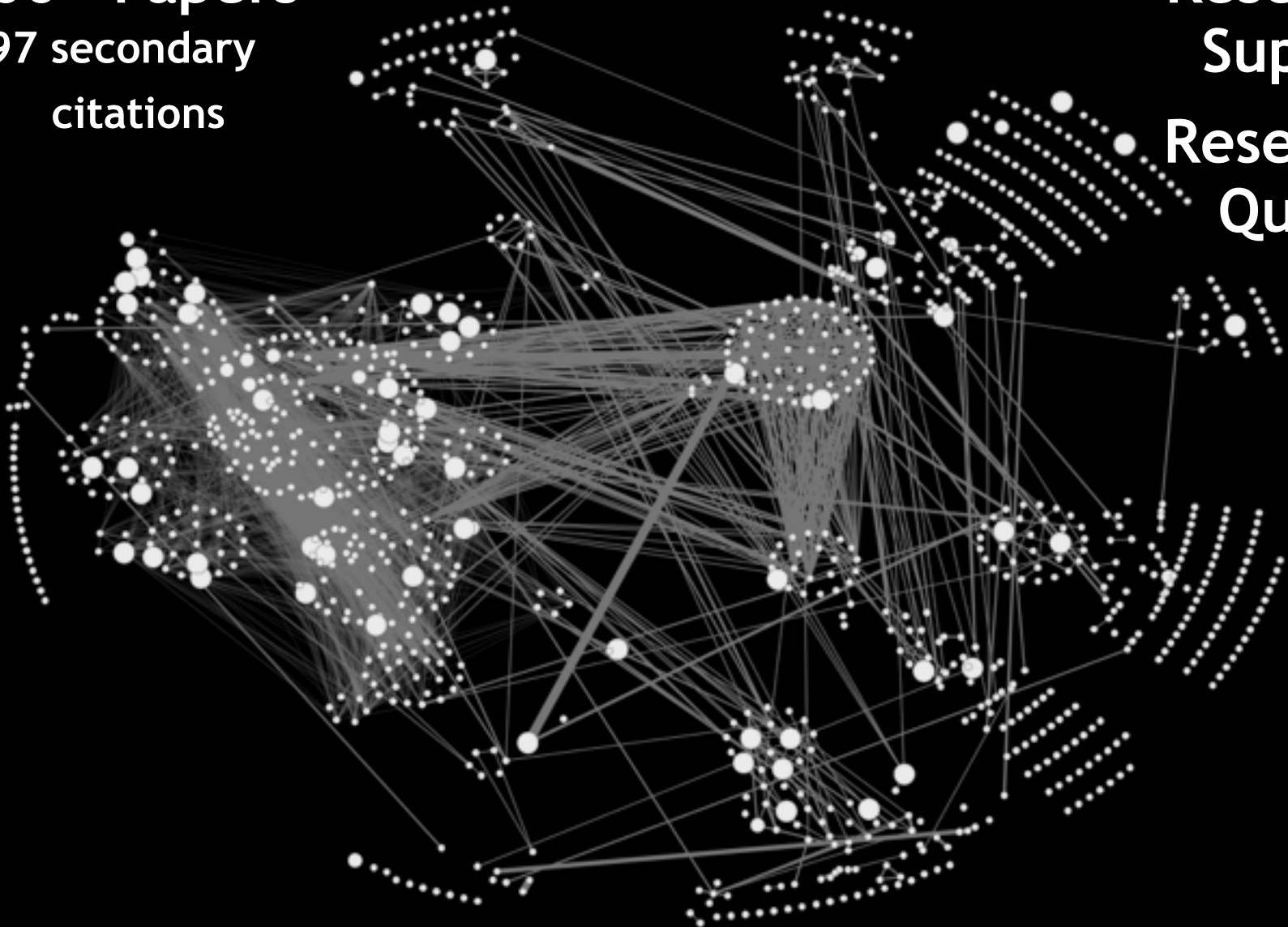
nanoHUB Citation Network (2000–2014)

1,100+ Papers

**13,997 secondary
citations**

**Research
Support**

**Research
Quality**



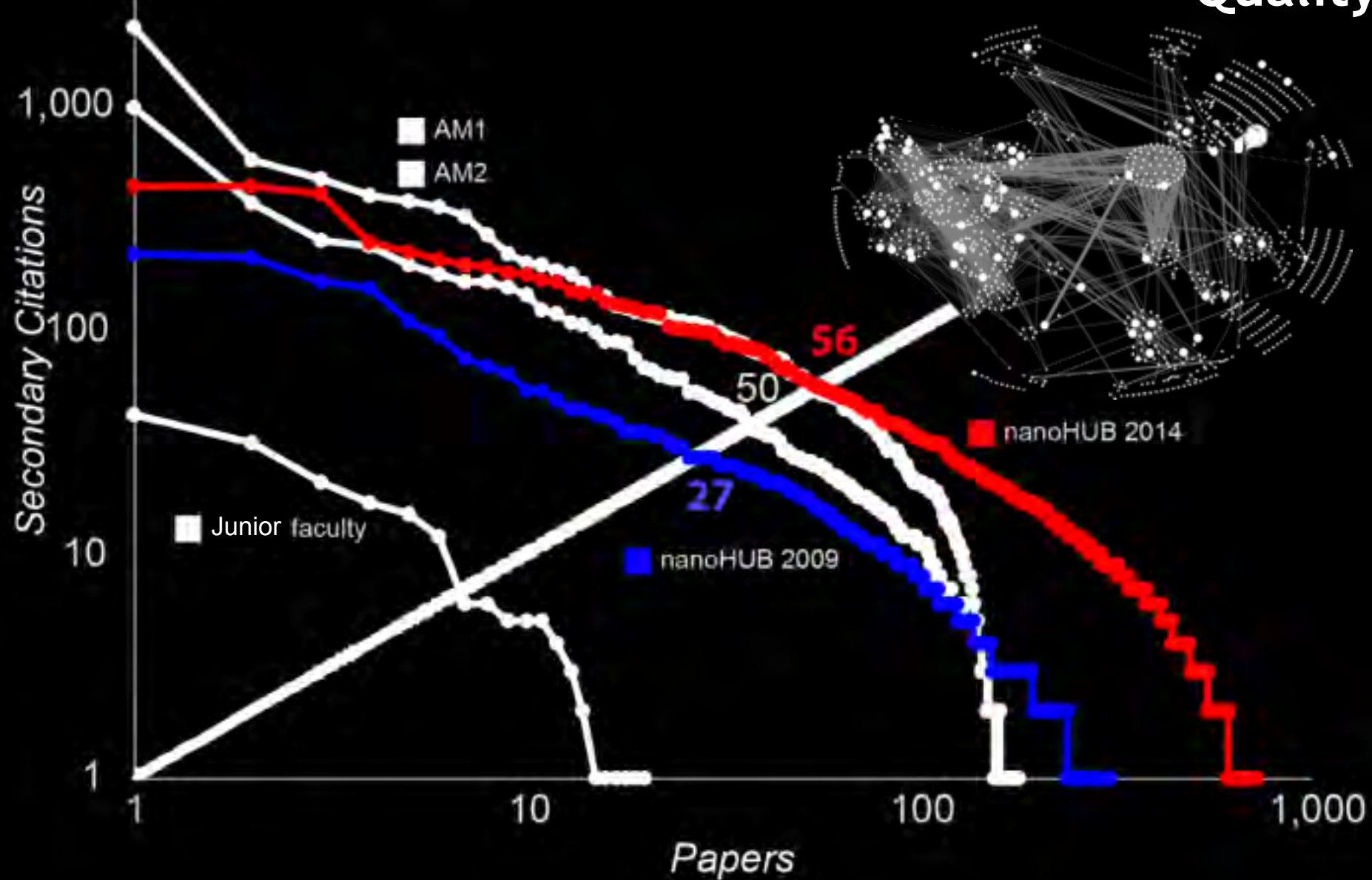
Three distinct dot sizes indicate the level of influence on h-index

- Papers with relatively low secondary citations
- Papers with potential to influence h-index
- Papers affecting the h-index

nanoHUB 2014: 1,108 Papers

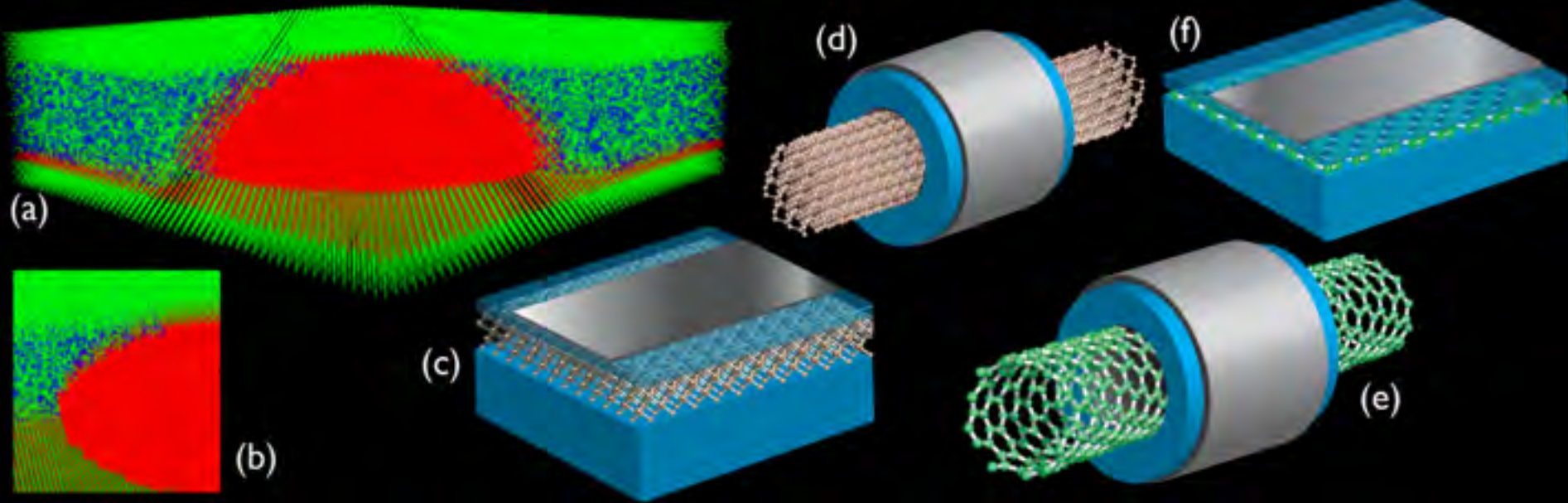
13,997 secondary citations h-index 56

Research
Quality





Compute Intensive: NEMO/OMEN

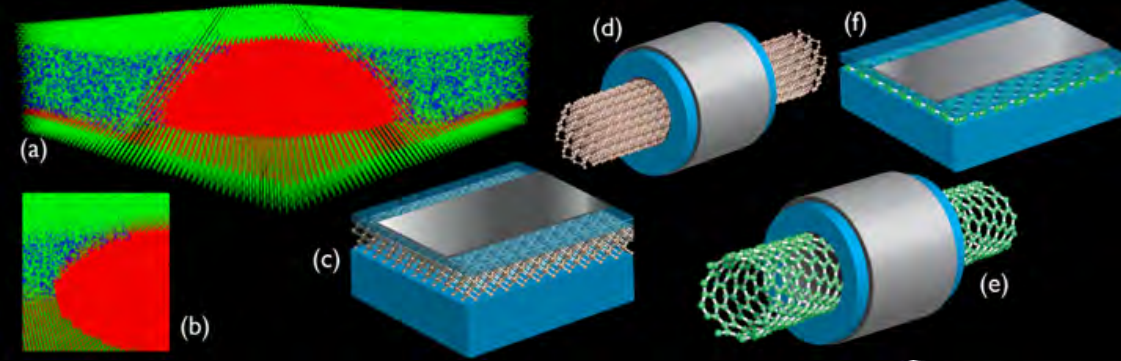


20 years development

- Texas Instruments
- NASA JPL
- Purdue

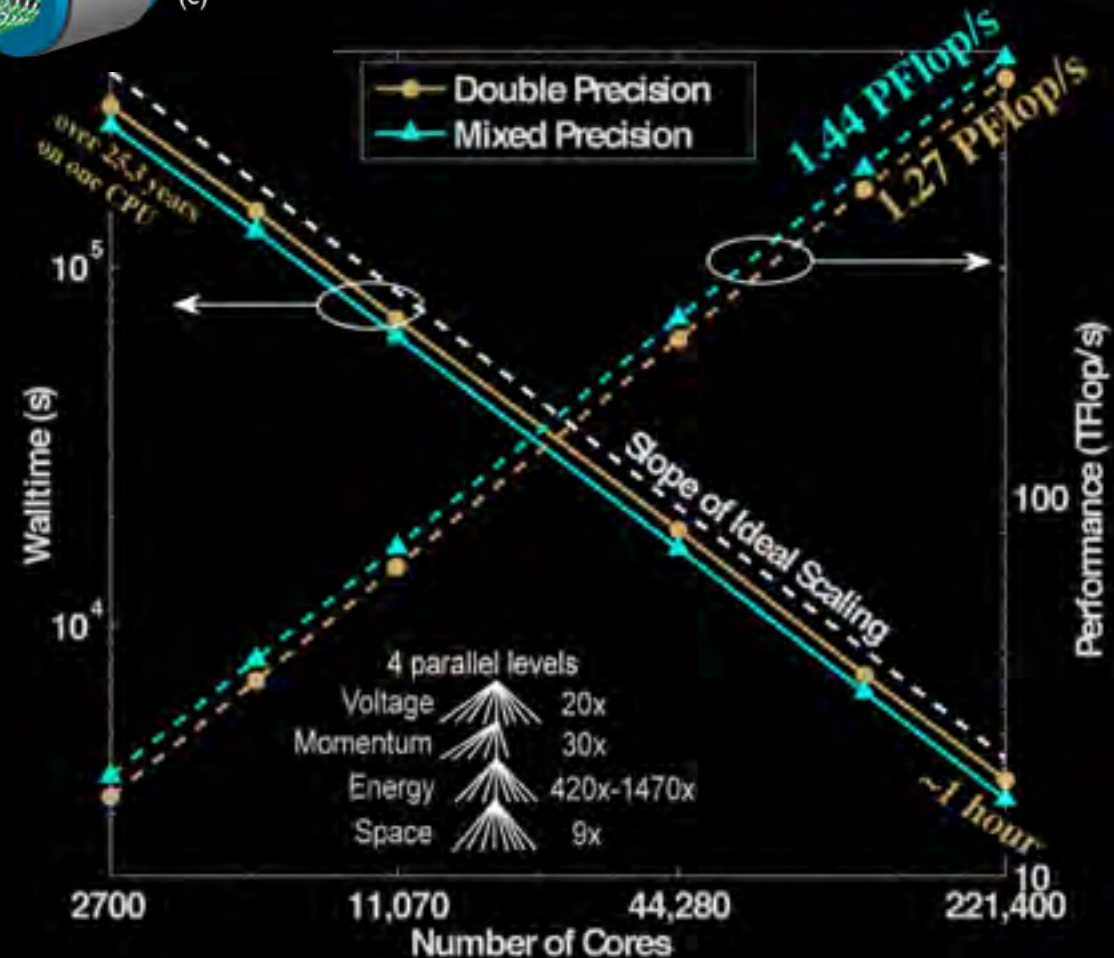


Compute Intensive: NEMO/OMEN



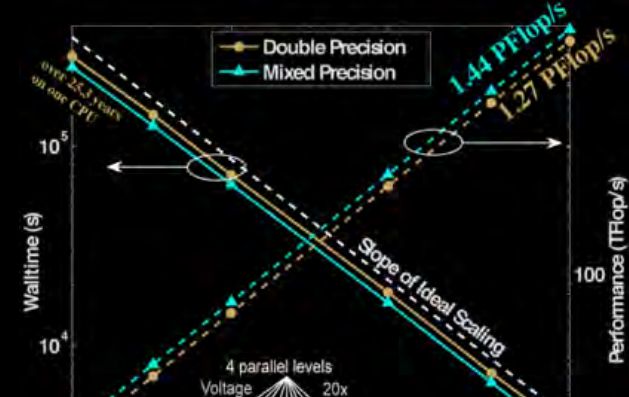
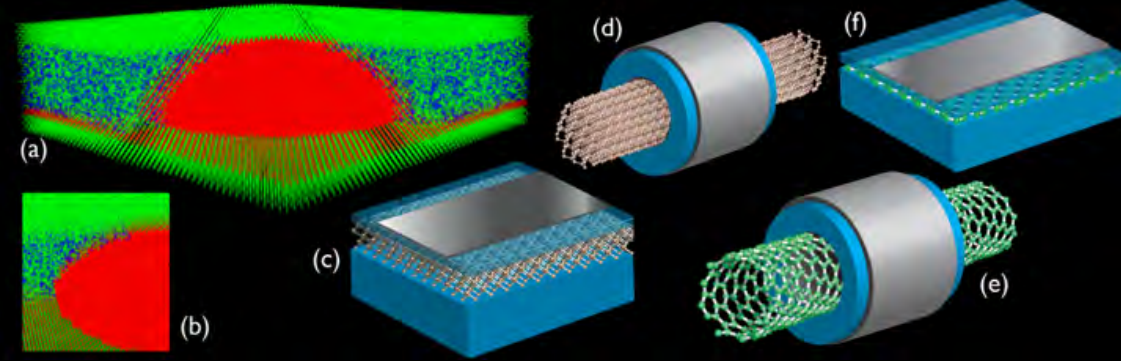
20 years development

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



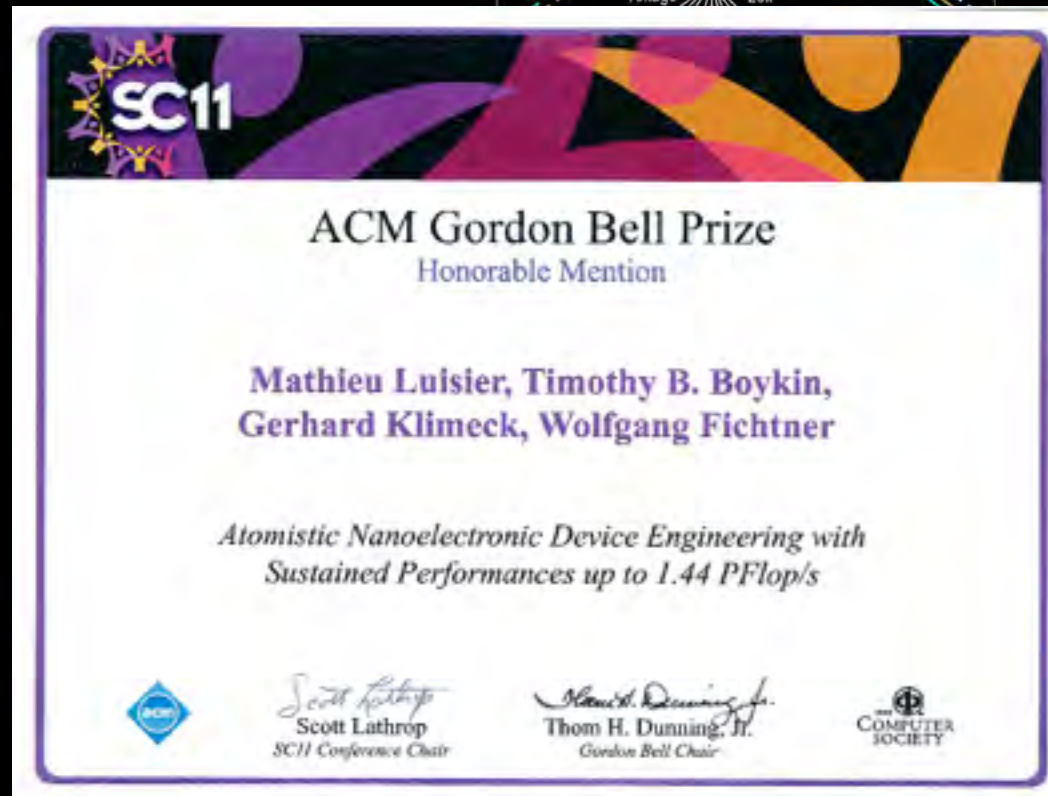


Compute Intensive: NEMO/OMEN

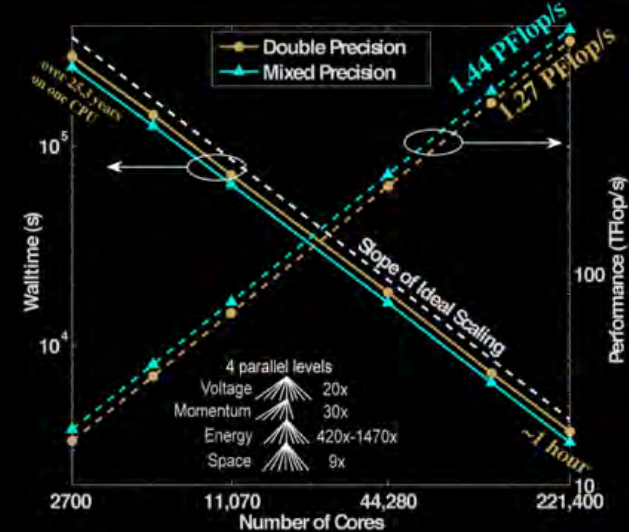
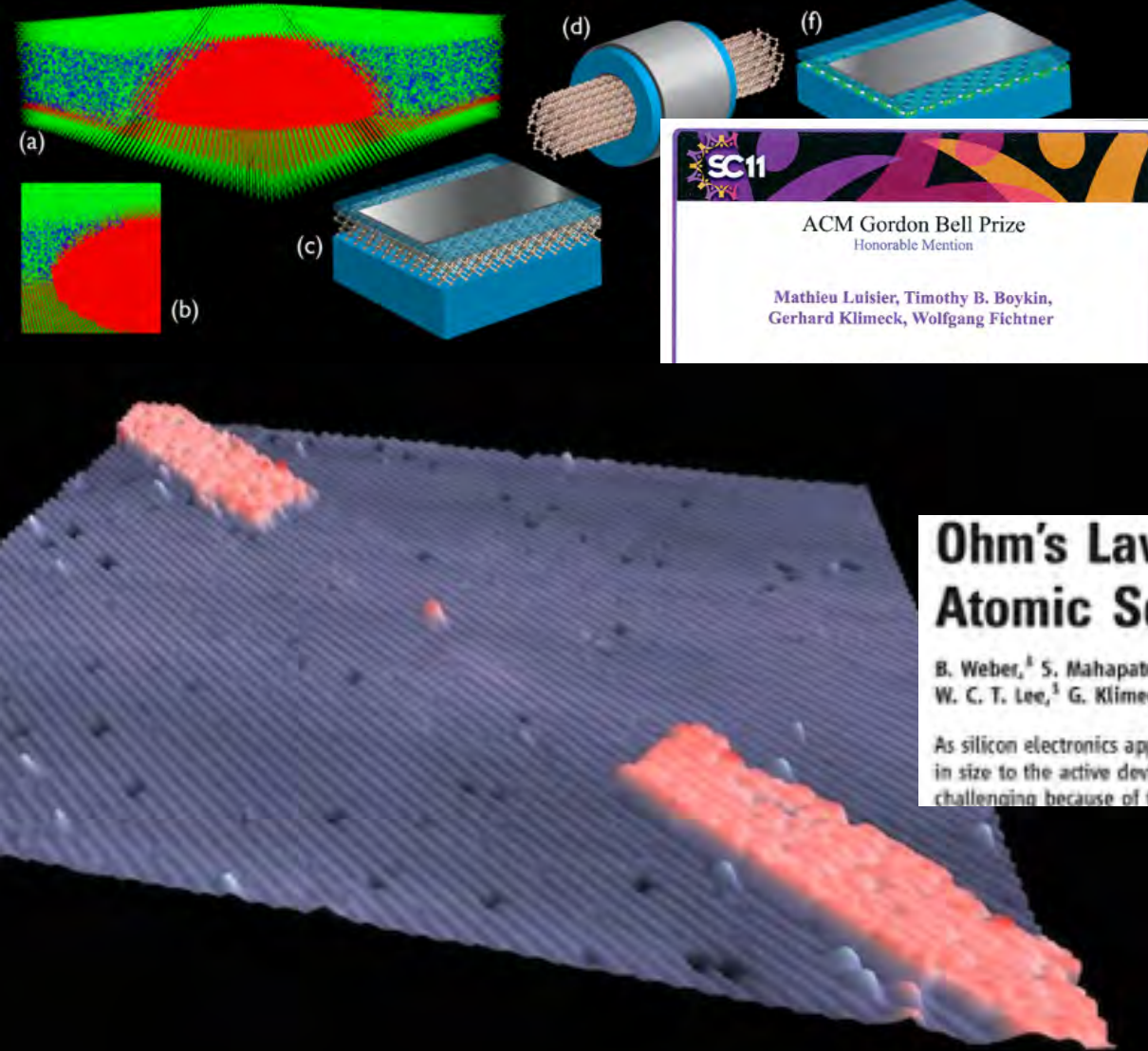


20 years development

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



Compute Intensive: NEMO/OMEN



Ohm's Law Survives to the Atomic Scale

B. Weber,¹ S. Mahapatra,¹ H. Ryu,^{2*} S. Lee,²
W. C. T. Lee,¹ G. Klimeck,² L. C. L. Hollenberg

As silicon electronics approaches the atomic scale, some comparable in size to the active device components. Maintaining this scale is challenging because of the presence of confining surfaces and interfaces. We report on the

nature
nanotechnology

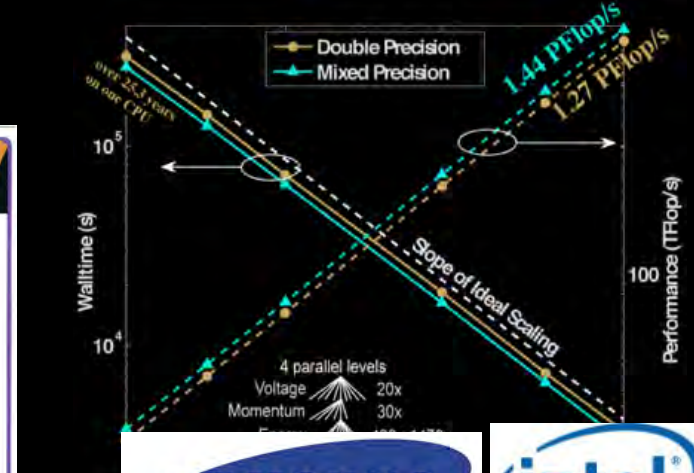
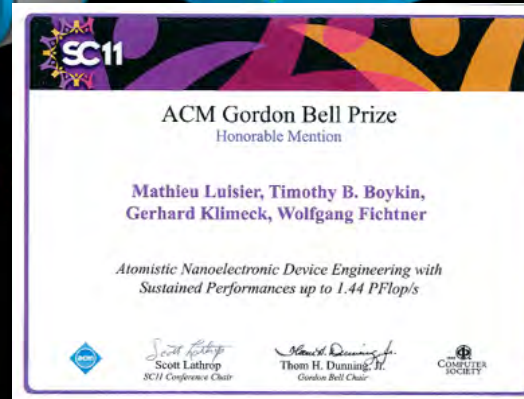
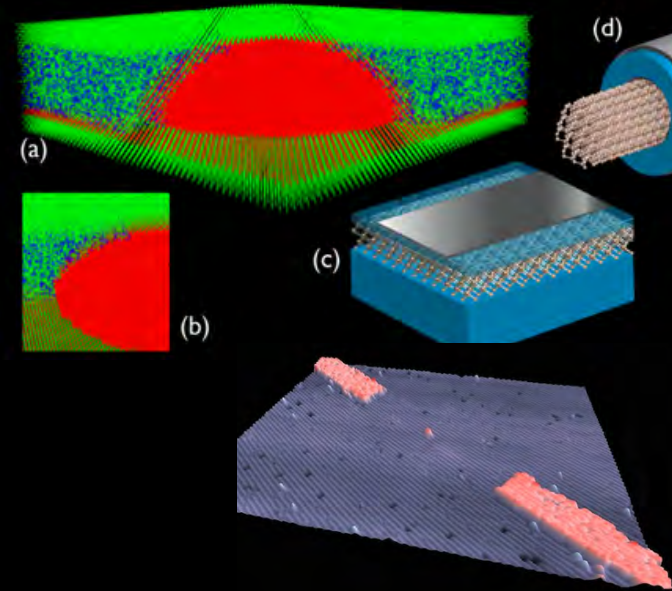
A single-atom transistor

Martin Fuechle¹, Jill A. Miwa¹, Suddhasatta Mahapa¹,
Oliver Warschkow¹, Lloyd C. L. Hollenberg², Gerhard

- Science, Nature Nano



Compute Intensive: NEMO/OMEN



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





compute Intensive

Myth Busted!
Prove
Computational Extensive Work

18 years development

• 267,362 Simulation Runs

• 10,786 Users

• 3,874 Users in 100 classes

• Peta

• Gord

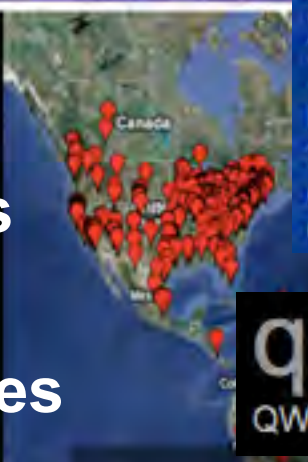
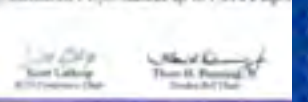
• Scie



(f)

...oykin,
...g Fichtner

...electronic Device Engineering with
...sustained Performances up to 1.44 PFlops



WANNIER90

siesta



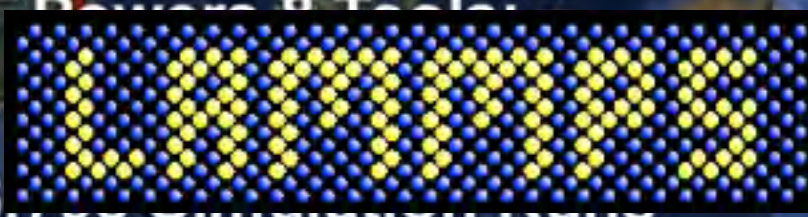
GAMMESS



SeqQuest

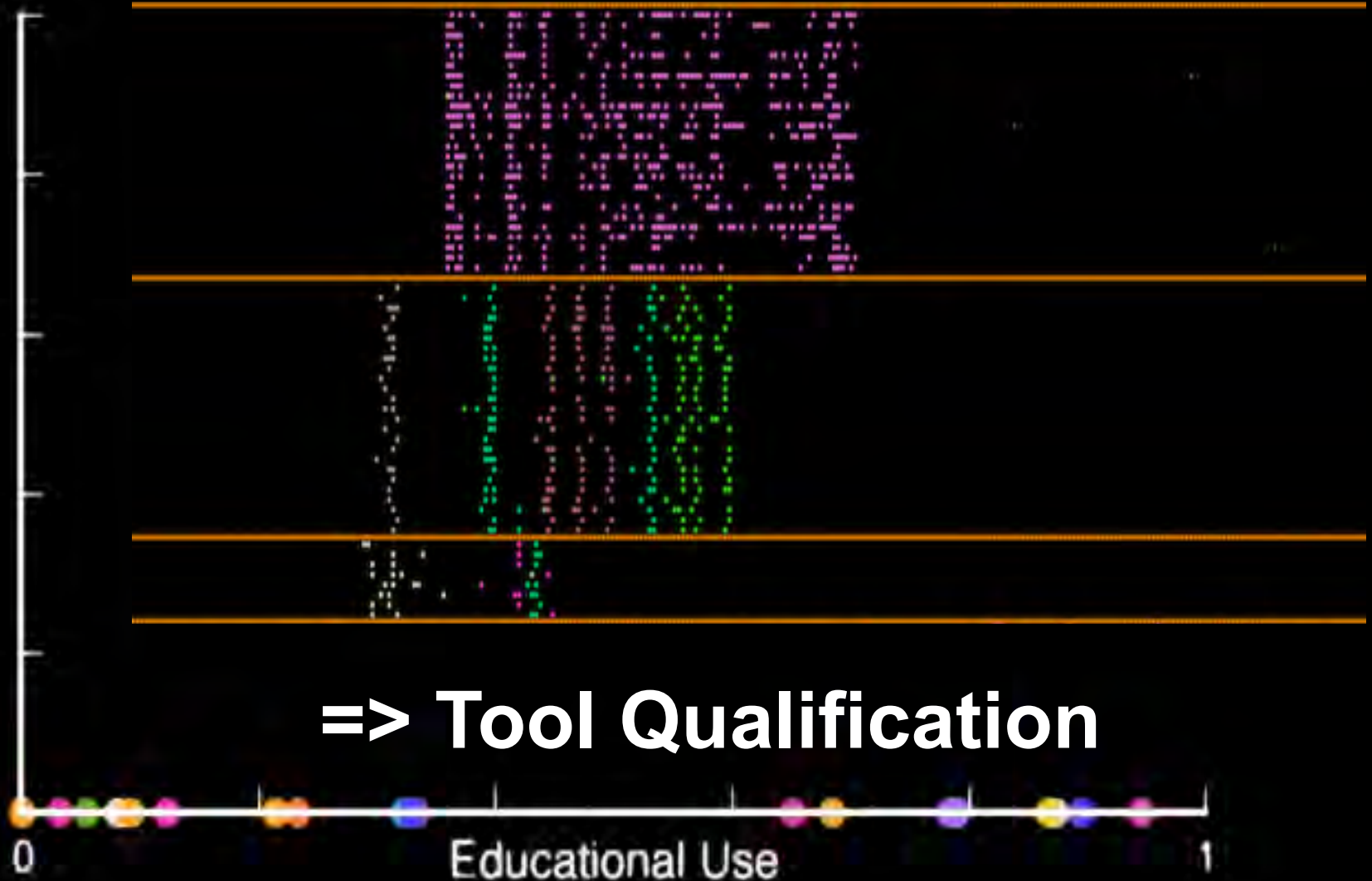
qwalk

QWalk: Continuum electronic structure quantum Monte C

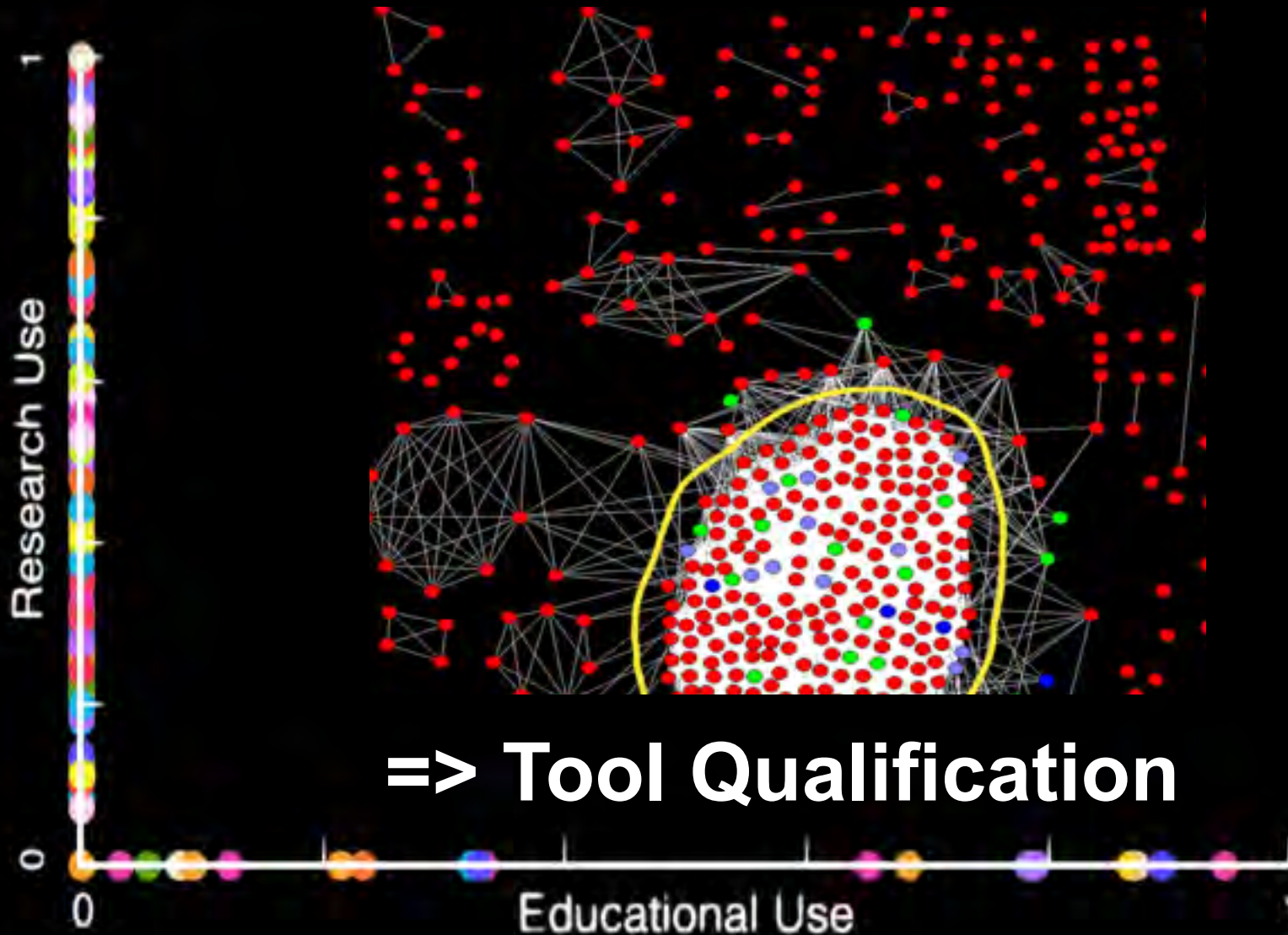


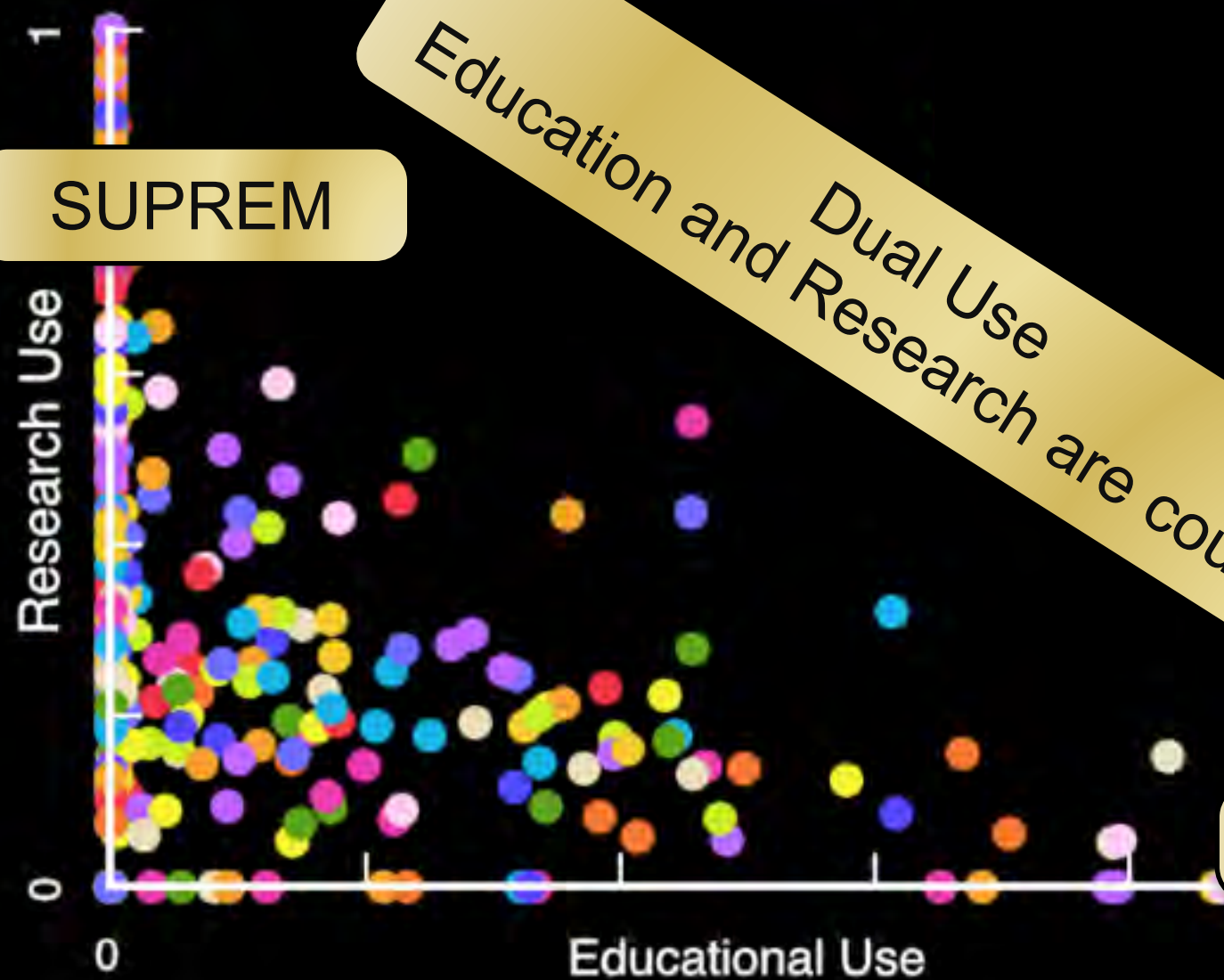
166,700 simulation runs

Usage Patterns



Literature Citations



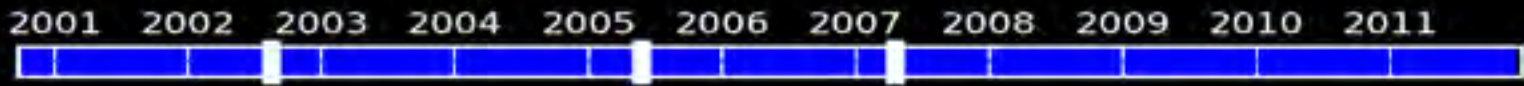


SUPREM

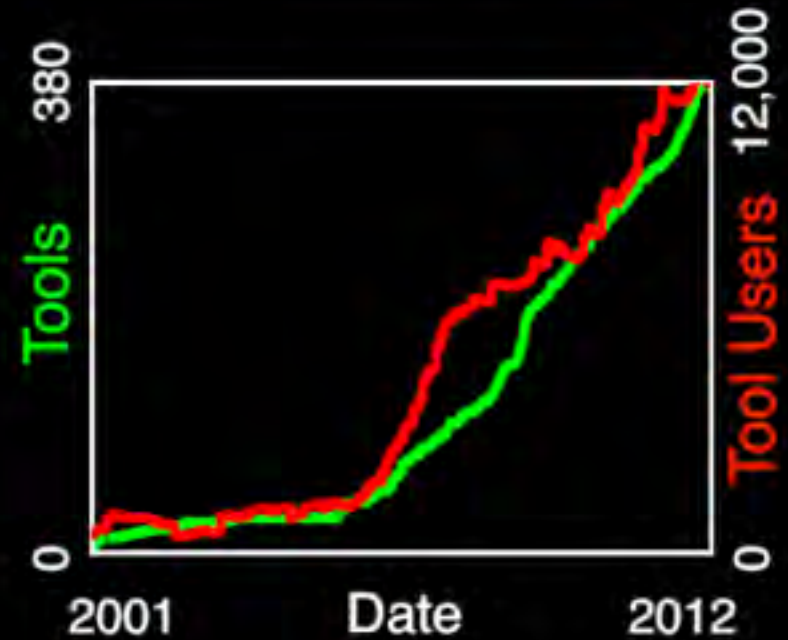
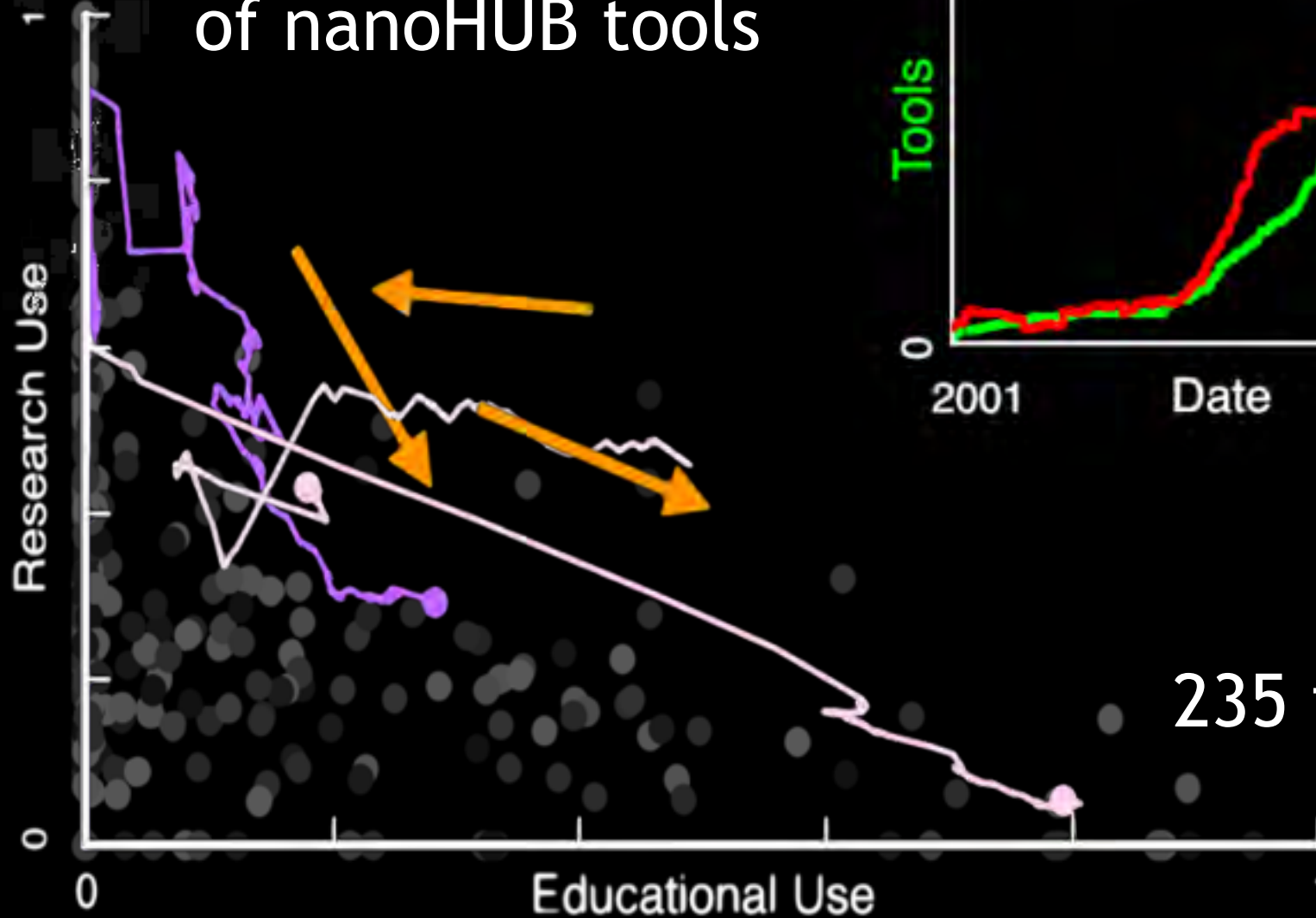
Education and Research are coupled!

235 tools!

SPICE

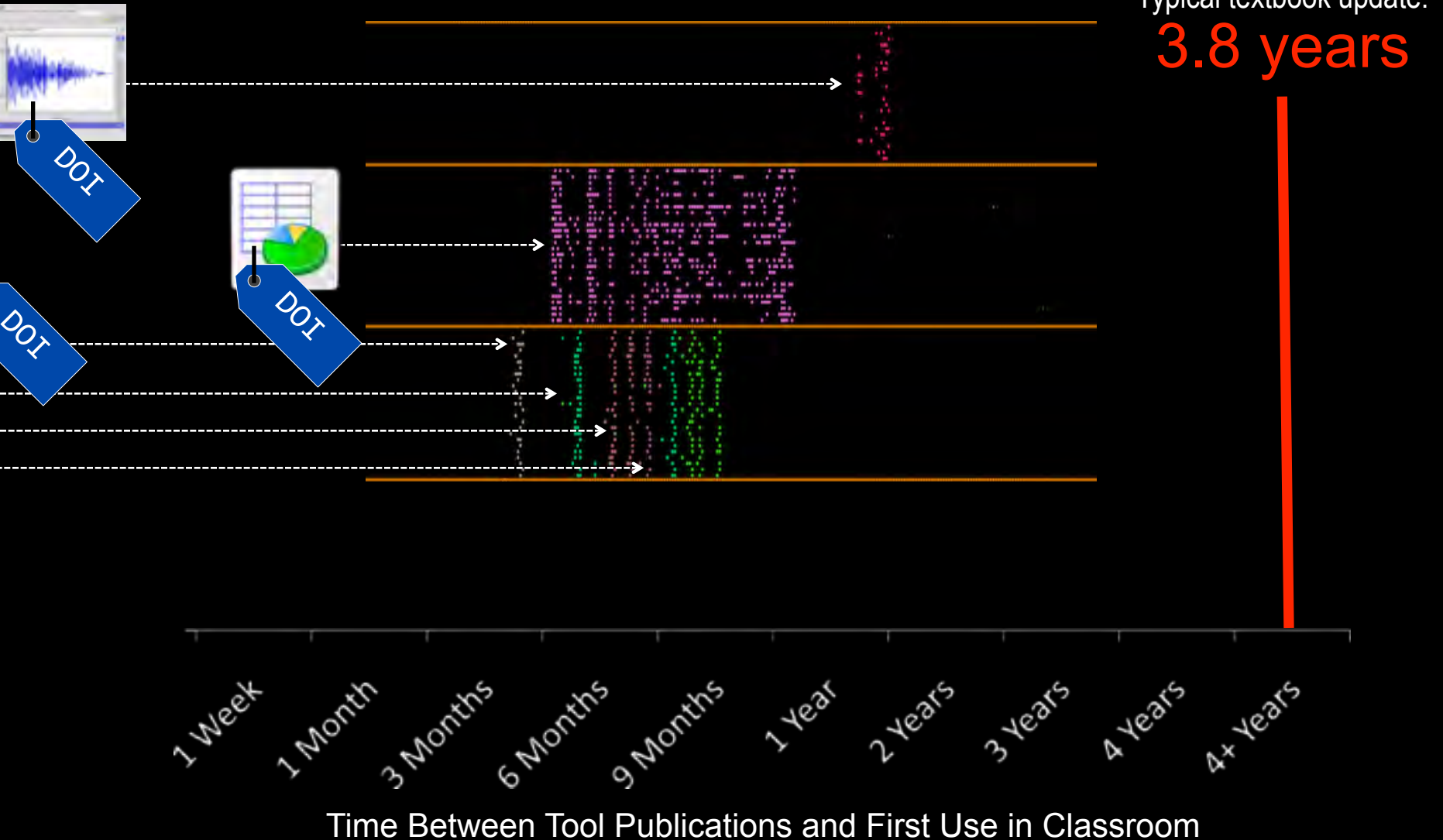


Time-evolution of nanoHUB tools



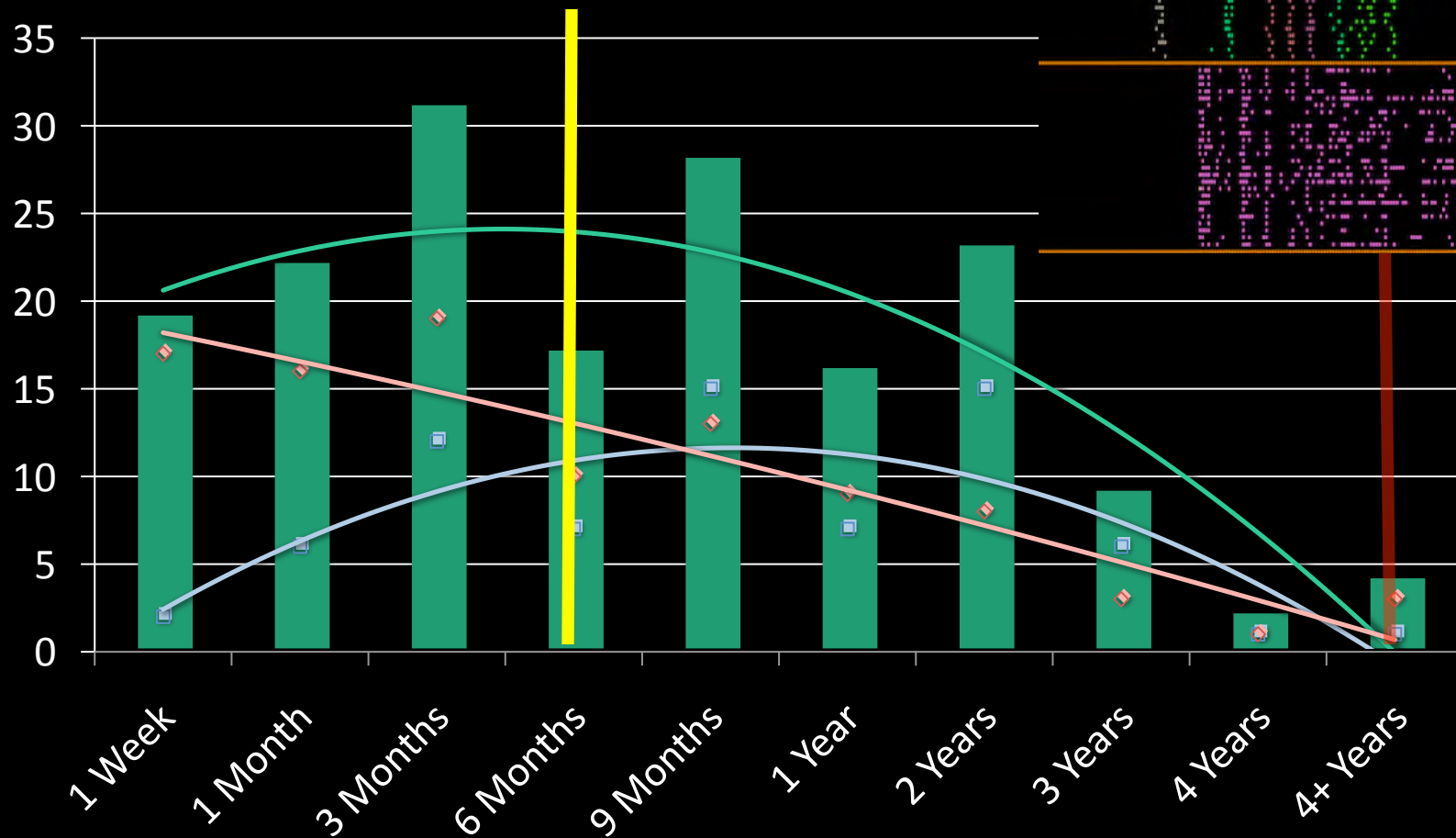
235 tools!

Time to First Adoption

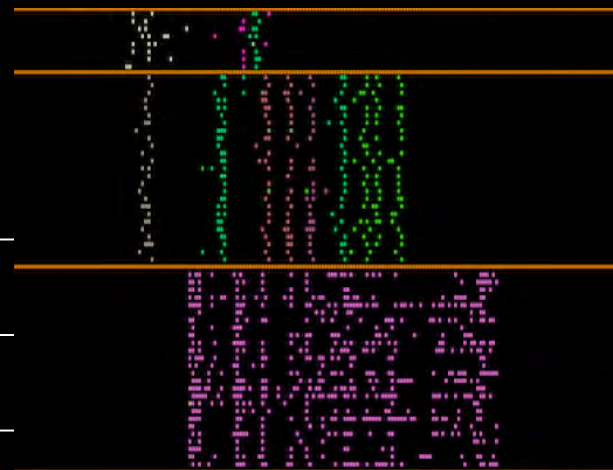


Revolutionizing Research → Classroom

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

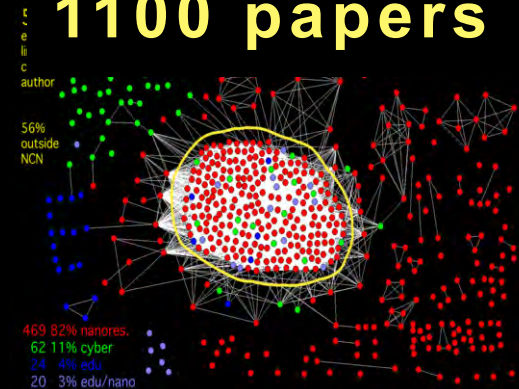
Fully operational 24/7

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

*In all areas of Nano Engineering and Science
Personalized Learning at all workforce levels
Become Part of the Day-to-Day Workflow*



*Reproducible
Nano Engineering*

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



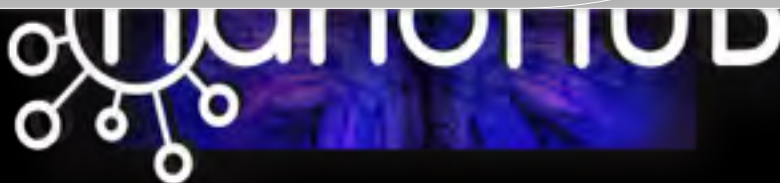


NANOMATERIALREGISTRY

Have: Experimental Data
Hypothesis Driven Data Structure

Need: Broad Exposure
Data integration with Registry
Data analysis tools to answer questions

Experimental Data
Access
community
with supporting data
integration capability

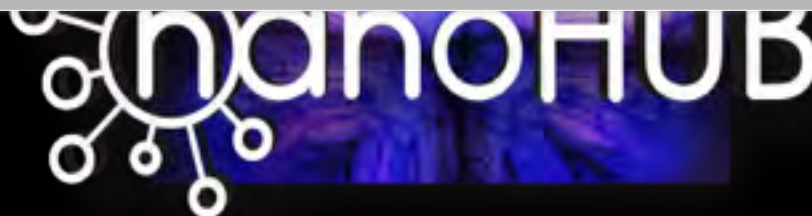


Analytics - Established User Community - Simulation Tools



Have: Rich nano content

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



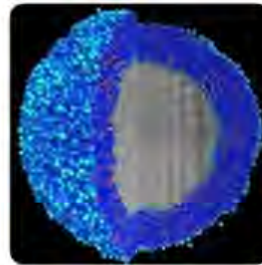
Established User Community - Flexible Content Hosting

Developing a Materials Innovation Infrastructure

Col
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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.



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

algorithms or 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.

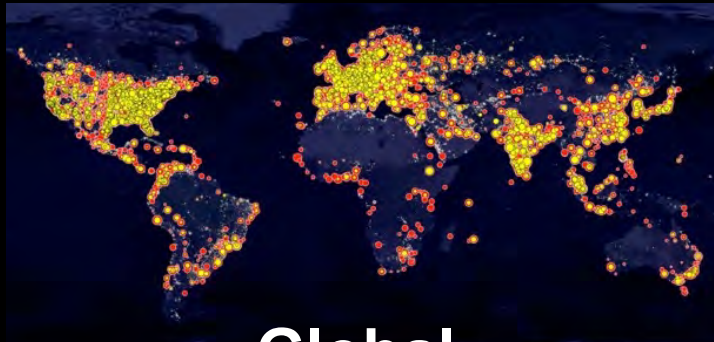
Achieving these objectives will require a focus in three necessary areas: (1) creating accurate models of materials performance and validating model predictions from theories and empirical data; (2) implementing an open-platform framework to ensure that all code is easily used and maintained by all those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

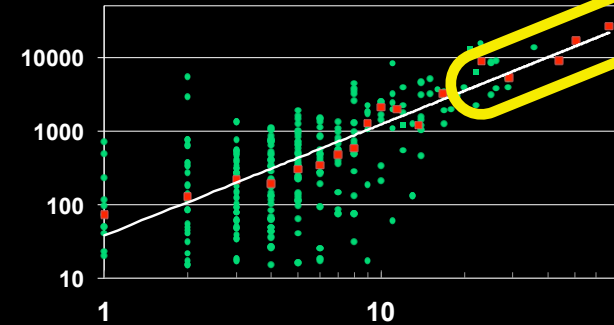
The Essence of a Research University



Global



Growing



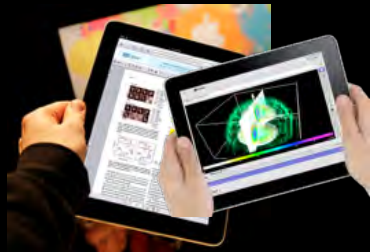
Collaboration
Focused



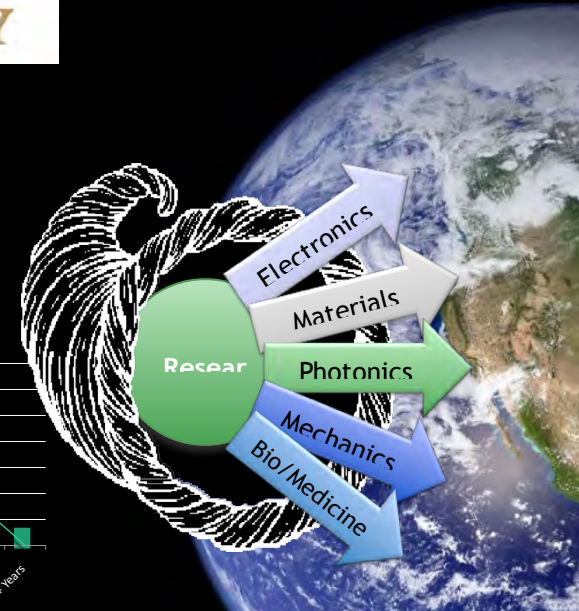
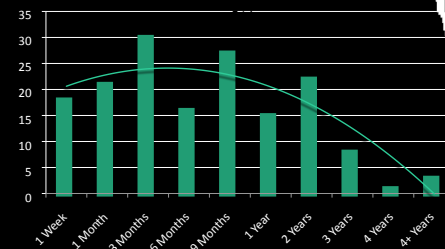
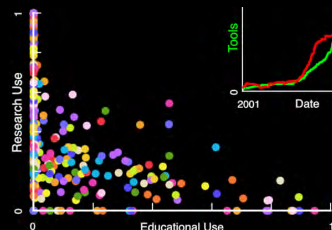
Recognized



Creative



Transformative



Thank
You!

