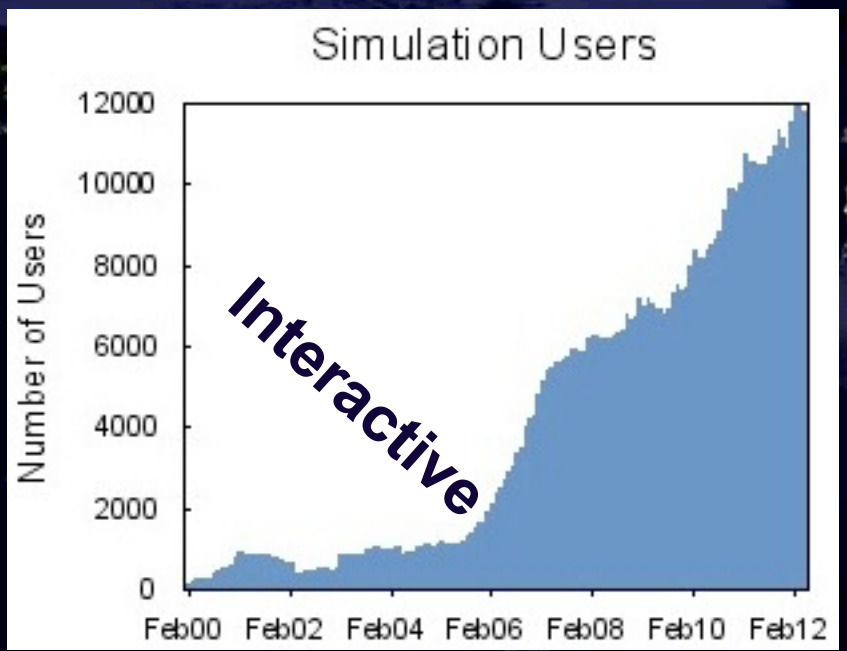
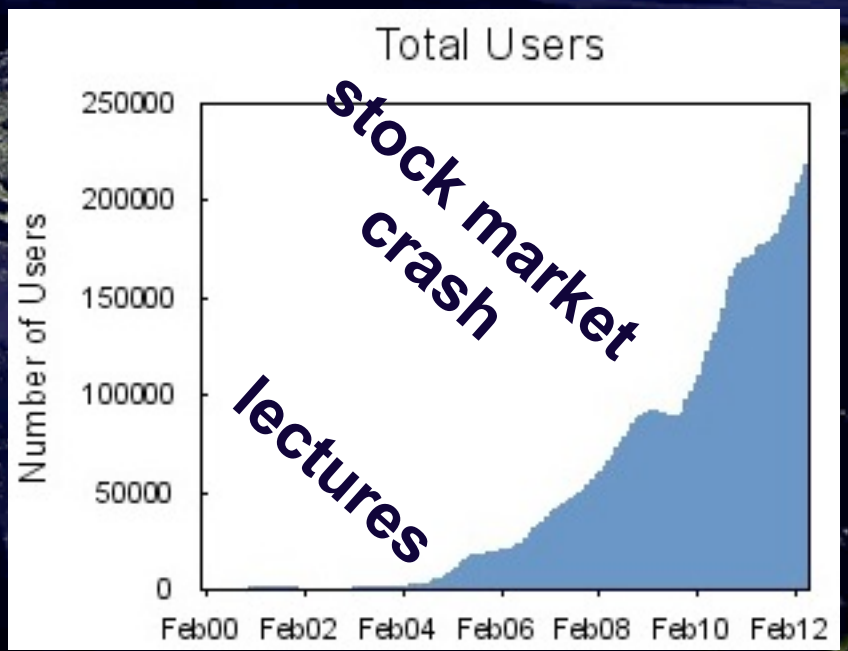
Mythbusting Scientific Knowledge Transfer with nanoHUB.org

Gerhard Klimeck, Purdue University, gekco@purdue.edu





Over 12,000 / 230,000 Users Annually

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

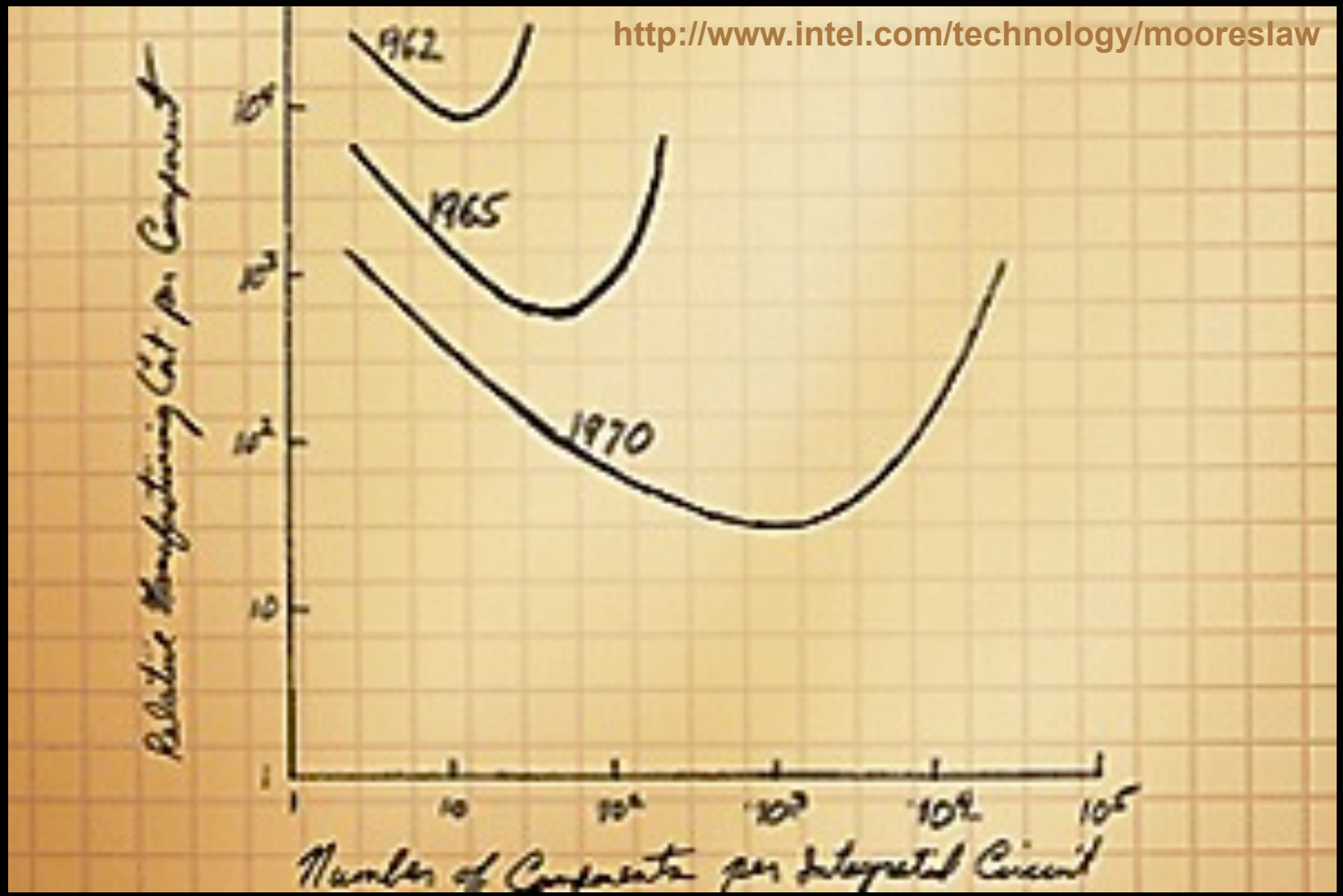
Thanks to

nanoHUB contributors:
330+ tool authors
1,000+ content authors

nanoHUB and HUBzero Team

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

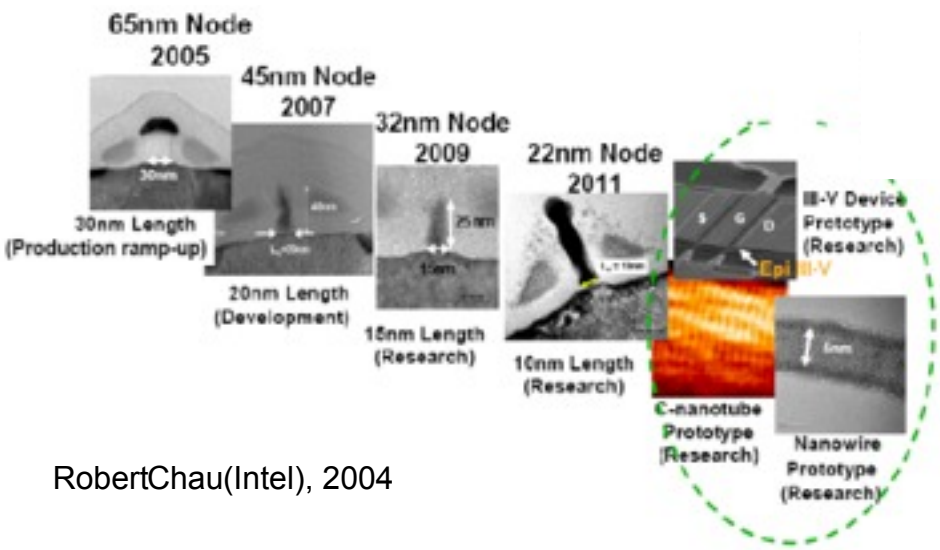
1965
Gordon Moore



Relative Manufacturing Cost per Component

Number of Components per Integrated Circuit

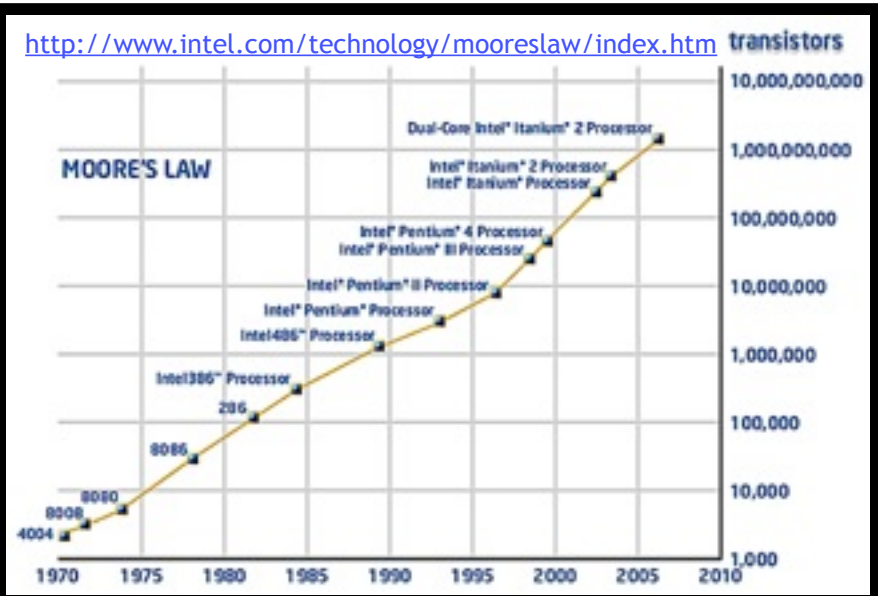
Intel in 2009



RobertChau(Intel), 2004

Device Size:
Tens of nanometers

Stanford SUPREM



Device Integration:
>2 Billion

Berkeley SPICE

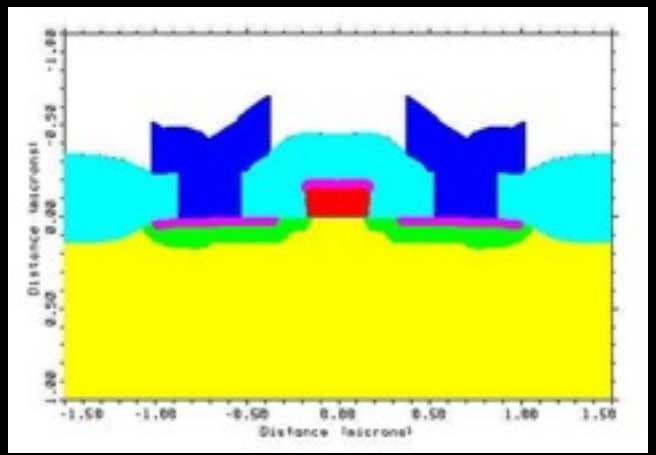
Berkeley
Simulation Program with Integrated Circuit Emphasis.

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

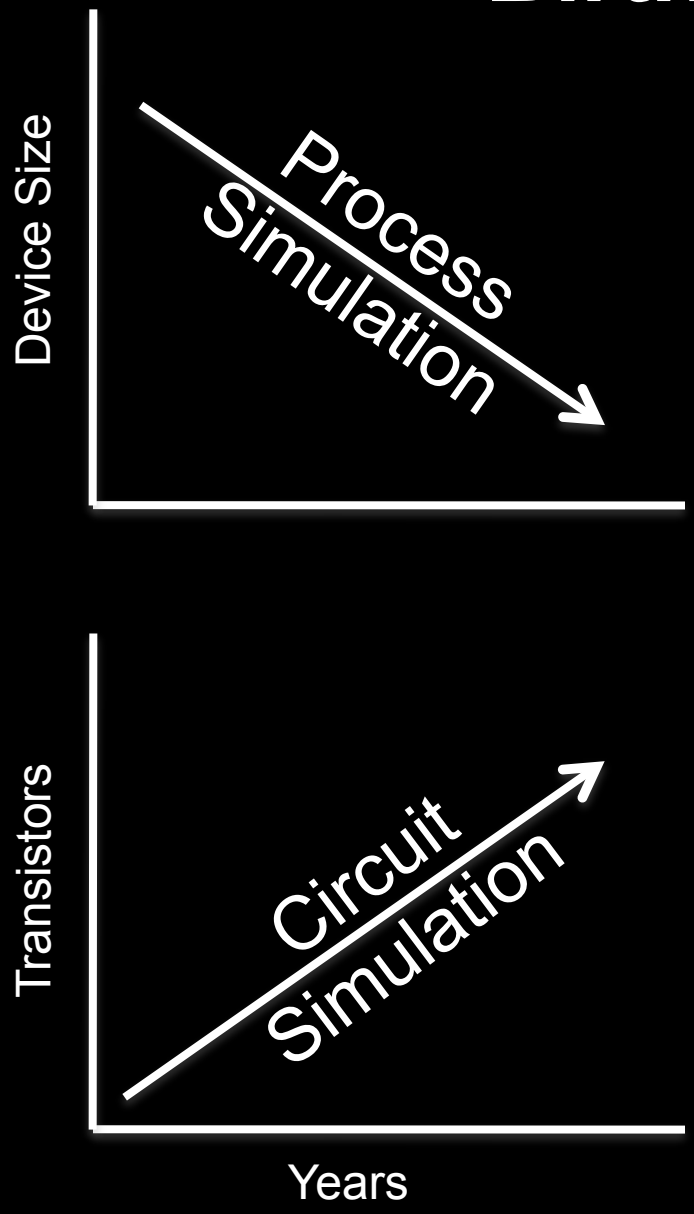
- Released 1972

Stanford
Stanford University PRocEss Modeling



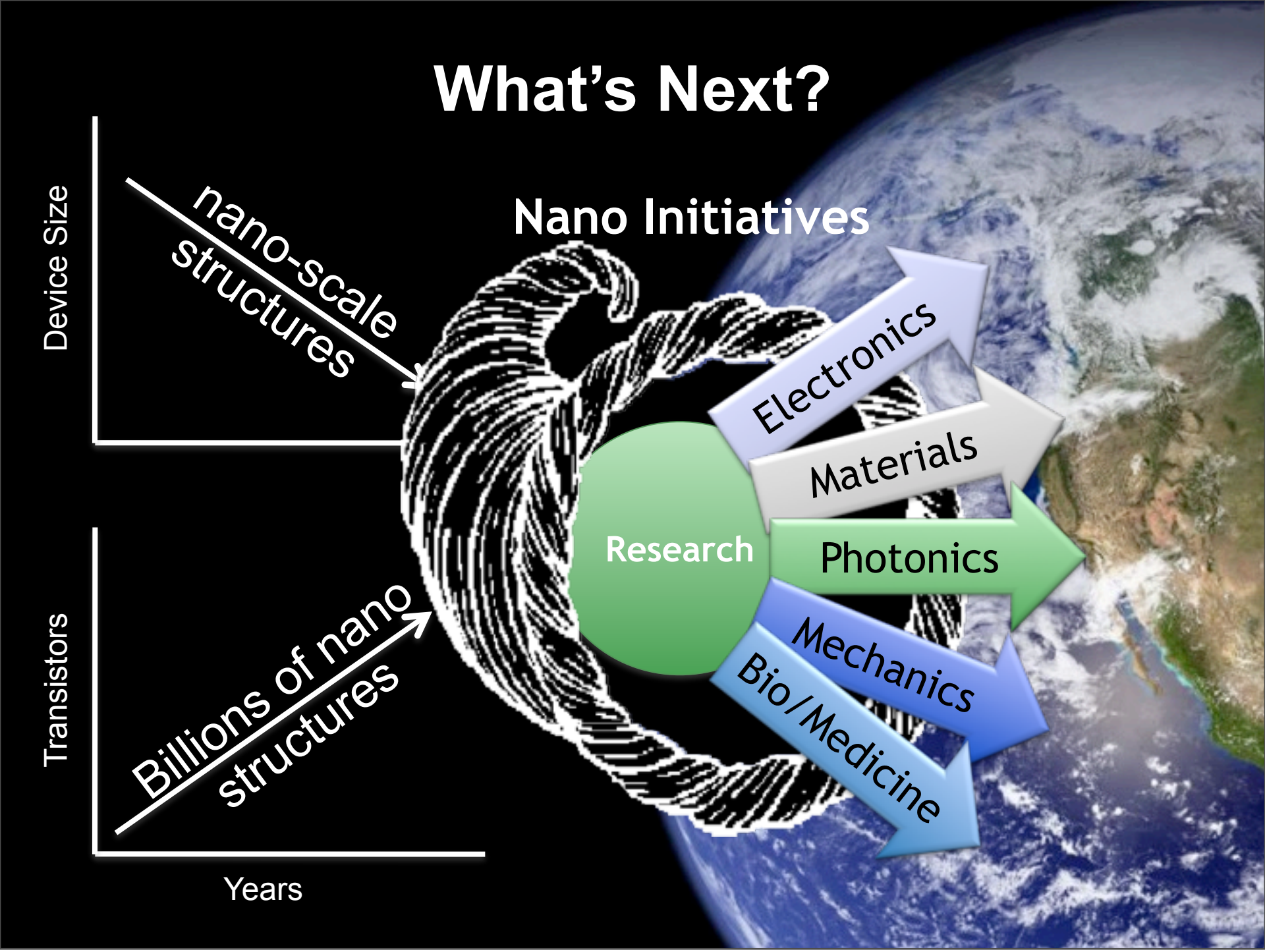
- Stanford wanted to mimic Berkeley success
- Combine various existing models
- Dissemination:
  - Public domain code
  - Community workshops
  - Students took it along to industry and academia

Birth of an Industy

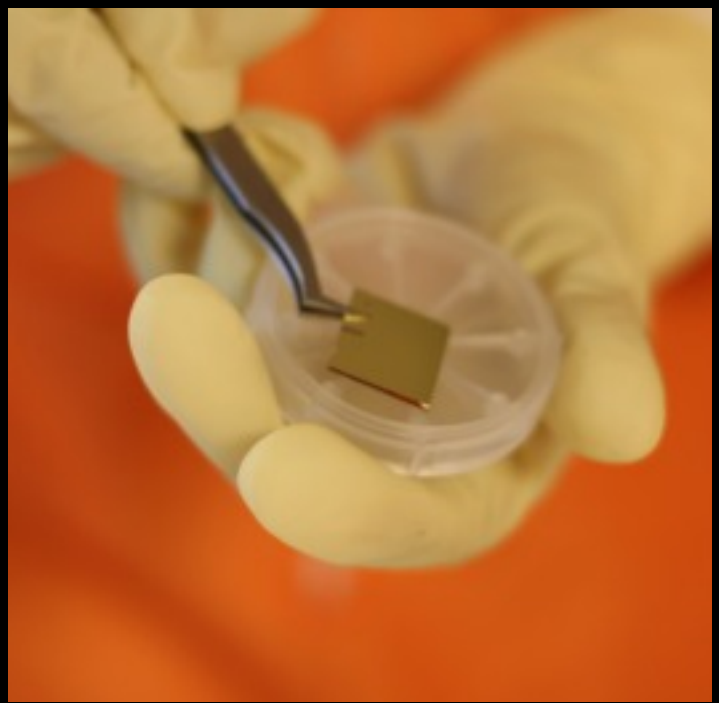


Intel Capitalization:
$85B
Total Industry:
$280B

What's Next?

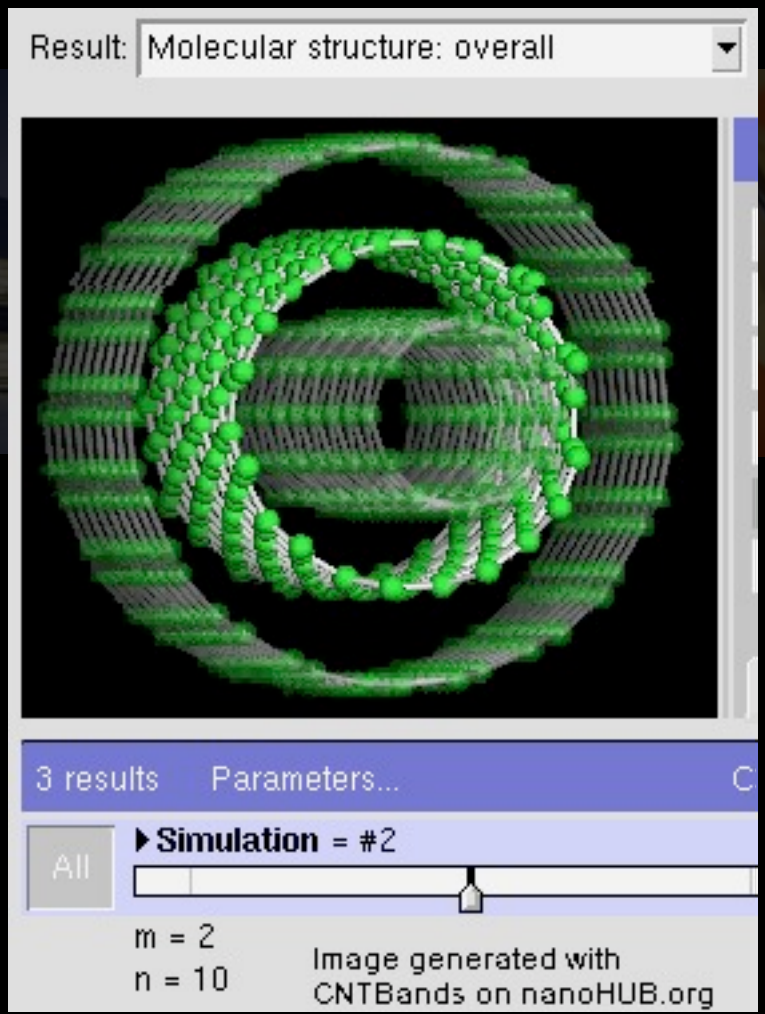


Nanotechnology

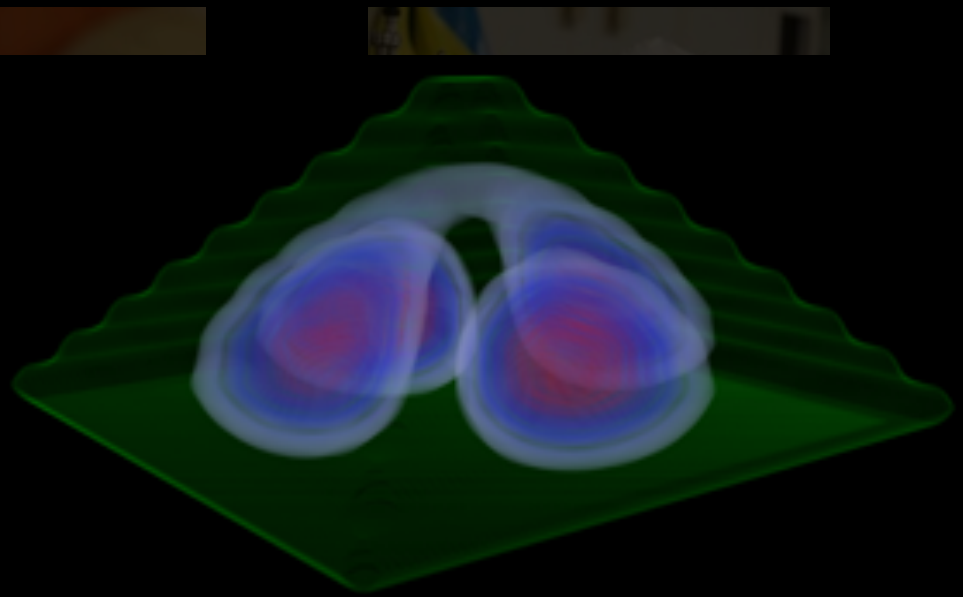


Extensive Facilities

Nano Models

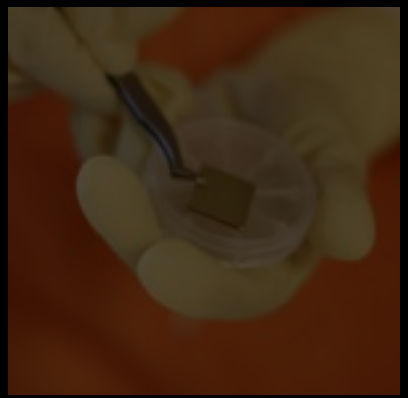


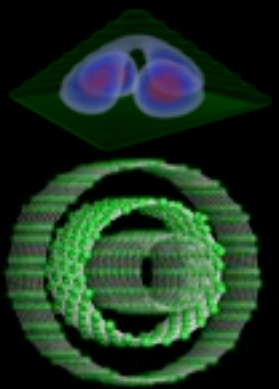
Carbon Nanotubes



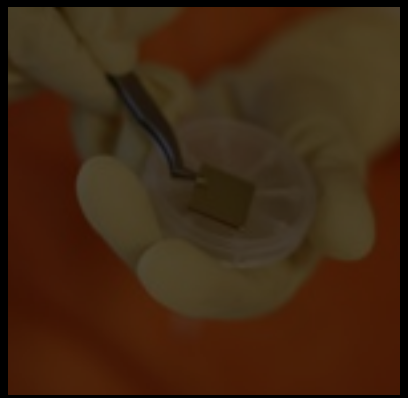
Quantum Dots
Artificial Atoms

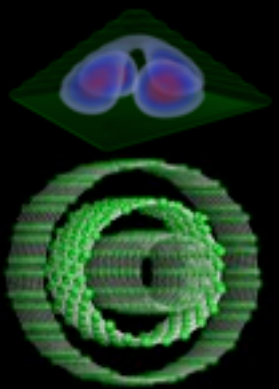
Computational Nano



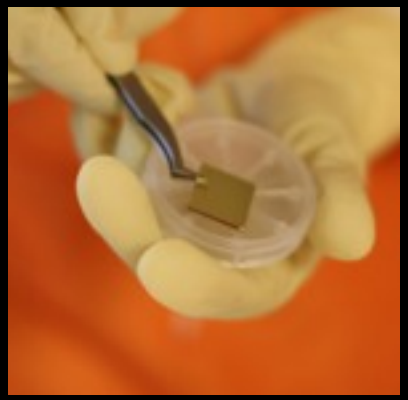


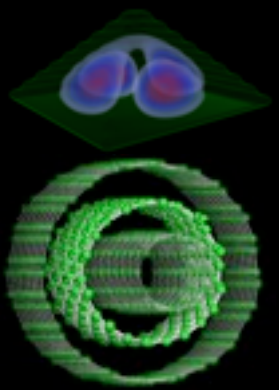
Computational Nano



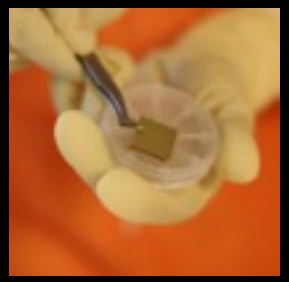


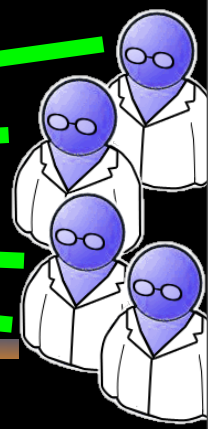
Different Worlds





Imagine Breaking Barriers



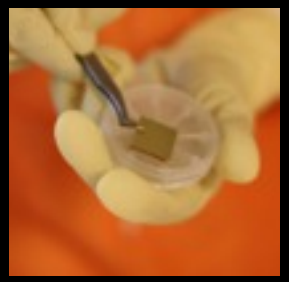


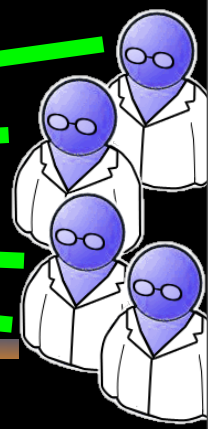
Easy use

No Install

Any Browser

Industries Breaking Barriers





Easy use

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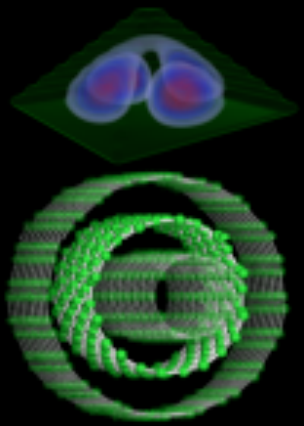
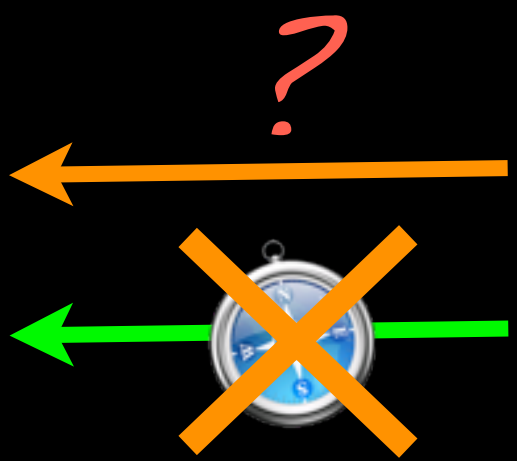
Why is this so hard?





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        s_H = -20
        Bands:TB:s:nanohub:p        ial         = 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

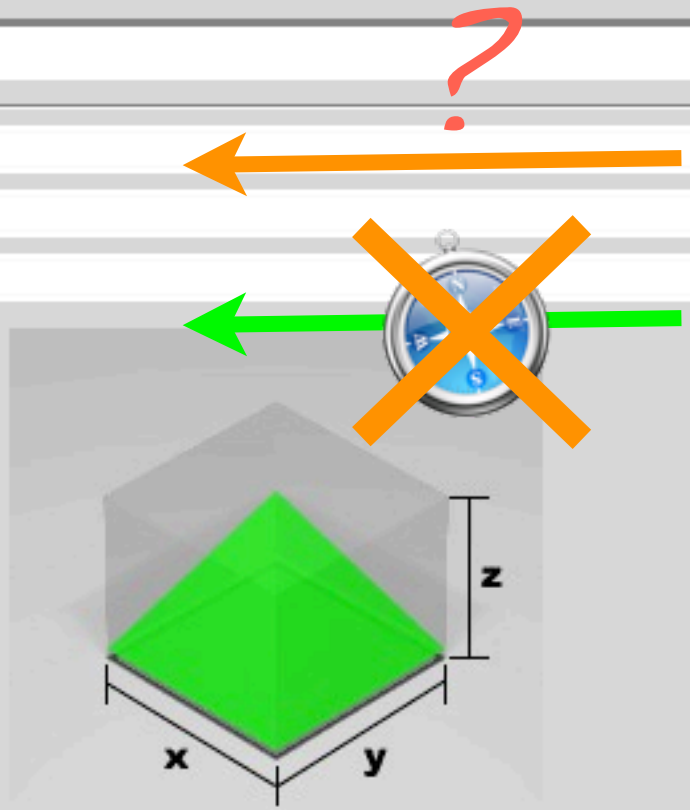
About this tool
Questions?

Number of States: 7

Surface passivation: yes

Device Structure | Light Source

Geometry: Pyramid



X dimensions: 10nm

Y dimensions: 10.5nm

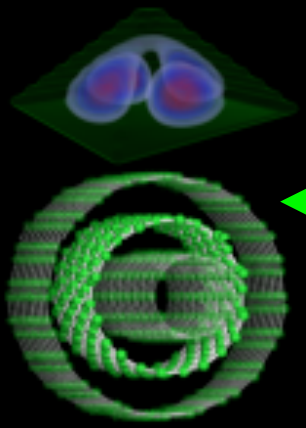
Z dimensions: 5nm

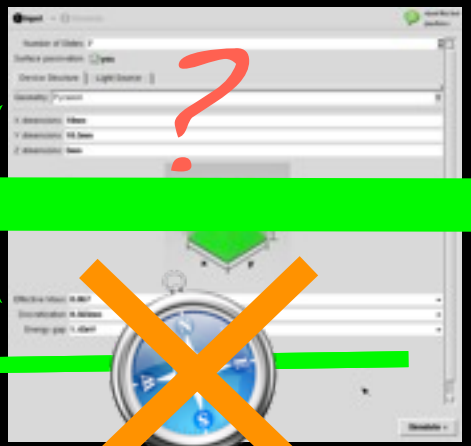
Effective Mass: 0.067

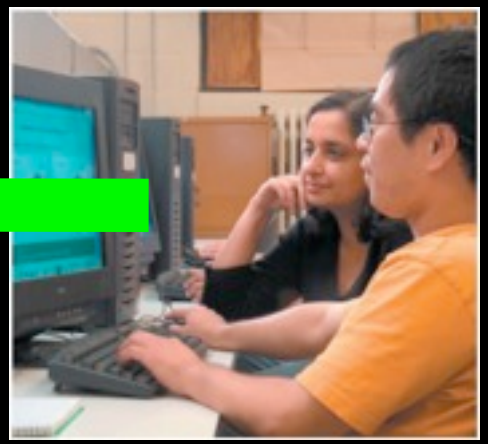
Discretization: 0.565nm

Energy gap: 1.43eV

Why is this so hard?







Most research codes

Accessible (no installation)

are written by one user

HUBzero

Developer Friendly

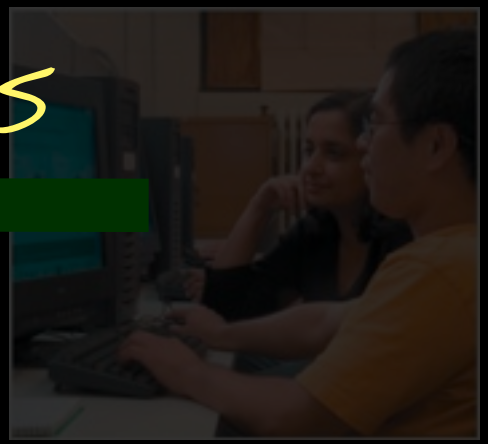
for one user

Rappture

User Friendly

It has been very hard!

Emerged Myths



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Cannot use research codes for education

Must write own code to do research

Experimentalists cannot use research codes

Developer Friendly

Building User Interfaces too Difficult

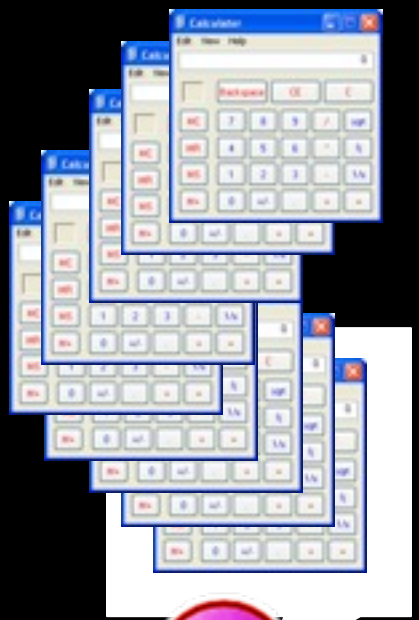
Must rewrite code for web deployment

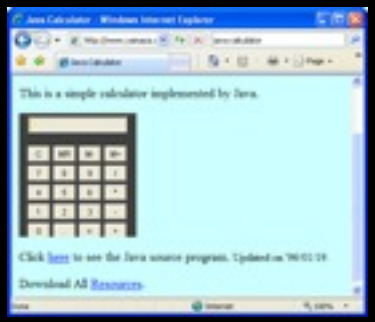
There is no incentive to share codes

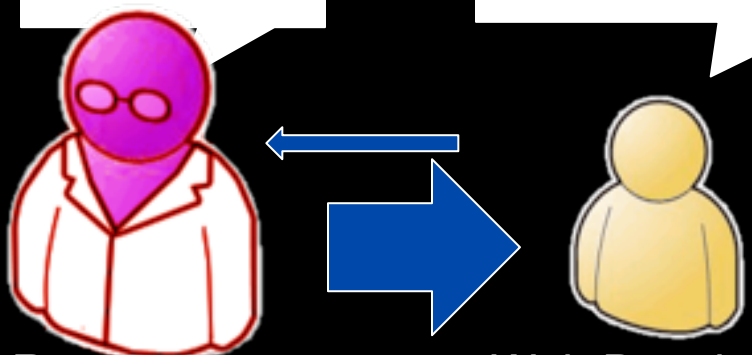
Accessible (no installation)

NO End-to-end Science Cloud Possible

Usual Science Gateway Process







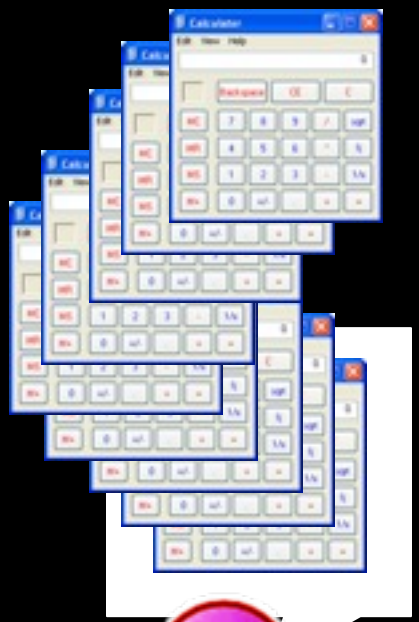
Researcher

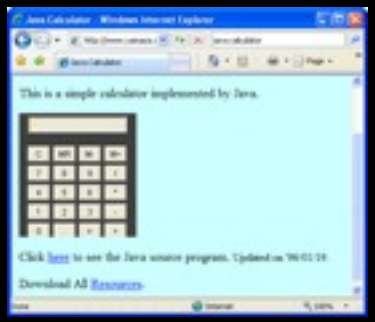
Web Developer

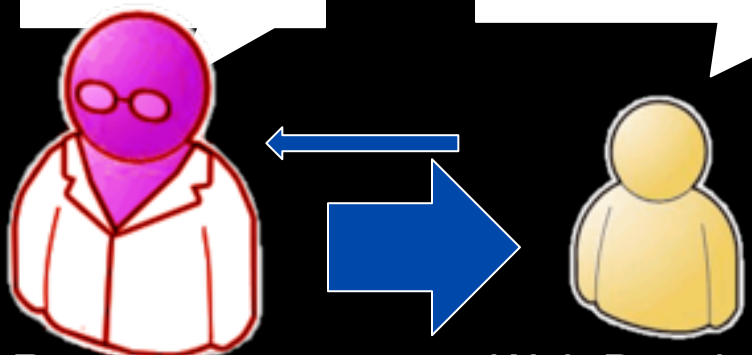
- 175 tools / 4 years: => ~~$8M~~
- $500k/tool
- NO new research!
- Not validated by researcher (disowned)
- Researcher has much better version
- Code rewrite takes 2-3 years

Many Proposals read alike

Usual Science Gateway Process







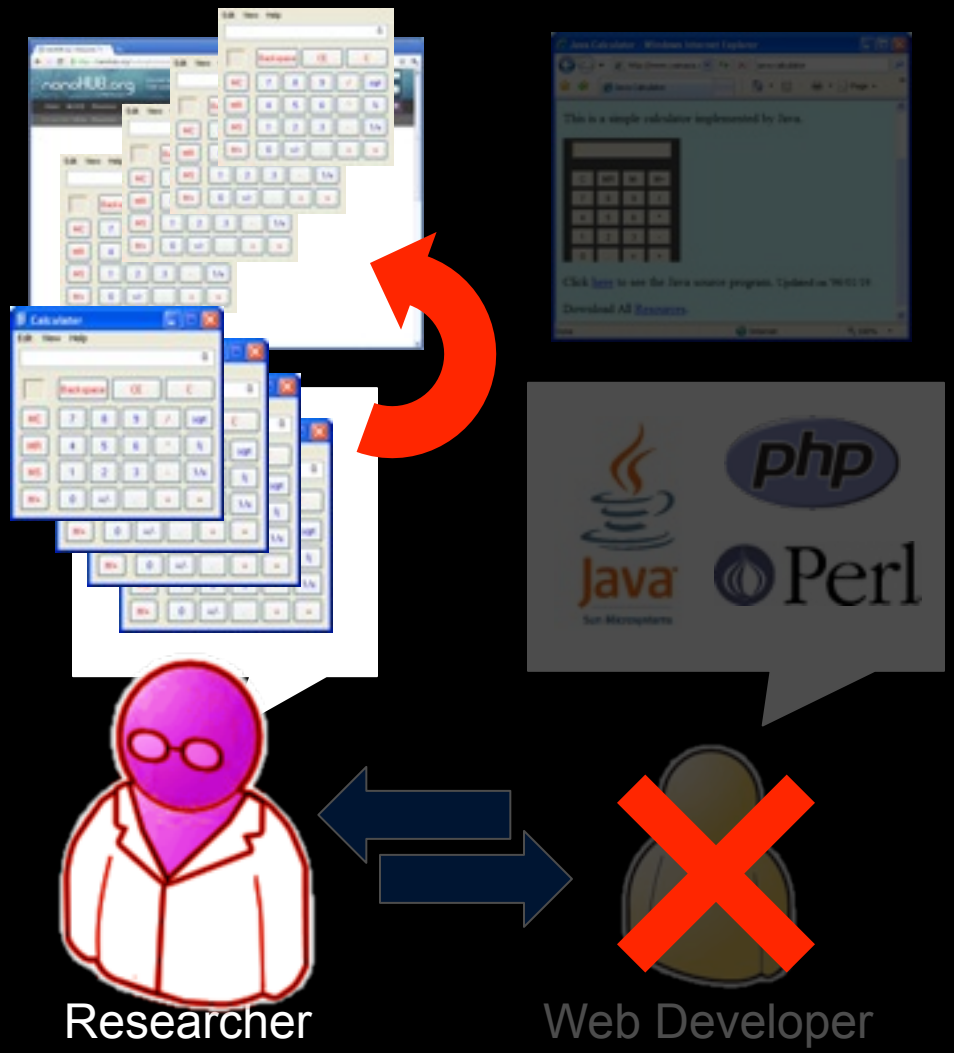
Researcher

Web Developer

- 175 tools / 4 years: => ~~$8M~~
- $500k/tool
- NO new research!
- Scale back expectations
- Not research codes
- Toy applications
- Not deep research
- Maybe for education?

Generating a Bad Reputation

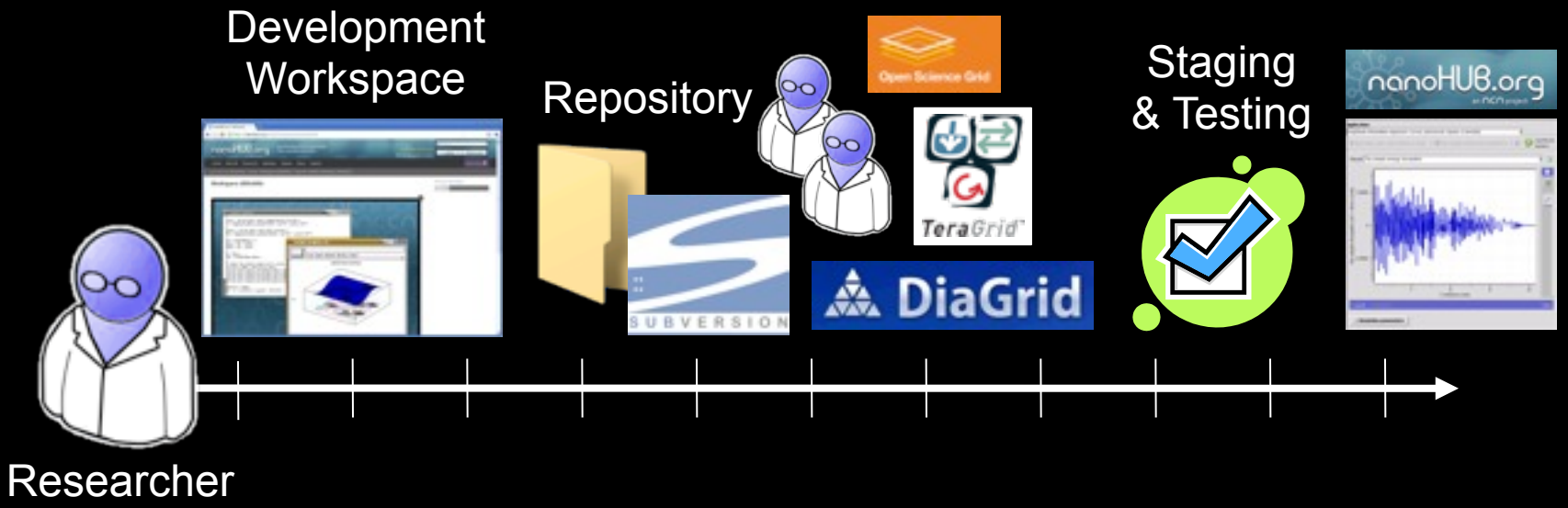
nanoHUB Process

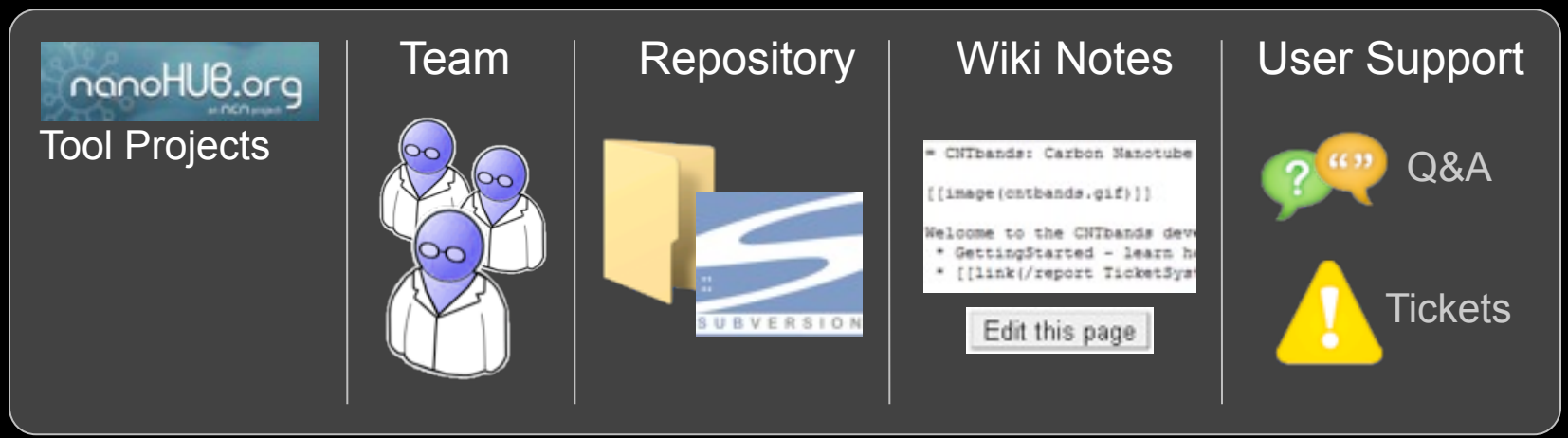


- **175 tools / 4 years without $88M**
- Eliminate bottlenecks
  - No Middleman
  - No Rewrite
  - Retain ownership
- Rapid Deployment: 2-3 years → 1-2 weeks
- Rappture toolkit
- S/W Dev. Ecosystem

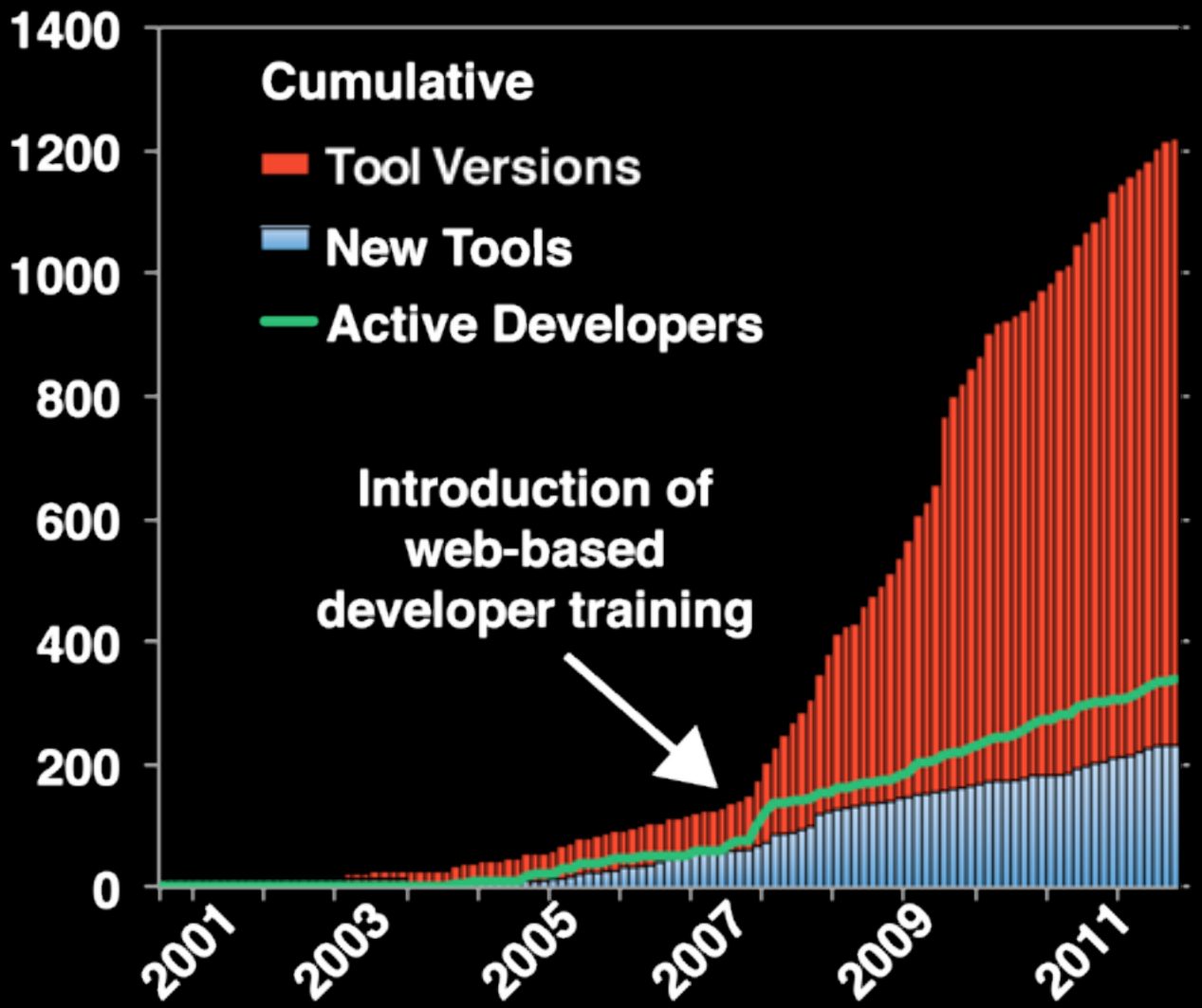
nanoHUB is different

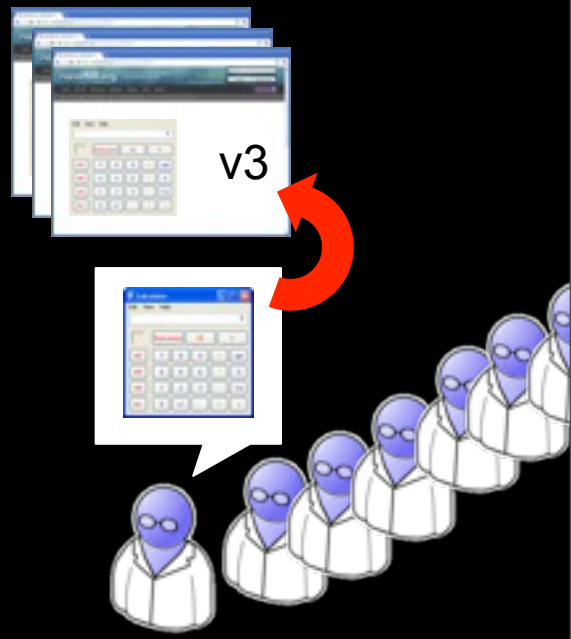
Software Development Ecosystem





nanoHUB - nowhere else!



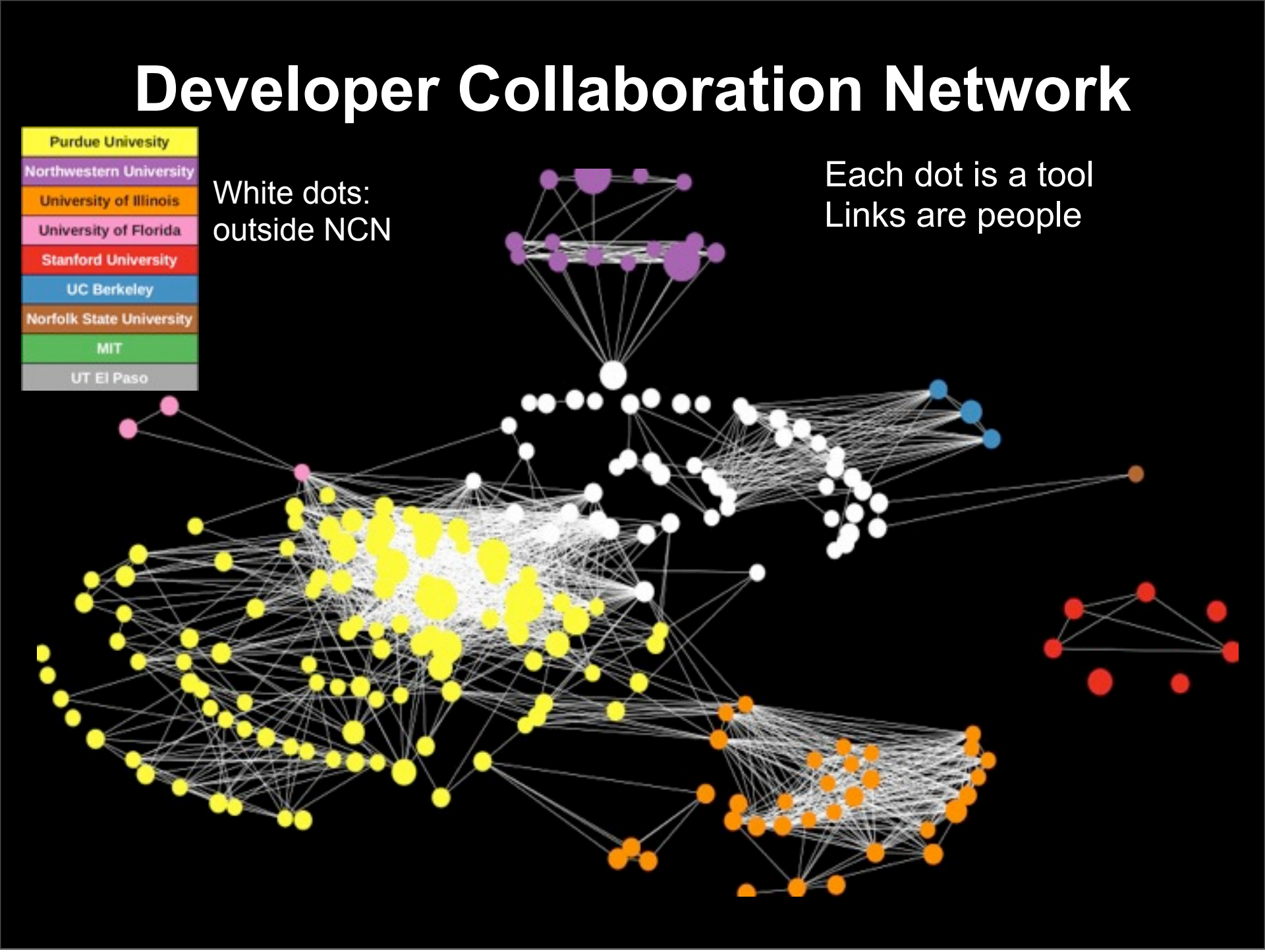


Continual Engagement

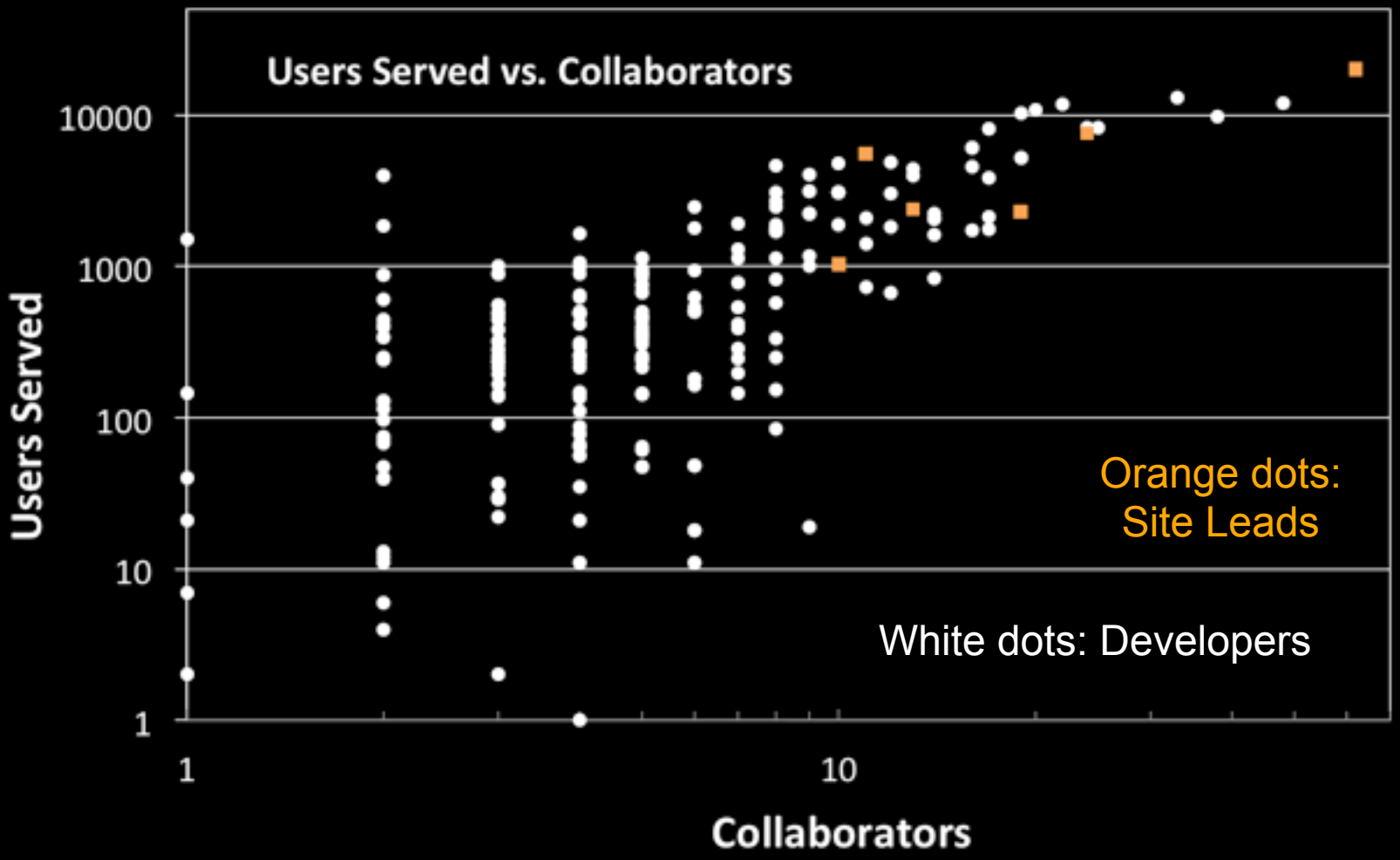
Over 300 Developers NOT PAID by NCN

nanoHUB can prove it

Developer Collaboration Network



Developer Collaboration Impact



Next Generation Publications
Research Incentives

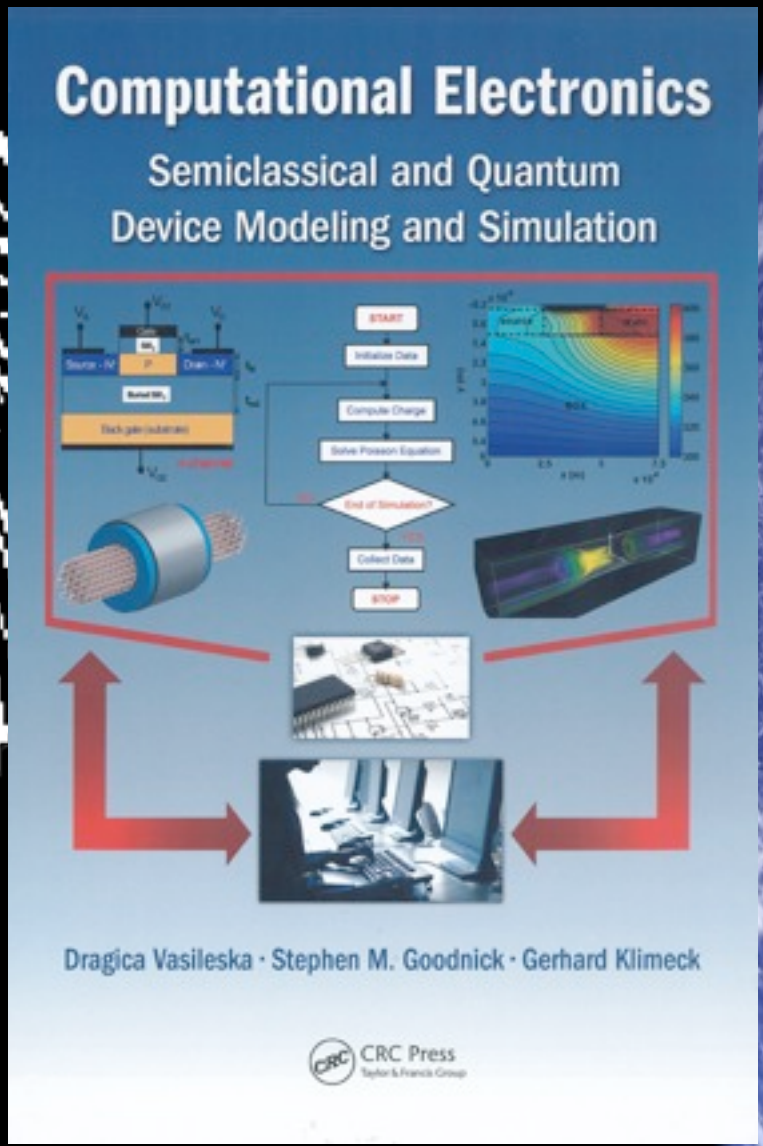
Tool Usage ≈ reading papers

Dragica Vasileska

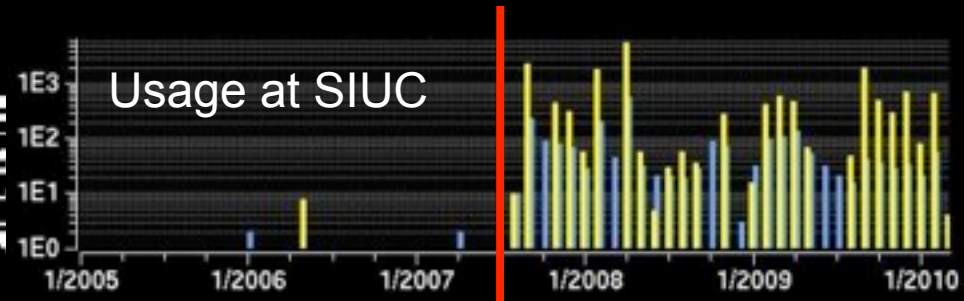
17 tools

➔ 11,570 users

➔ 123 citations



Next Generation Faculty:



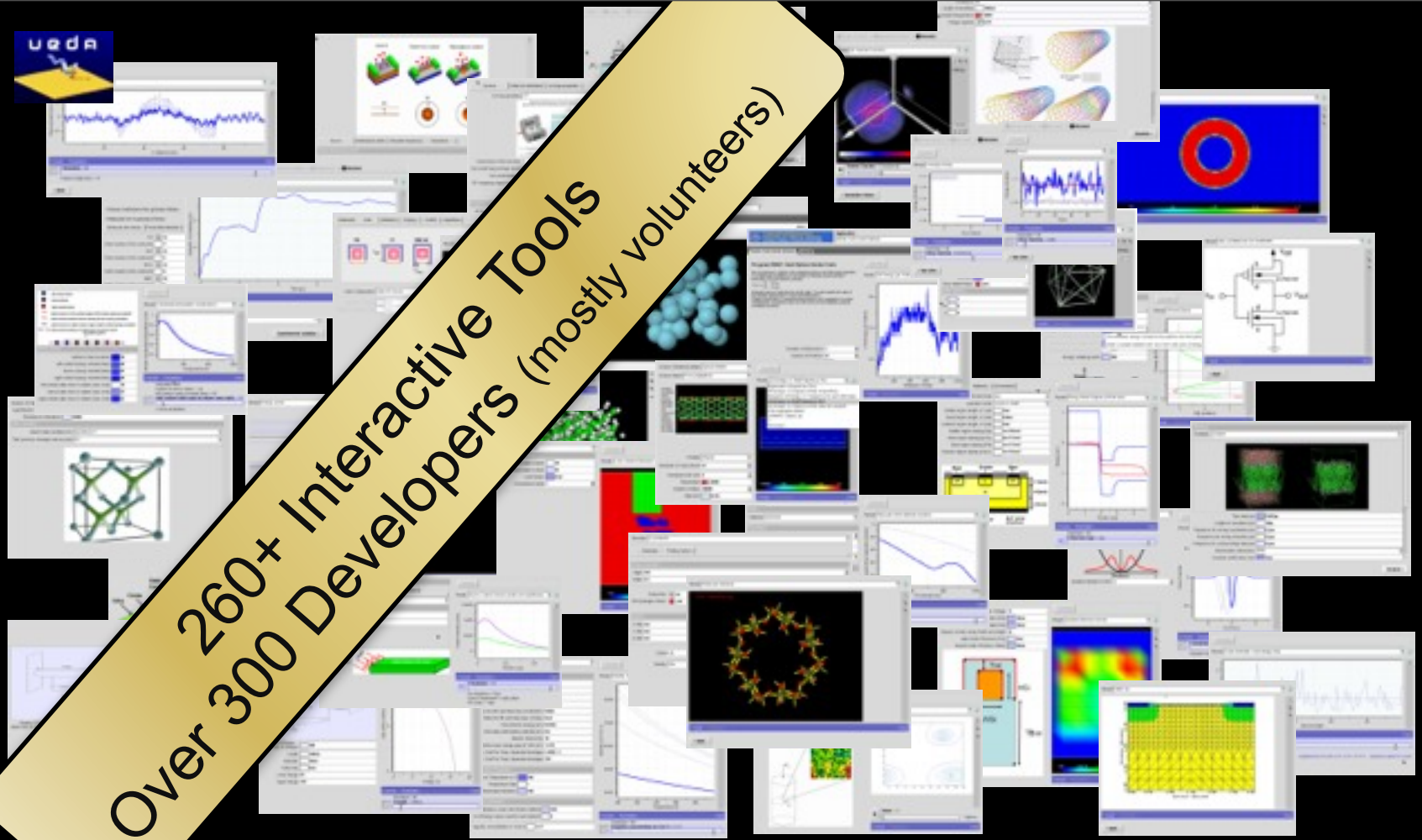
Shaikh Ahmed

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



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Myths Busted

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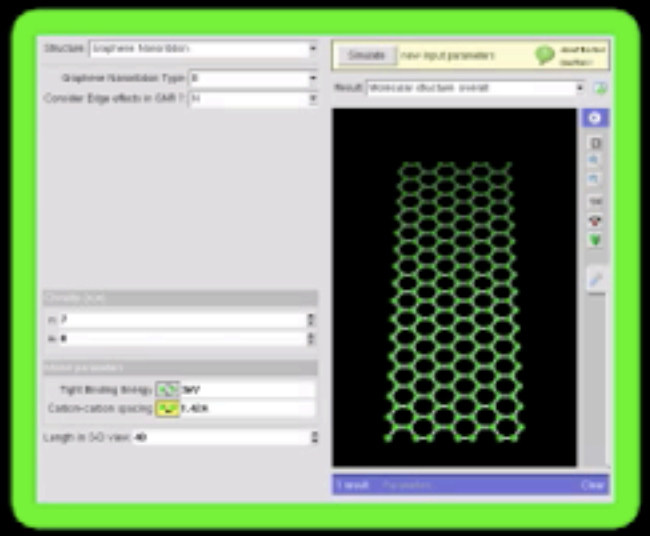
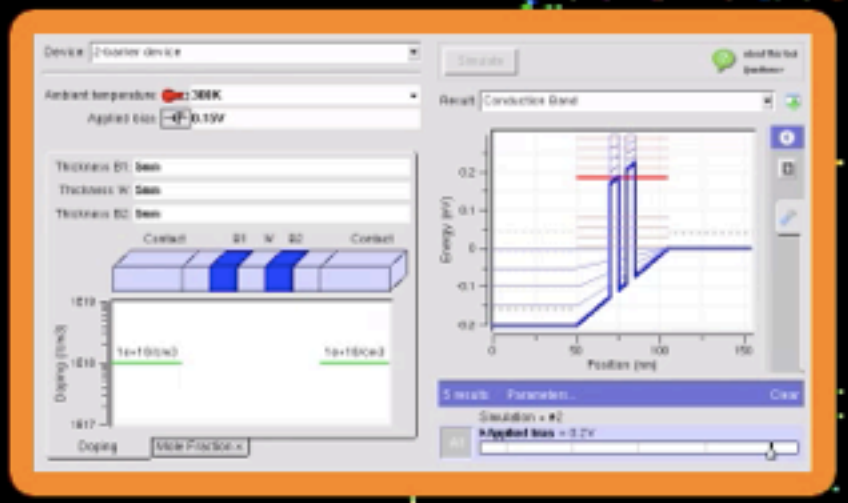
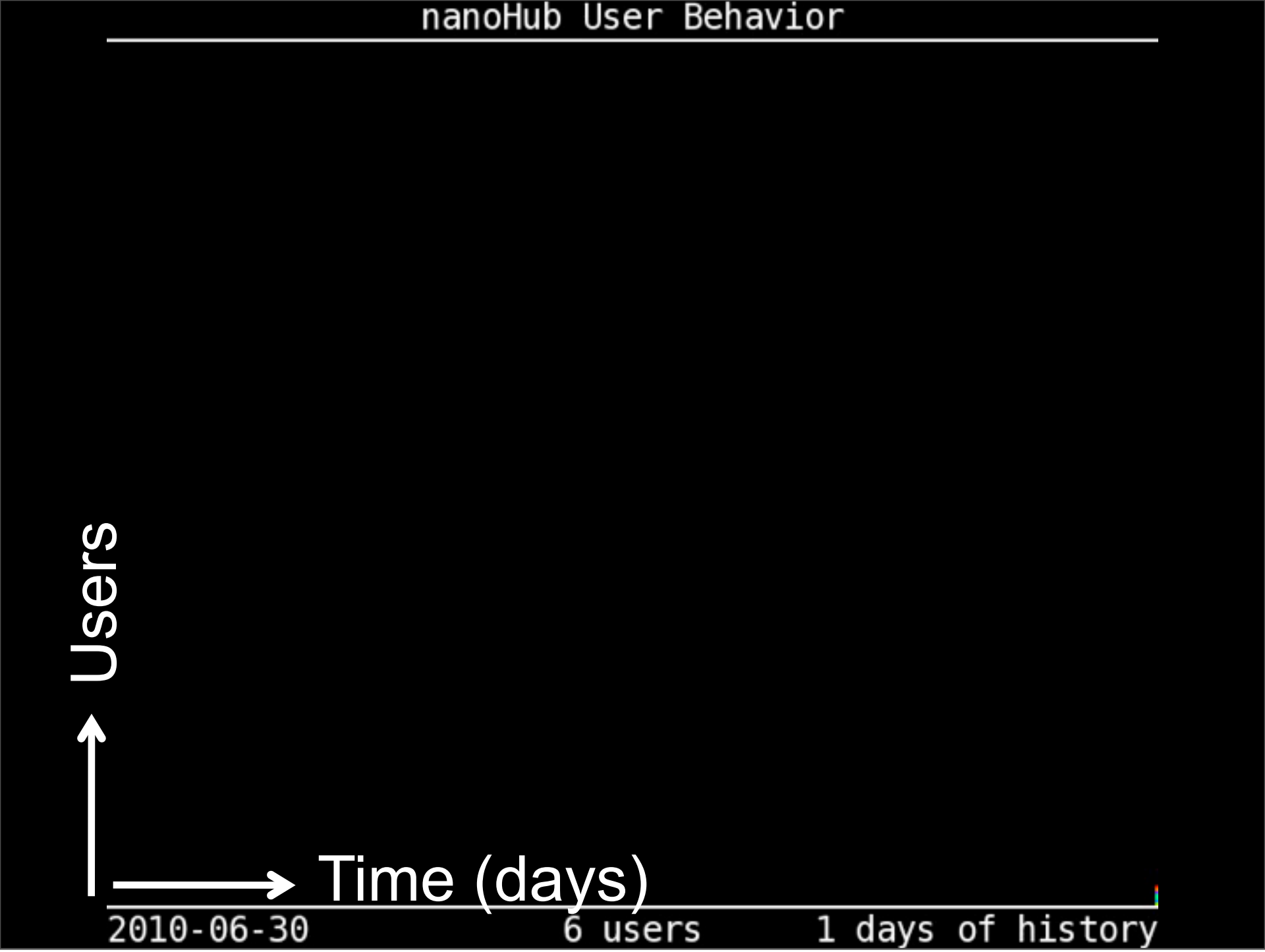
User Behavior Analysis





Users

Time (days)



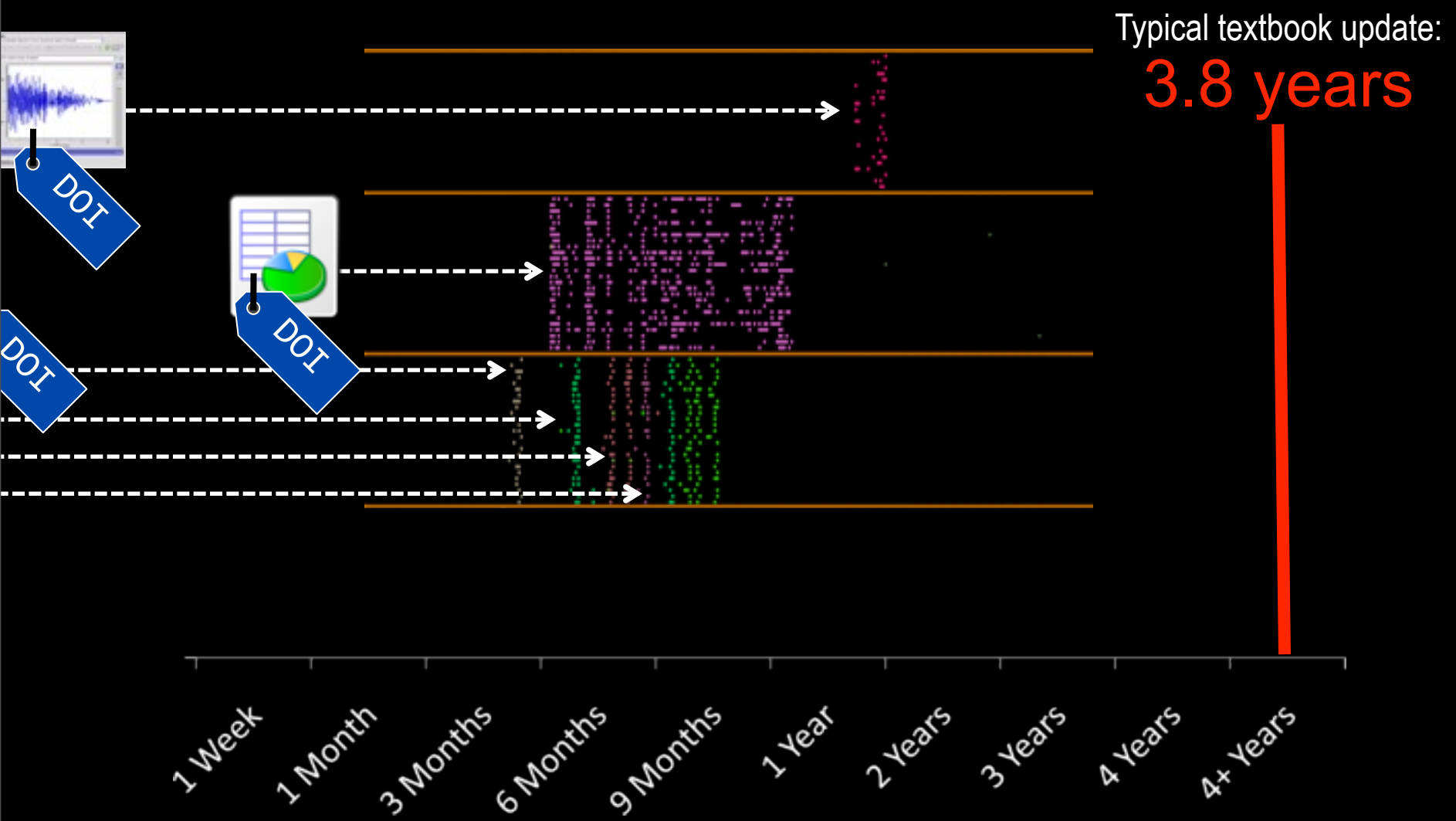
User Behavior Analysis

single tool,
single use /
homework

Users

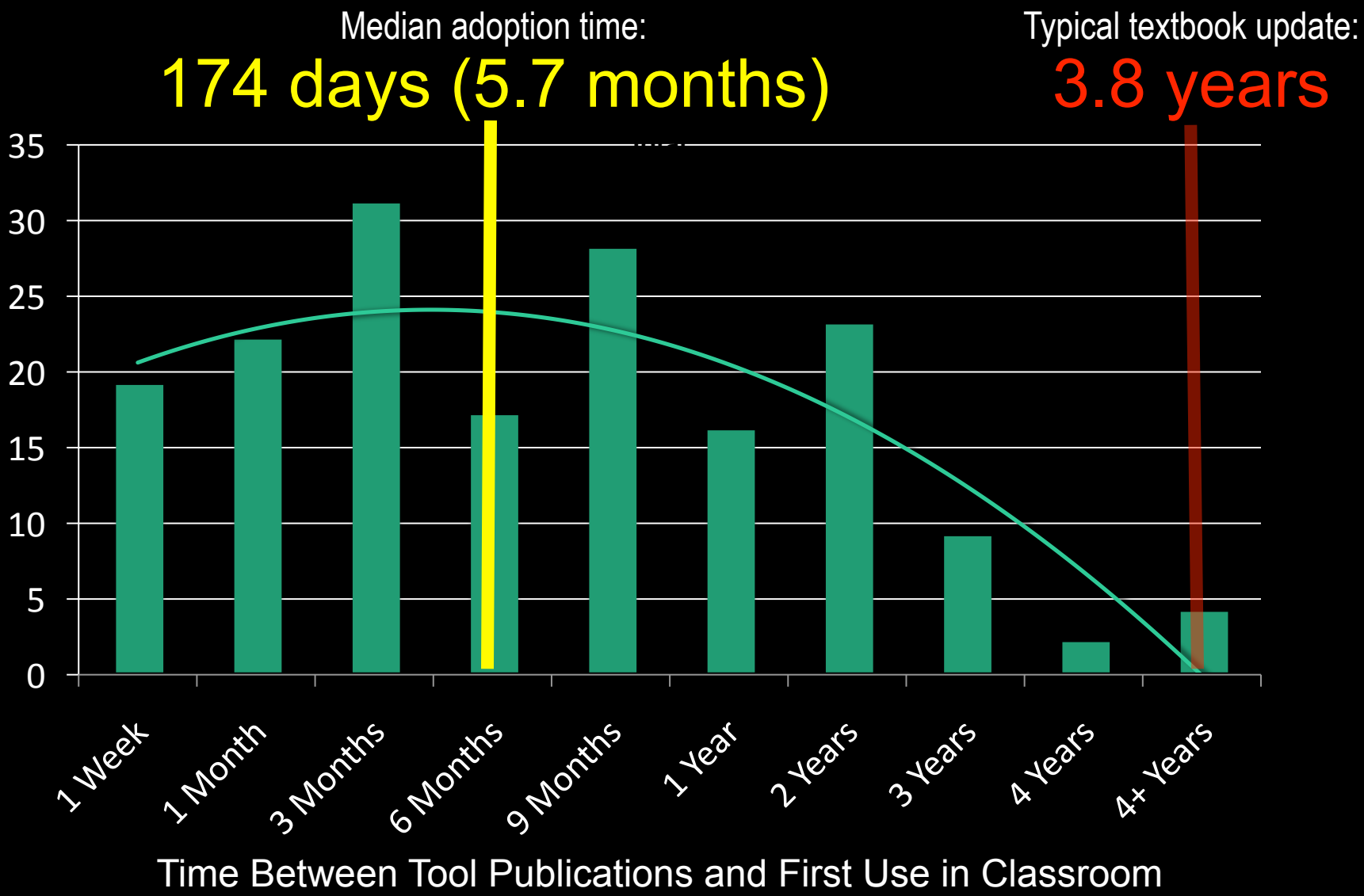
Myth Busted:
Proof of use in EDUCATION!
Knowledge Transfer out of Research
14,000 students, 185 institutions
Voluntary / Viral Use

Time to First Adoption

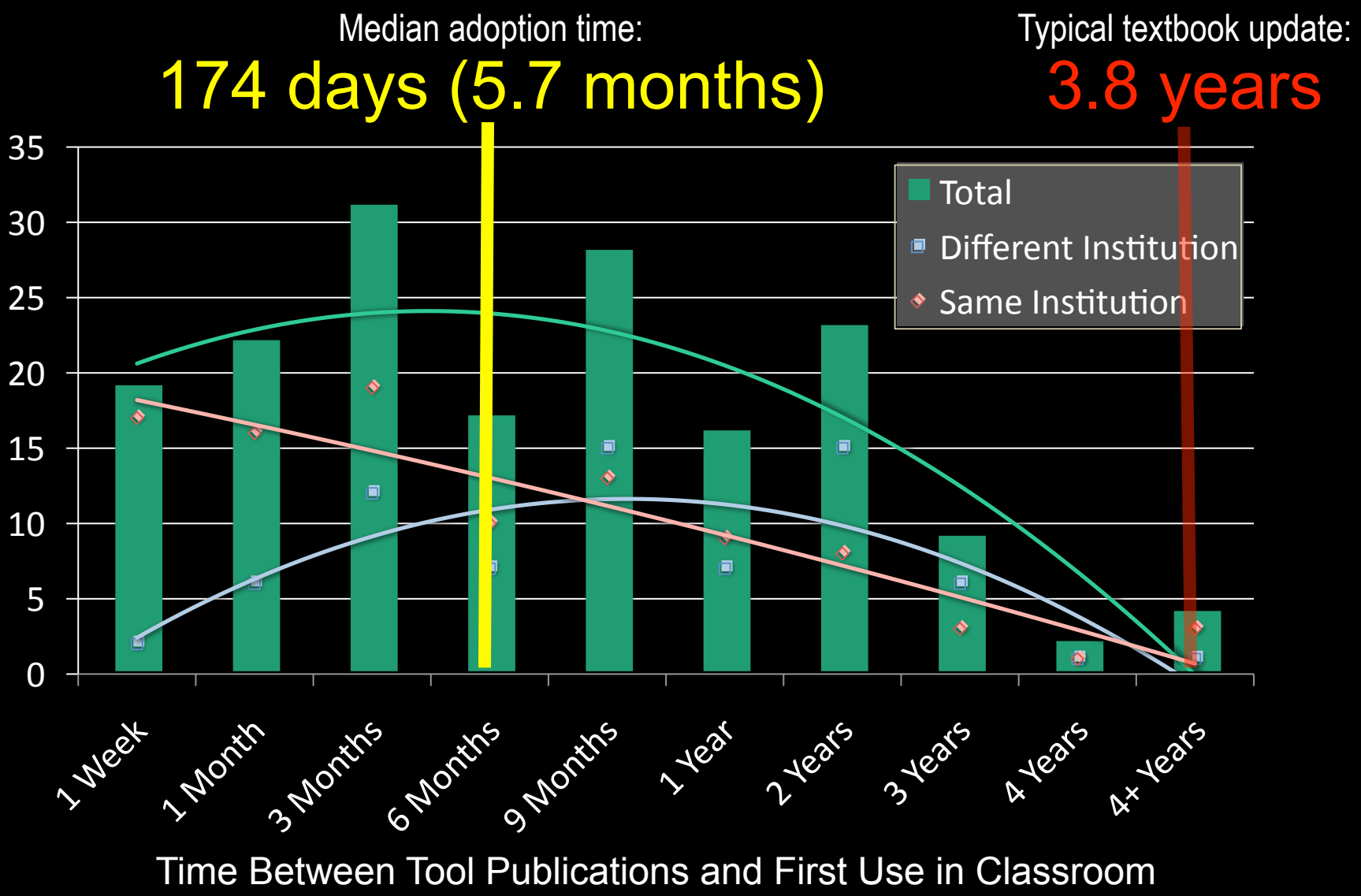


Time Between Tool Publications and First Use in Classroom

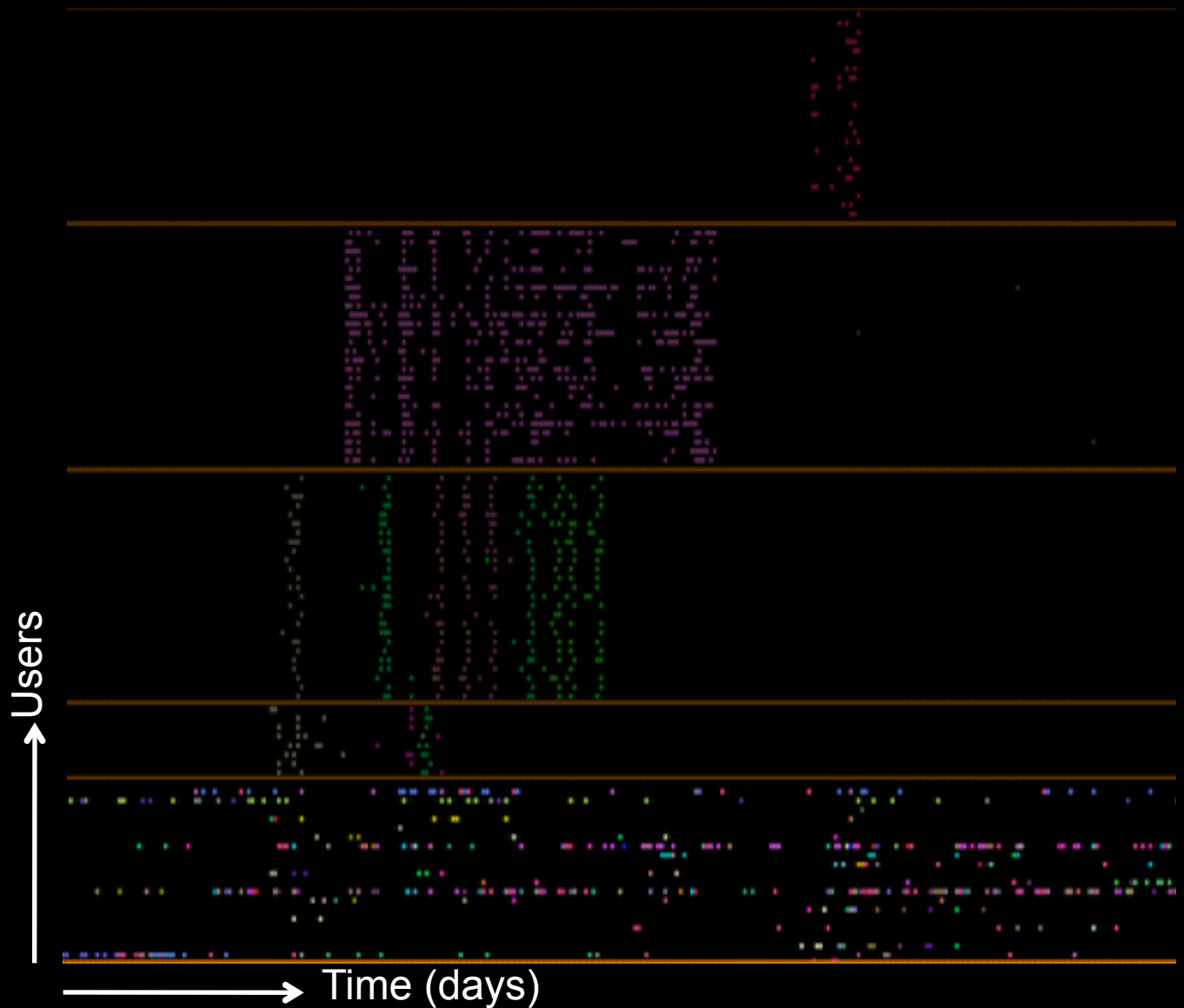
Rapid Adoption of Research



Revolutionizing Research → Classroom



User Behavior Analysis
=> Is Research Possible?



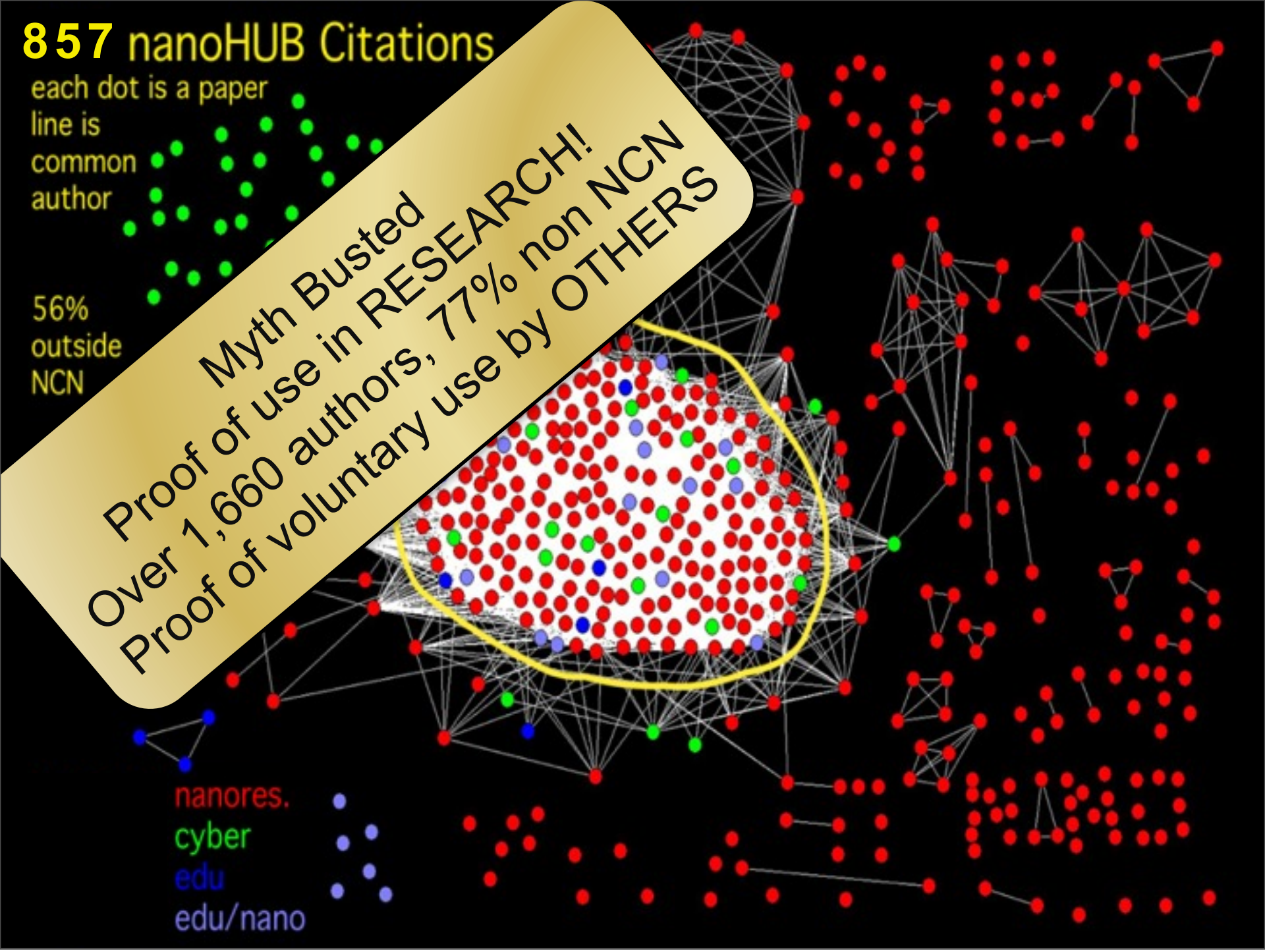
single tool, single use / homework

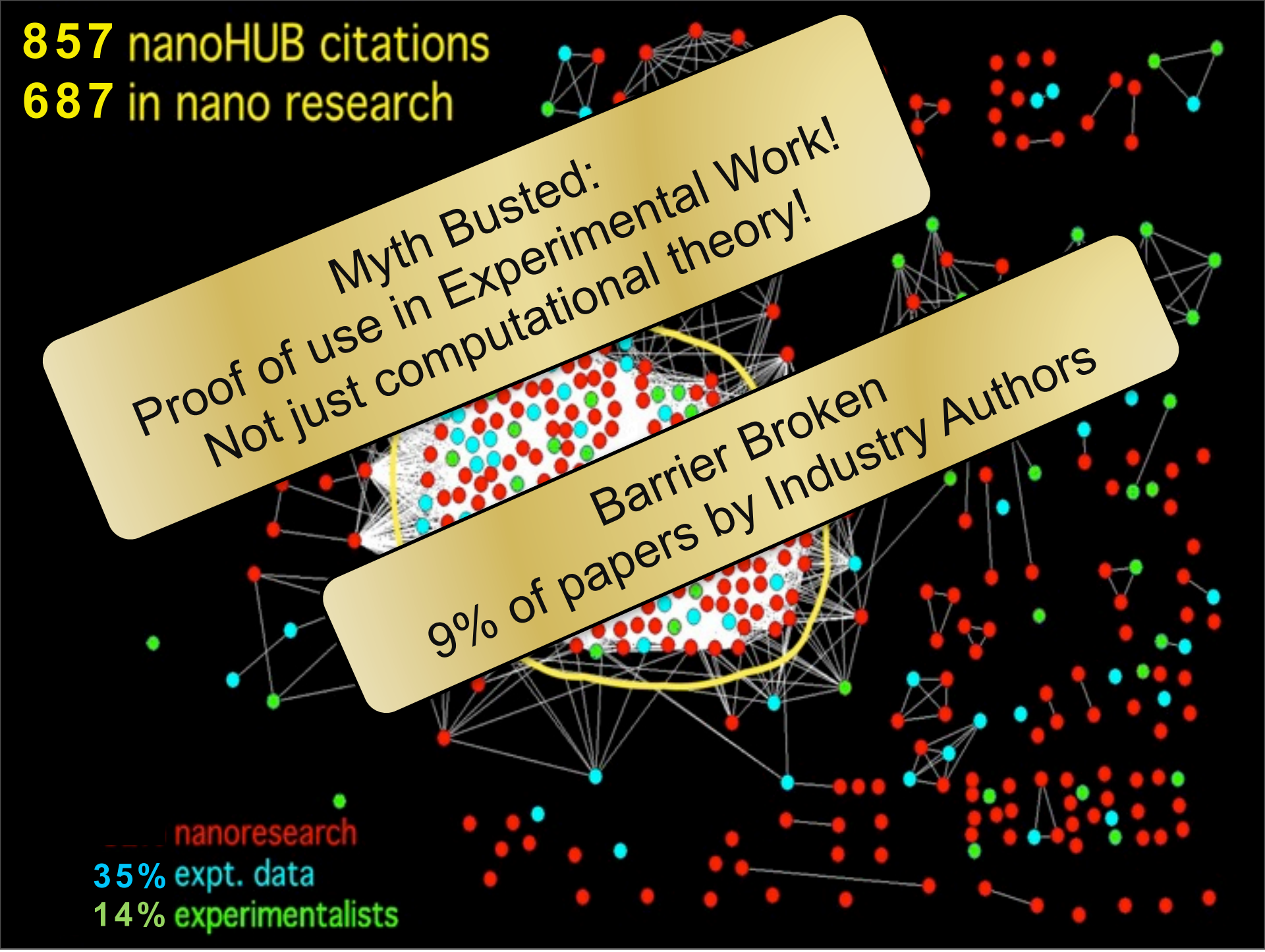
single tool, sustained, intense

multiple tools, sustained, periodic

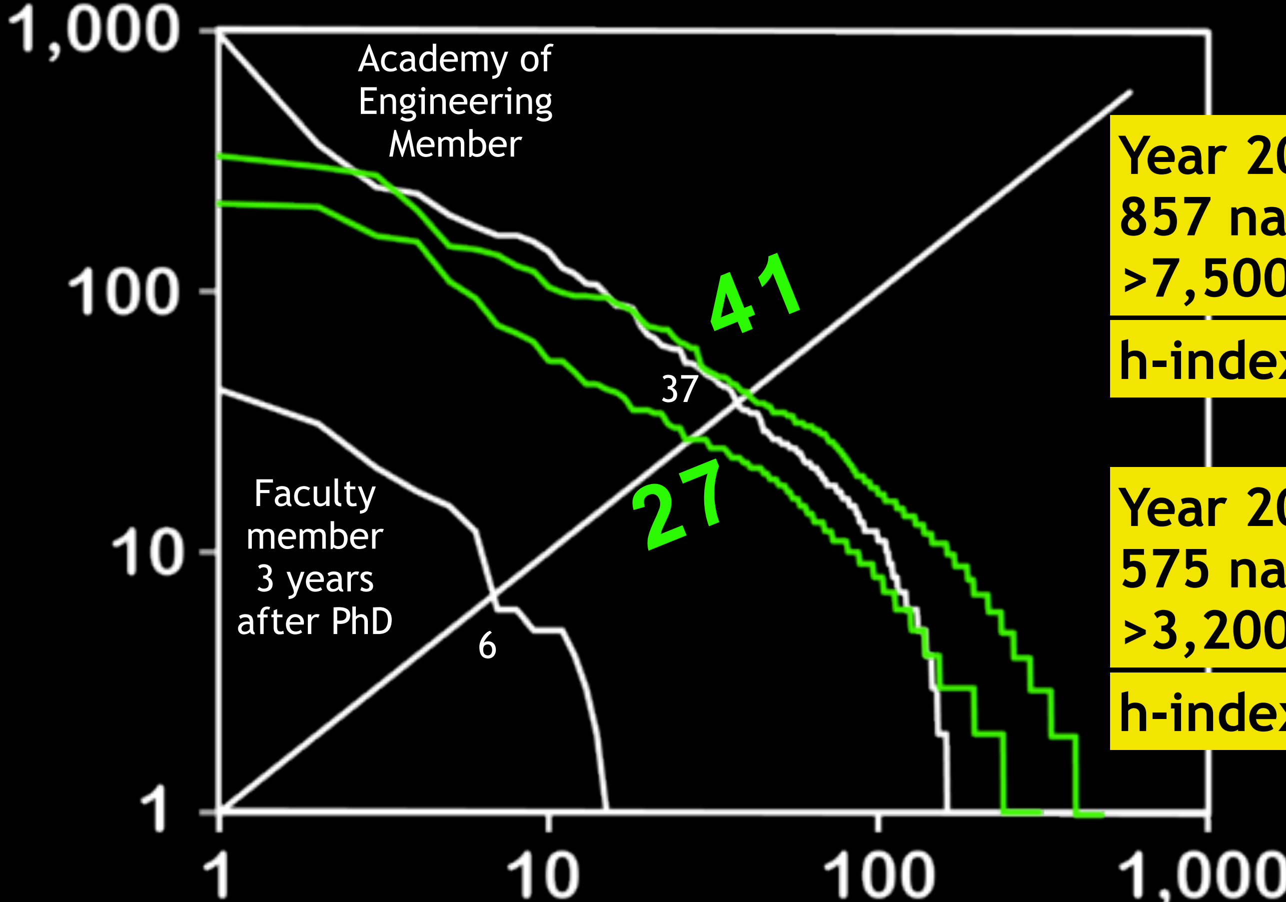
multiple tools, small class

research, self-study





h-index: Research Quality Indicator



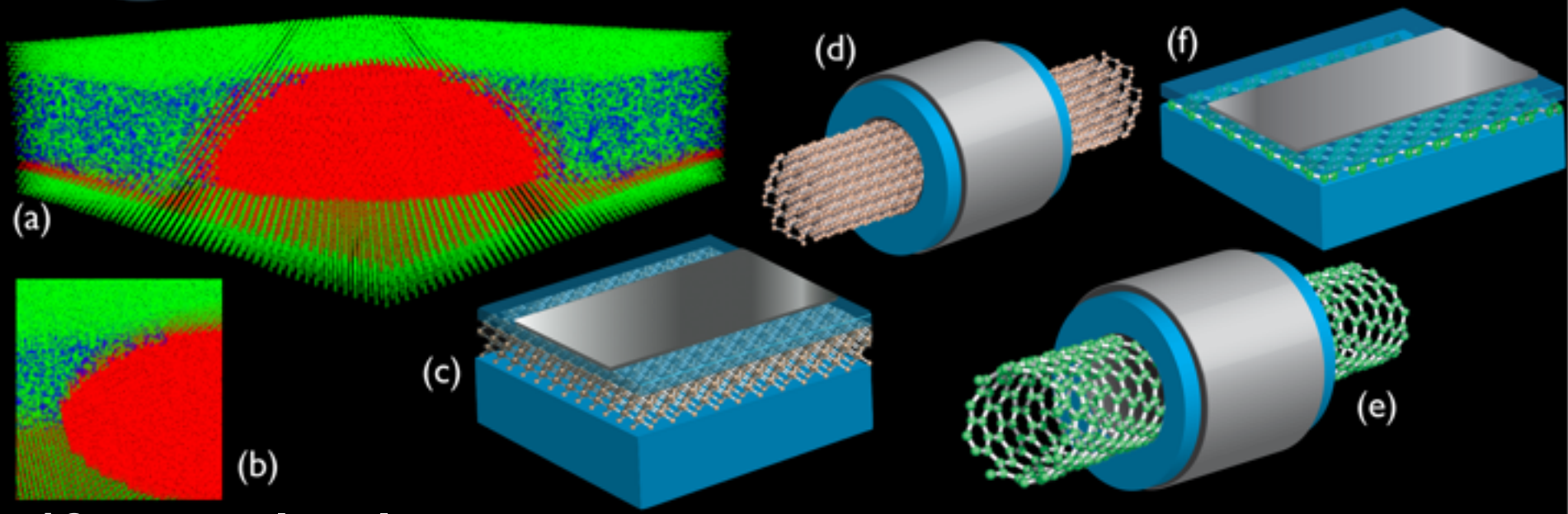
Year 2012
857 nanoHUB citations
>7,500 secondary citations

h-index: 41

Year 2009
575 nanoHUB citations
>3,200 secondary citations

h-index: 27

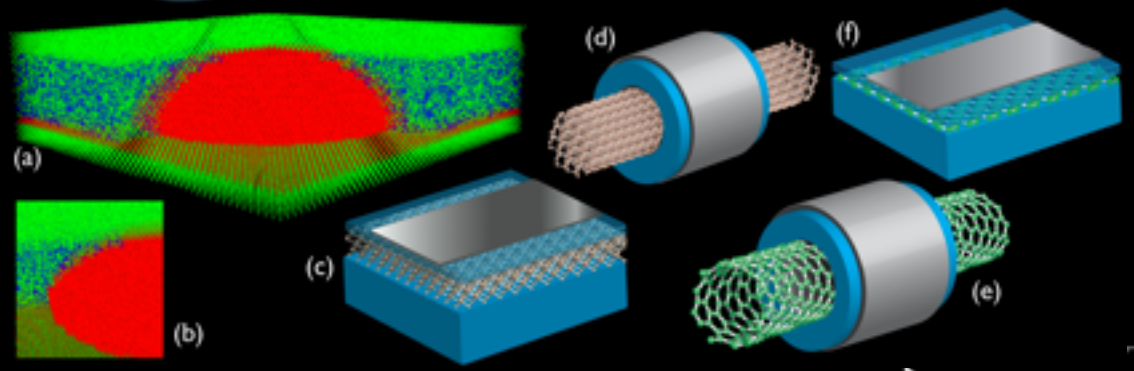
Compute Intensive: NEMO/OMEN

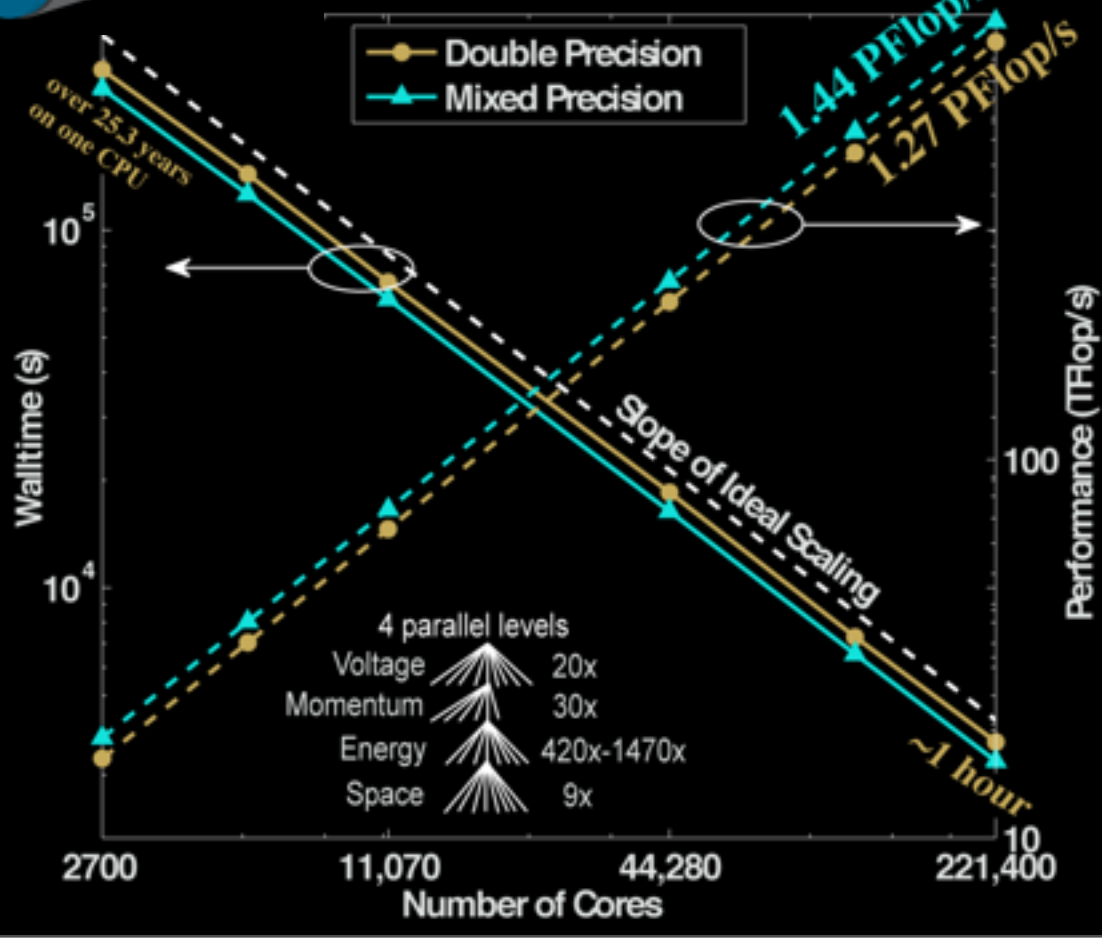


18 years development

- Texas Instruments
- NASA JPL
- Purdue

Compute Intensive: NEMO/OMEN





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- Texas Instruments
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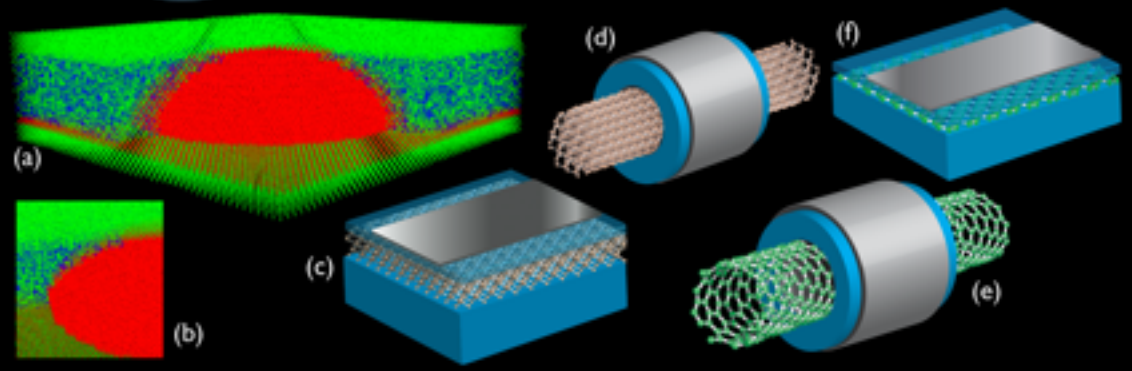
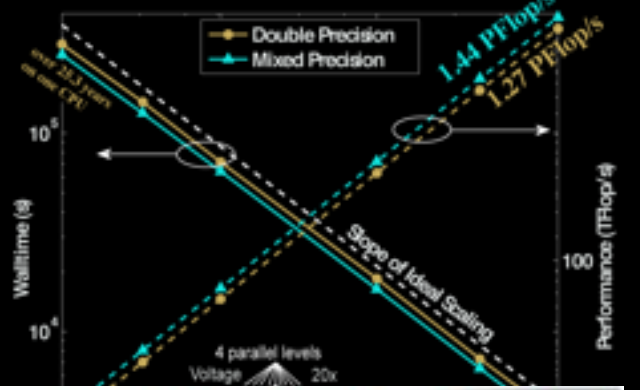
- Peta-scale Engineering

Compute Intensive: NEMO/OMEN





18 years development

- Texas Instruments
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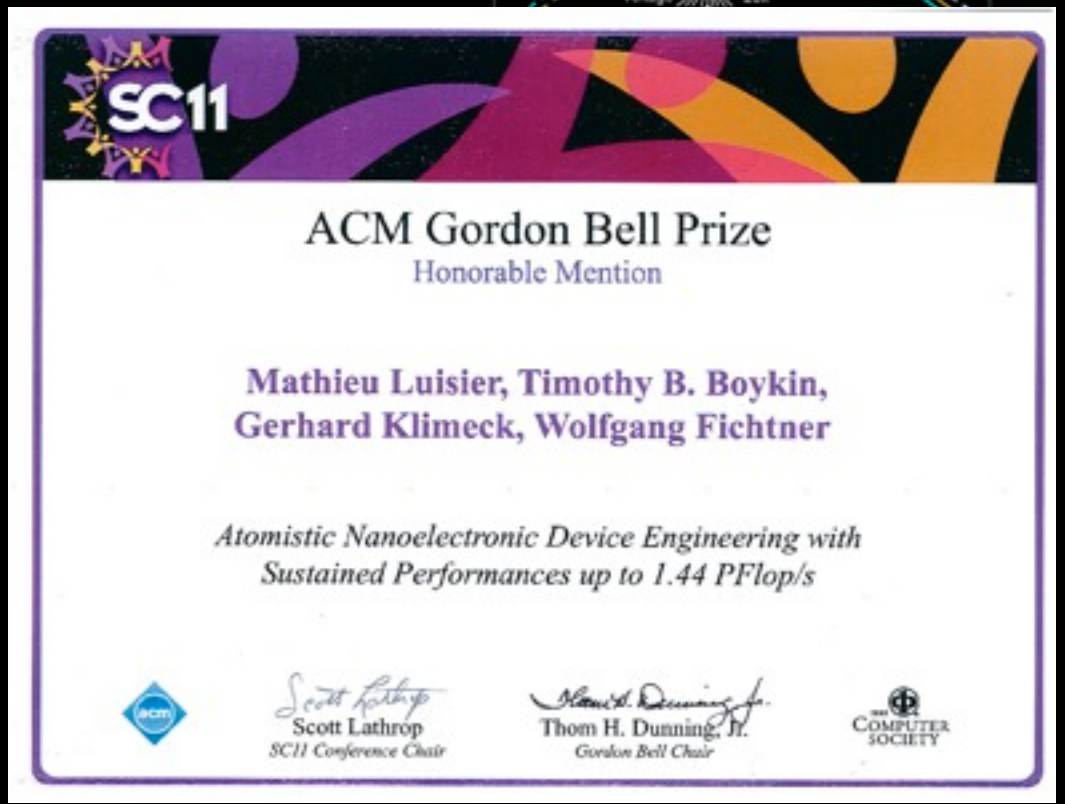
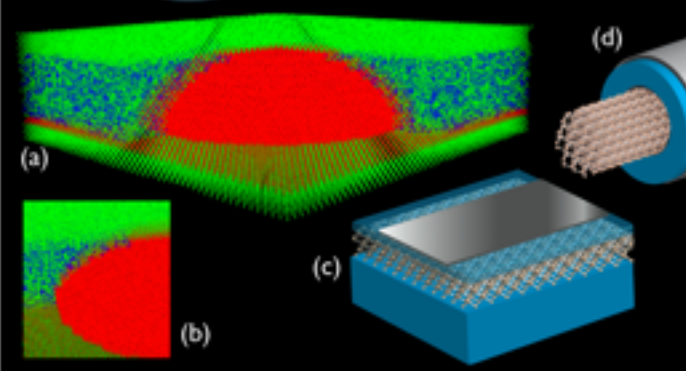
- Peta-scale Engineering
- Gordon Bell



Compute Intensive: NEMO/OMEN

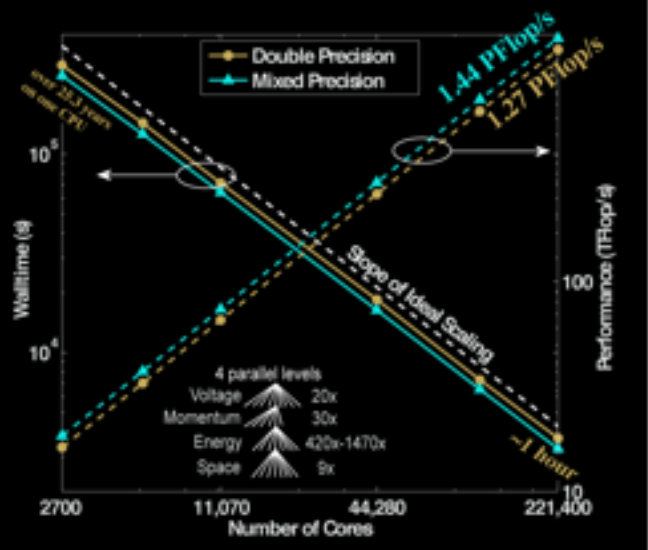


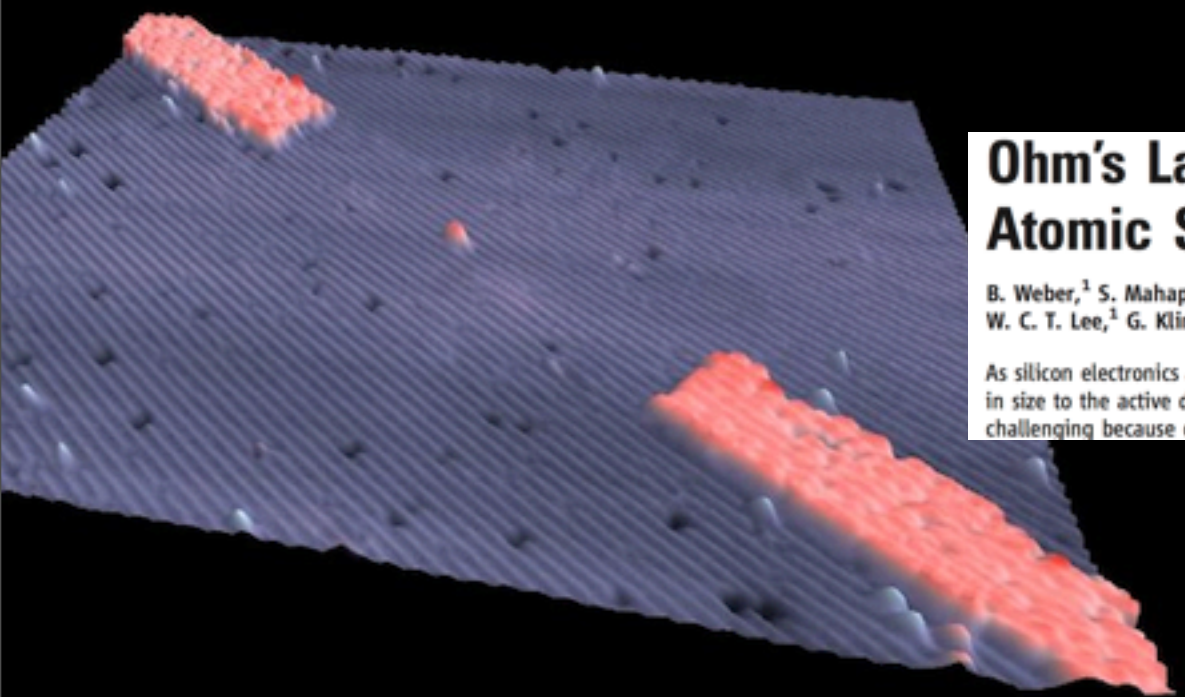
SC11

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. Hollenber

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

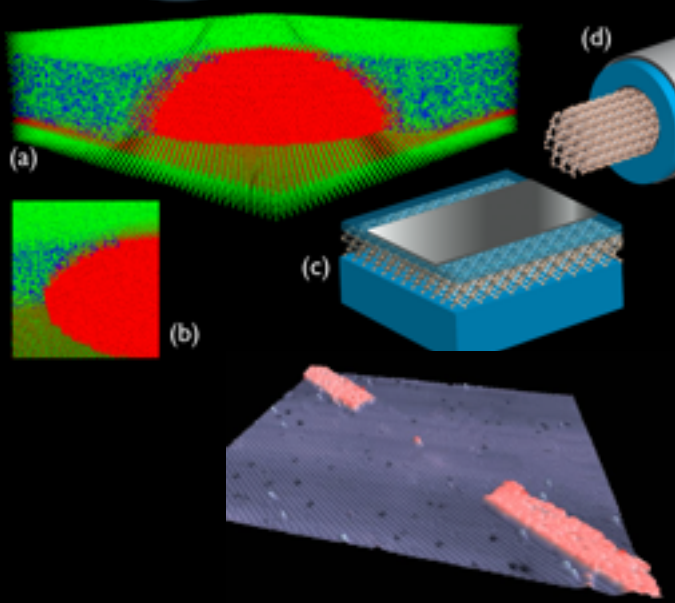
nature nanotechnology

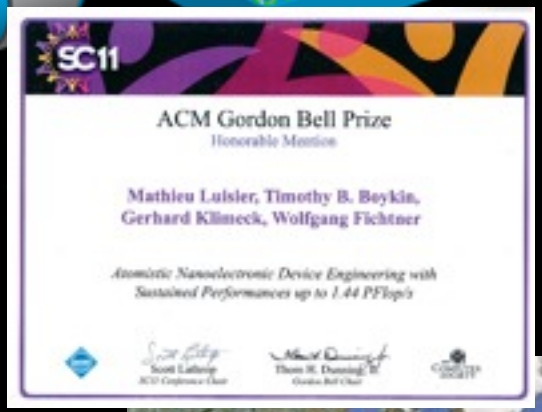
A single-atom transistor

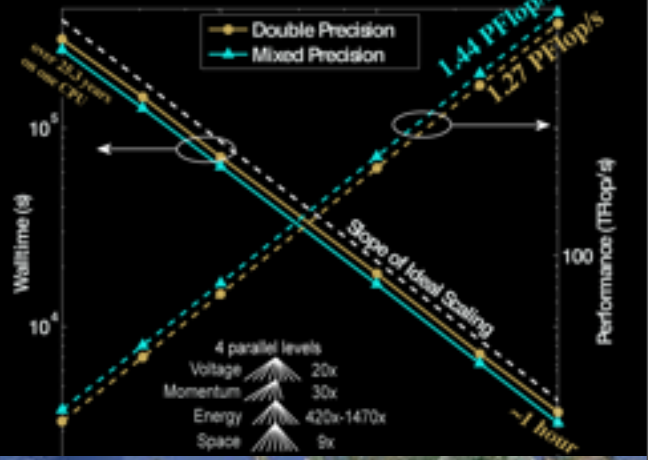
Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard

- Science, Nature Nano

Compute Intensive: NEMO/OMEN







18 years development

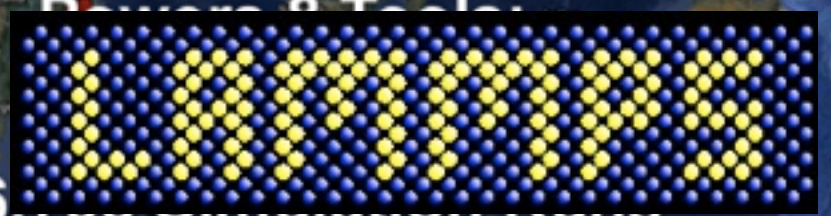
- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell
- Science, Nature Nano

pute Intensive

Myth Busted!
Prove
Computational Extensive Work

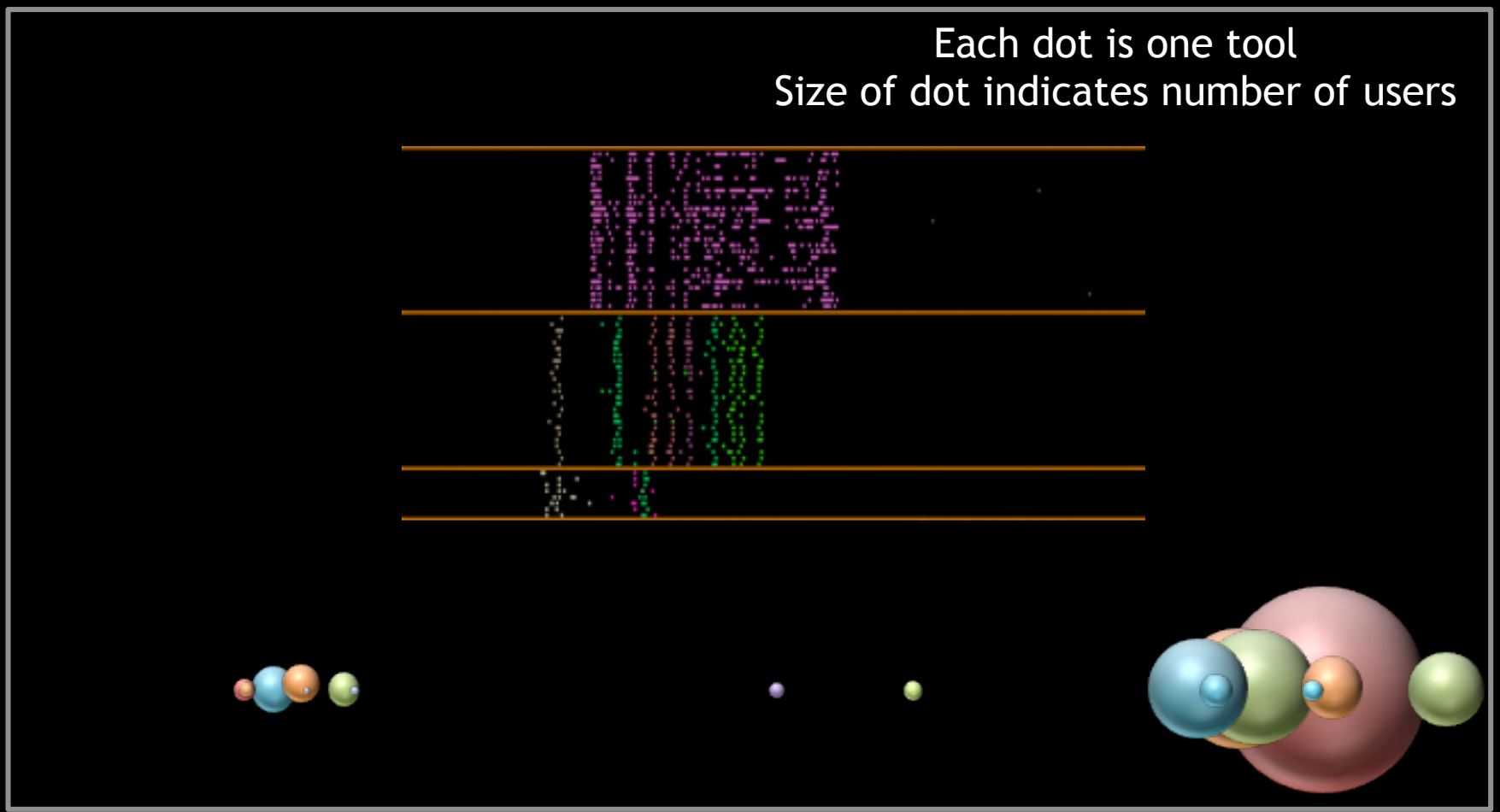
- 18 years development
- 267,362 Simulation Runs
- 10,786 Users
- 3,874 Users in 100 classes

- Peta
- Gord
- Scie



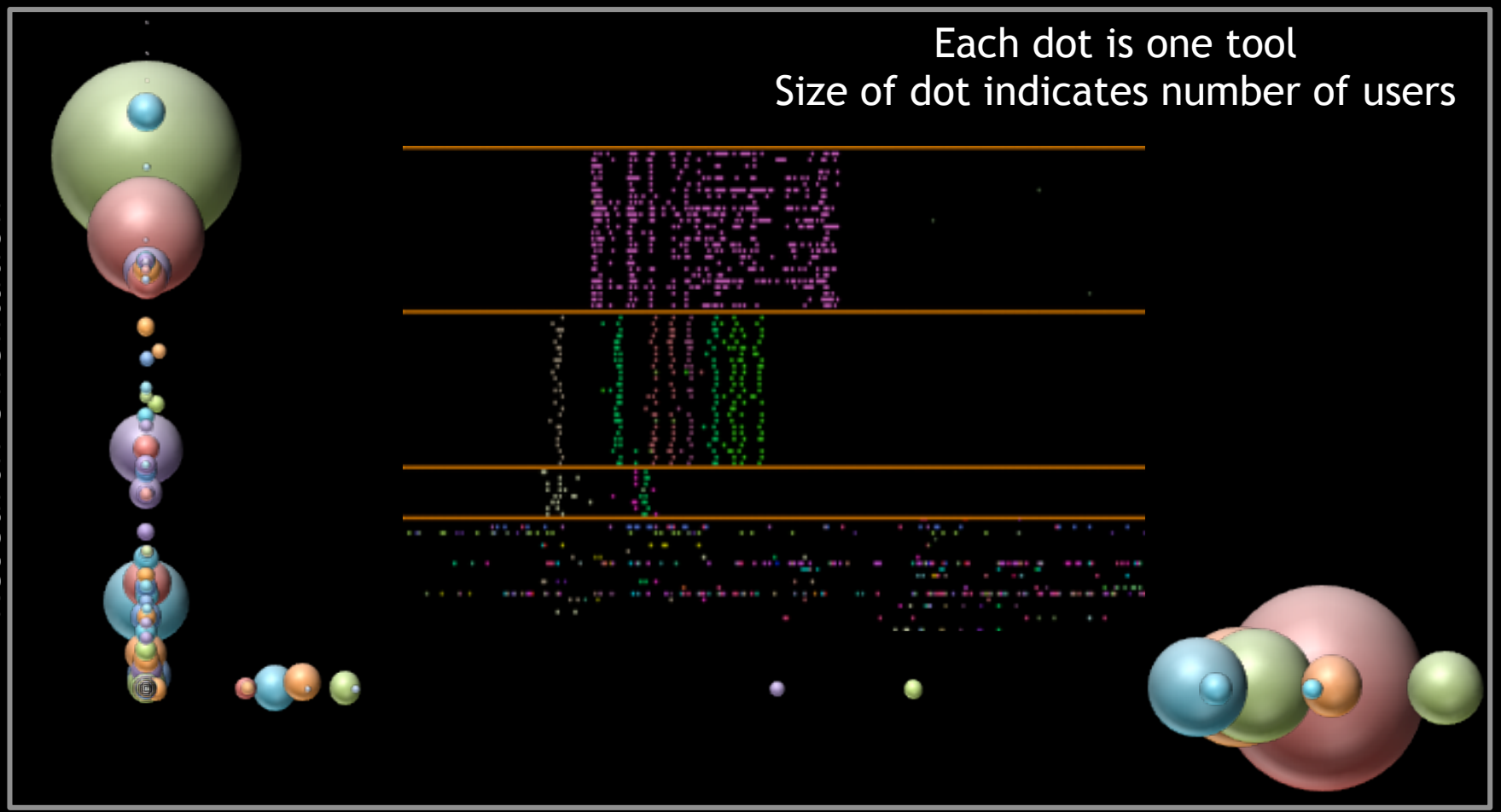
166,

Usage Patterns
=> Tool Qualification

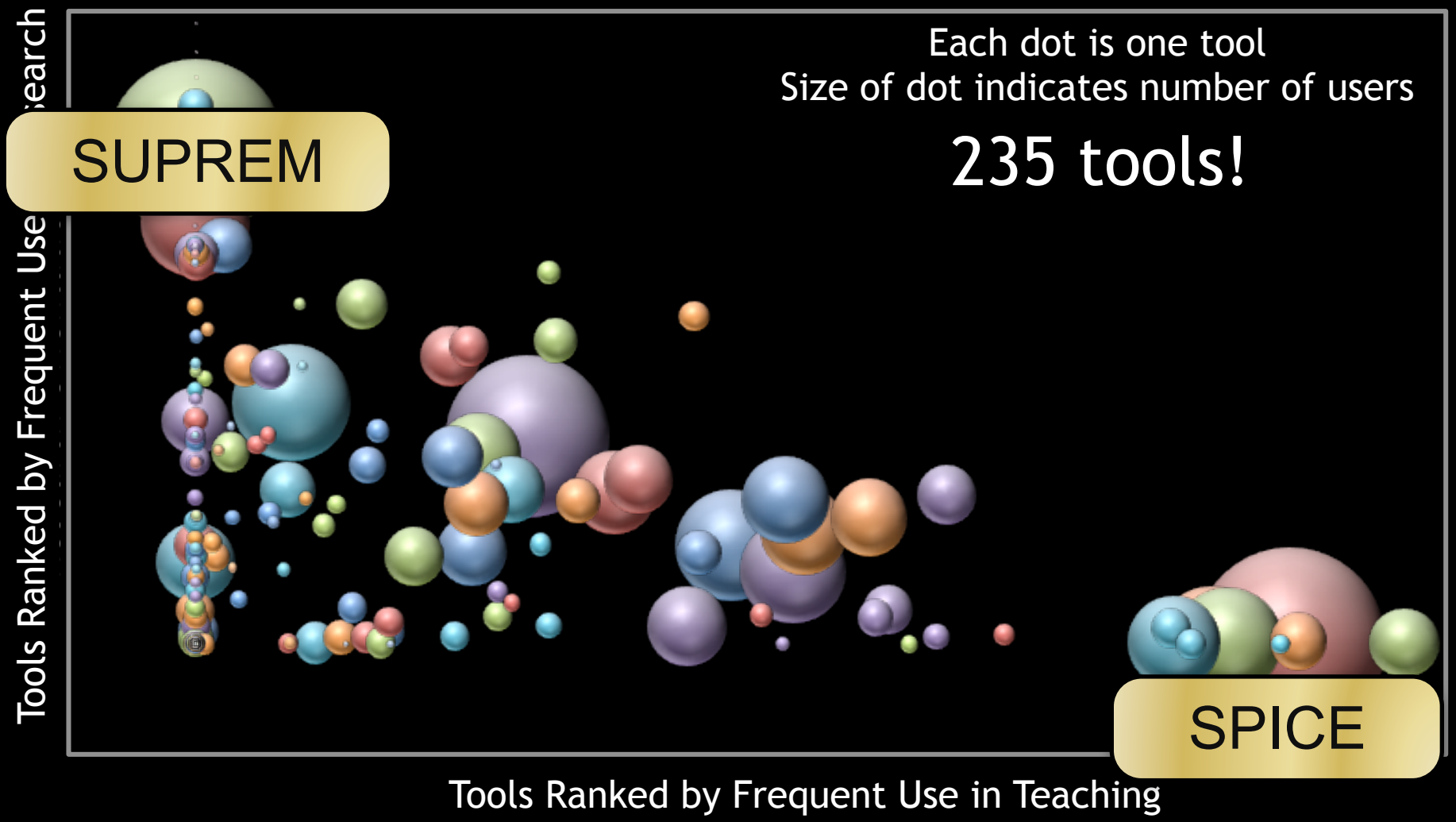


Tools Ranked by Frequent Use in Teaching

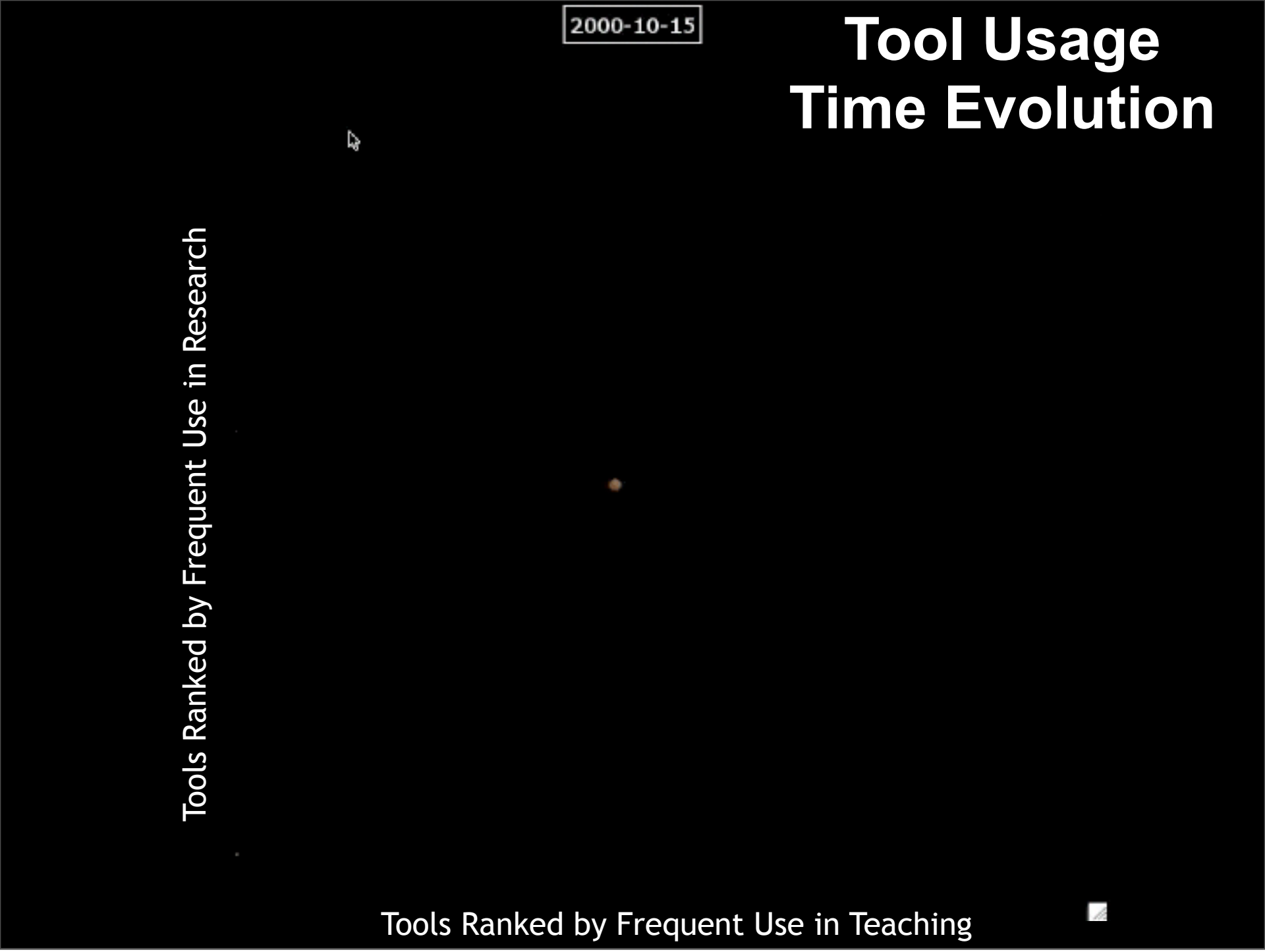
Usage Patterns
=> Tool Qualification



Dual Use
Education and Research are coupled!



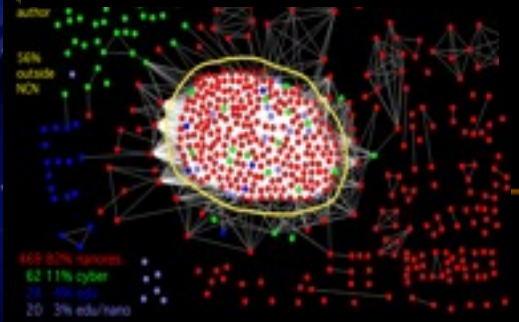
Tool Usage Time Evolution



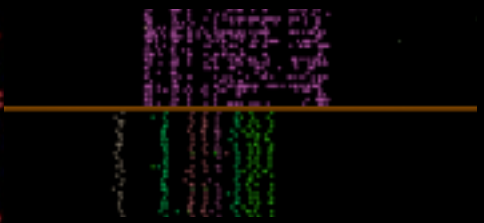
Scientific Knowledge Transfer on nanoHUB.org
Making Research Useful for Others

Over 230,000 Users Annually

857 papers



14,000 students



What's Next?

HUBzero & Rappture

Accessible (FREE, no installation)

In Research

In Education, Accelerate Innovation

Developer Friendly

260+ tools
>300 developers

User Friendly

12,000 Sim. Users Annually

Imagine

Simulation Tools

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

In a scientific cloud

Without any installation

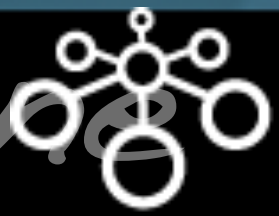
Fully operational 24/7

With assessed IMPACT

Many proposals read alike

The PowerPoints are identical

Imagine



nanoHUB.org

Simulation Tools

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- Used by experimentalists
- Used in education

In a scientific cloud

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Fully operational 24/7

With assessed IMPACT

We achieved that dream.

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nanoHUB.org

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nanoHUB.org

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Without any installation

Fully operational 24/7

Reproducible

Nano Engineering

In all areas of Nano Engineering and Science

With assessed IMPACT

Personalized Learning at all workforce levels

Become Part of the Day-to-Day Workflow

Many proposals look like

The PowerPoints are identical

Imagine

nanoHUB.org

Imagine

nanoHUB

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THE PROFESSIONAL nano SOCIETY

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

nanoHUB

THE PROFESSIONAL nano SOCIETY

Imagine!

Imagine

Simulation Tools **and Experimental Data**

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

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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