

nanoHUB
Network for Computational Nanotechnology

NSF Research Infrastructure since 2002

HUB usage 2016-01-01 00:00:00

~ERC

SI2-S2I2

However:
We gladly would accept an additional grant
Sustainability

nanoHUB

nanoHUB in a nutshell:
translating traditional research to **new paradigms** in publishing, computing, research, & education

What ?

- 494 nano-Apps in the cloud
- > 5,000 lectures and tutorials
- > 100 courses => MOOC

Cyberinfrastructure
24/7 operation with 99.4% uptime

Who?

- > 1.4 million users annually
- > 1,800 contributors
- 172 countries
- Faculty
- Students
- Industry practitioners

Research Impact:

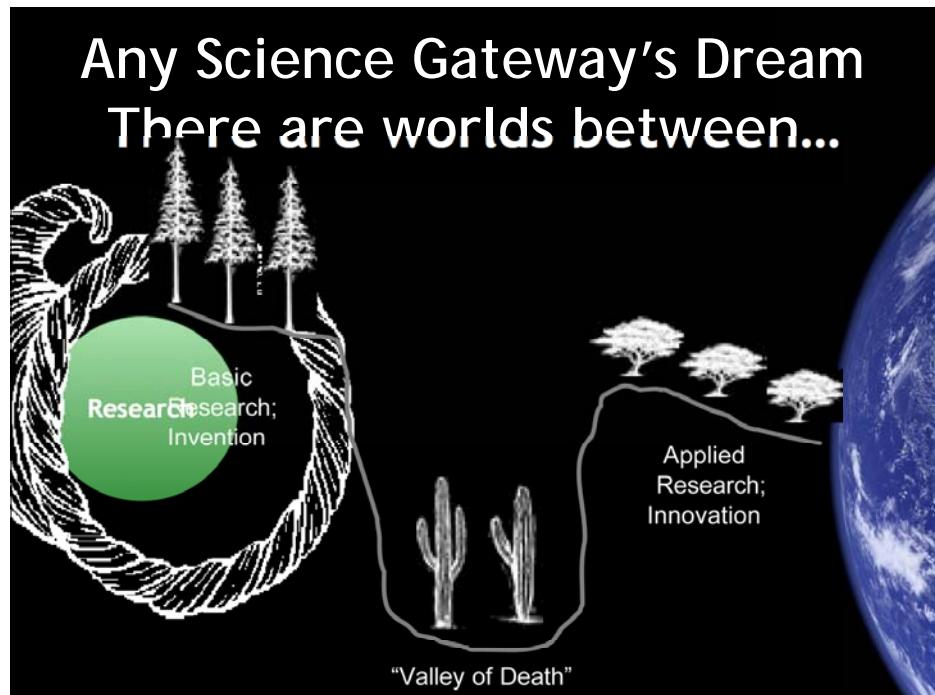
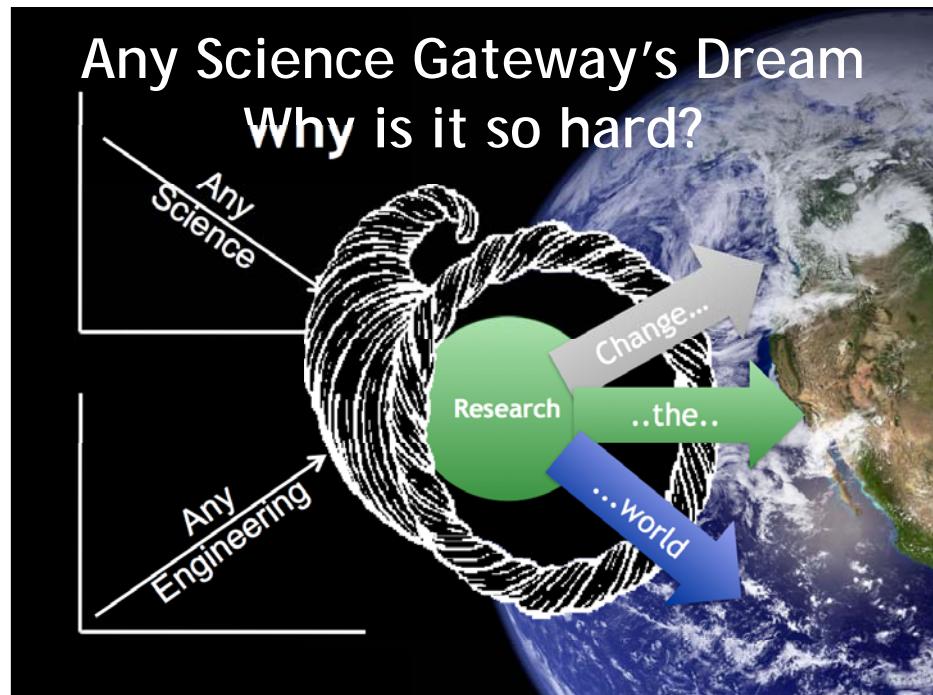
- nanoHUB tools now listed in **WEB OF SCIENCE**
- > 1,980 papers cite nanoHUB
- > 30,900 secondary citations
- h-index of 82

Educational Impact

- > 35,100 students use tools in classrooms, > 1780 classes, 185 institutions
- Rapid curriculum change <6 months adoption rate

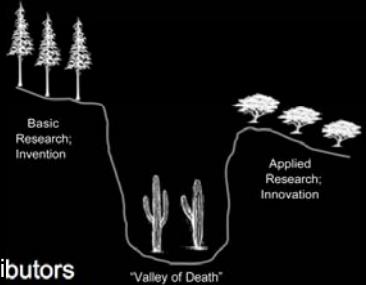
Fundamental changes in approach or underlying assumptions

=> Existence Proofs



nanoHUB is the world's first end-to-end Science & Engineering Cloud Computing Gateway

nanoHUB has bridged the “valley of death”
Research => applied users



Success Criteria

1. Understanding Stakeholders
2. Outstanding Science
3. Incentives for and commitment by contributors
4. Technology - HUB
5. Technology Transfer Processes
6. Open assessment / analytics
7. Business model

The next “valley of death”: Sustainability

3. Incentives for and commitment by contributors

nanoHUB recognized as Tool Publisher



- Web of Science and Google Scholar pull nanoHUB tool publications and list them as proper publications
- New incentives for academics
- New publication paradigm
- Culture change

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Usual Science Gateway Process

The diagram illustrates a communication gap between a researcher and a web developer. On the left, a researcher (represented by a pink person icon) and a web developer (represented by a yellow person icon) are connected by a blue double-headed arrow. Above them, several computer screens show various software interfaces, including a Java calculator and code snippets. To the right, a large red X is drawn over the following text:

- 175 tools / 4 years: => \$82M
- \$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

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Usual Science Gateway Process

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Customers / Users

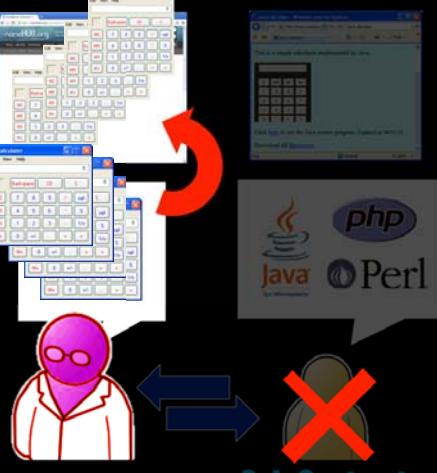
- Scale back expectations
- Not research codes
- Toy applications
- Not deep research
- Maybe for education?

Generating a Bad Reputation

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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



Supplier

Sub-Contractor Consultant

nanoHUB is different

Going Beyond Specialized Capabilities

Innovative Capability Examples



NEMO
Abinit
GAMESS
LAMMPS
Quantum Espresso
PWscf
Qwalk
SeqQuest

Innovative Usability & Accessibility => Impact




Going Beyond Specialized Capabilities

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Innovative Usability & Accessibility => Impact



nanoHUB

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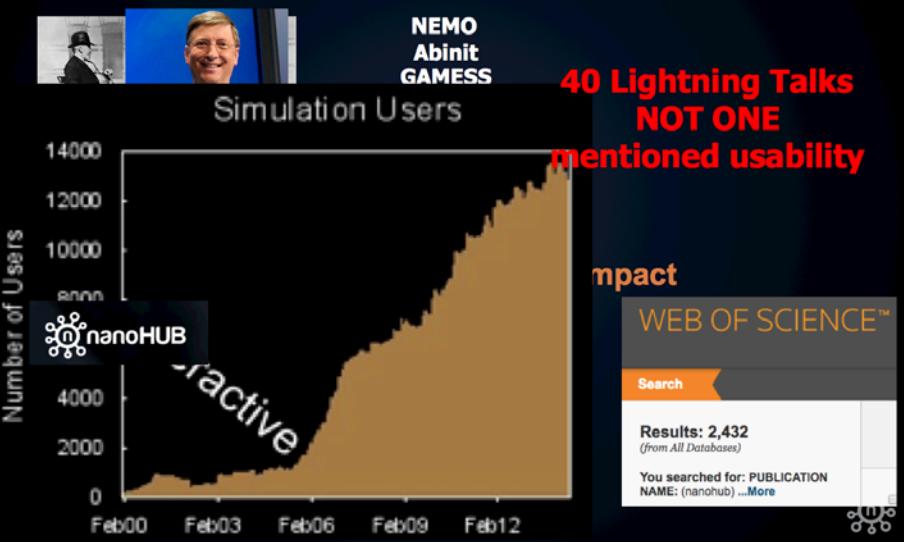
nanoHUB

Simulation Users

Interactive

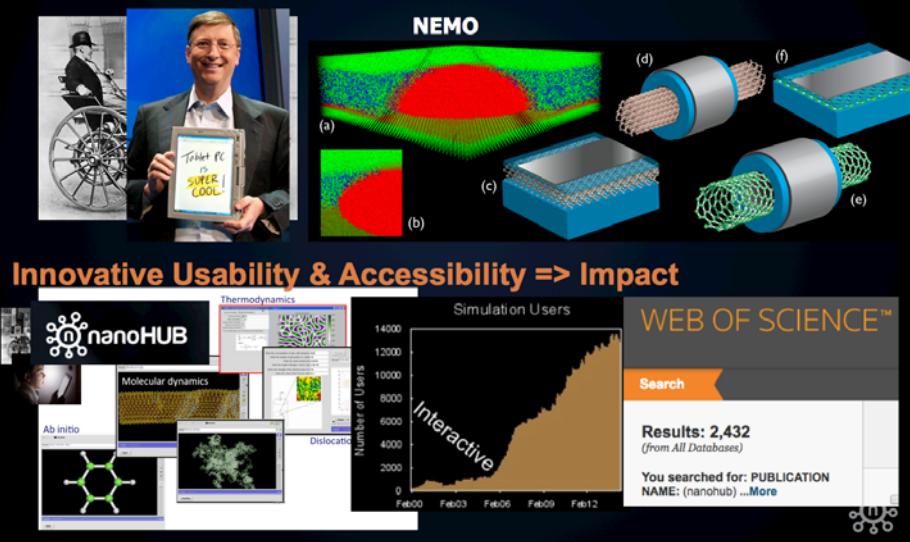
Going Beyond Specialized Capabilities

Innovative Capability Examples

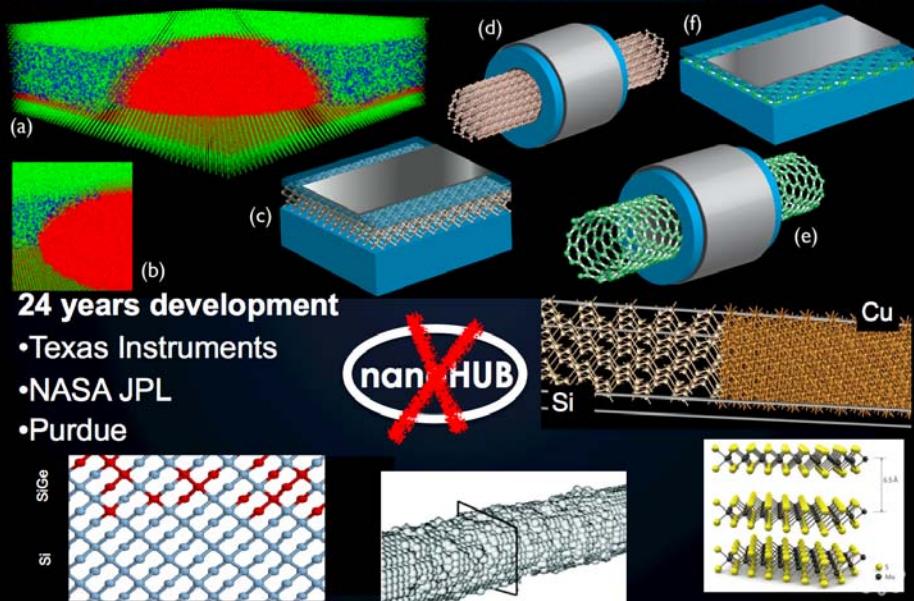


Going Beyond Specialized Capabilities

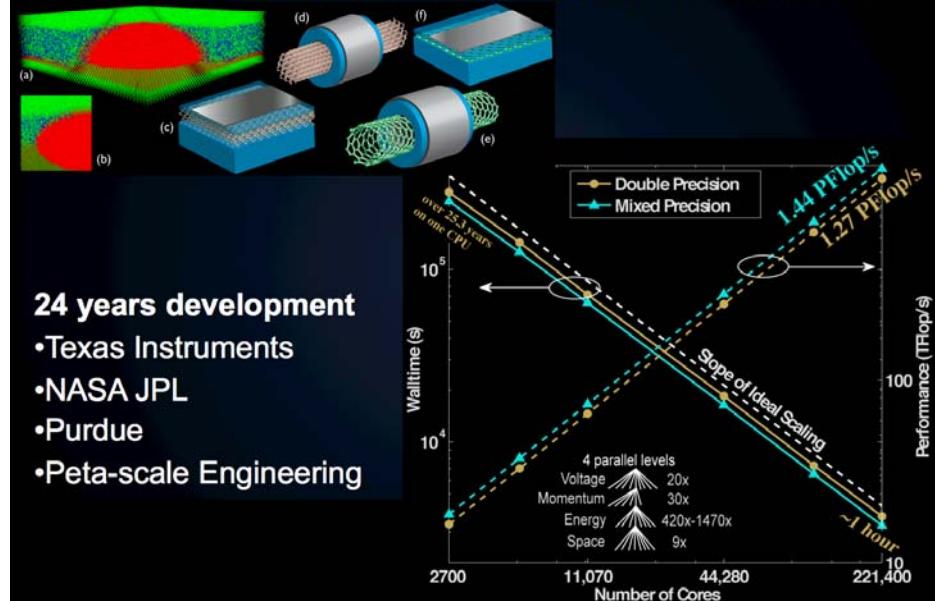
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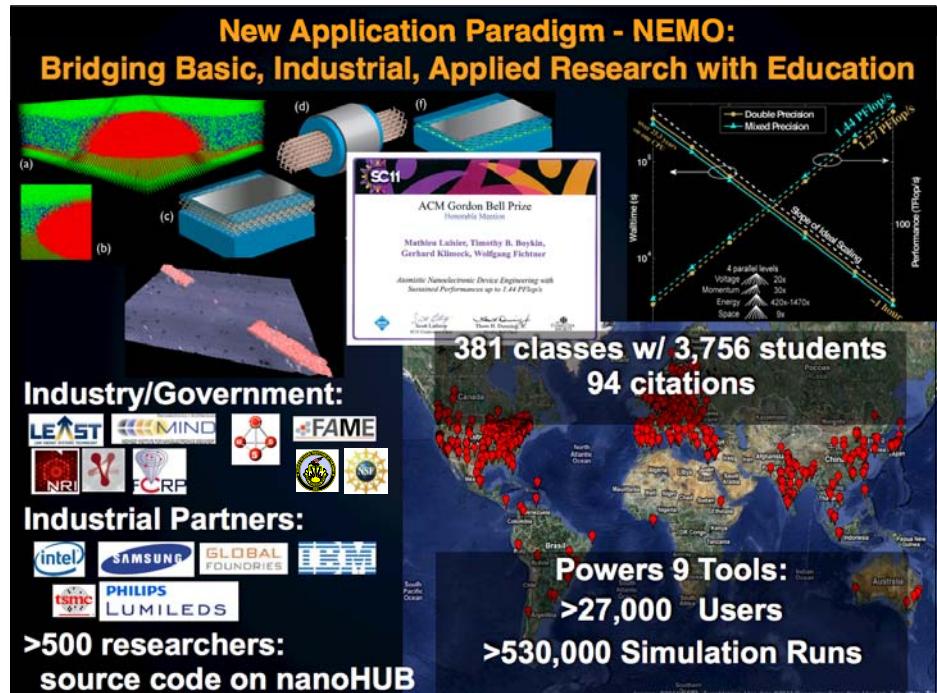
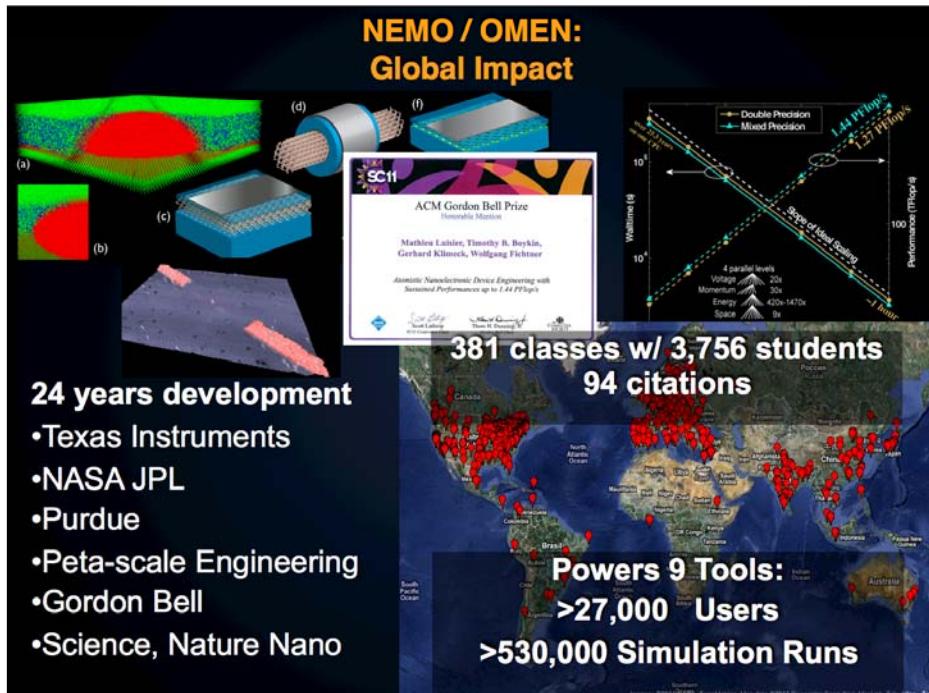
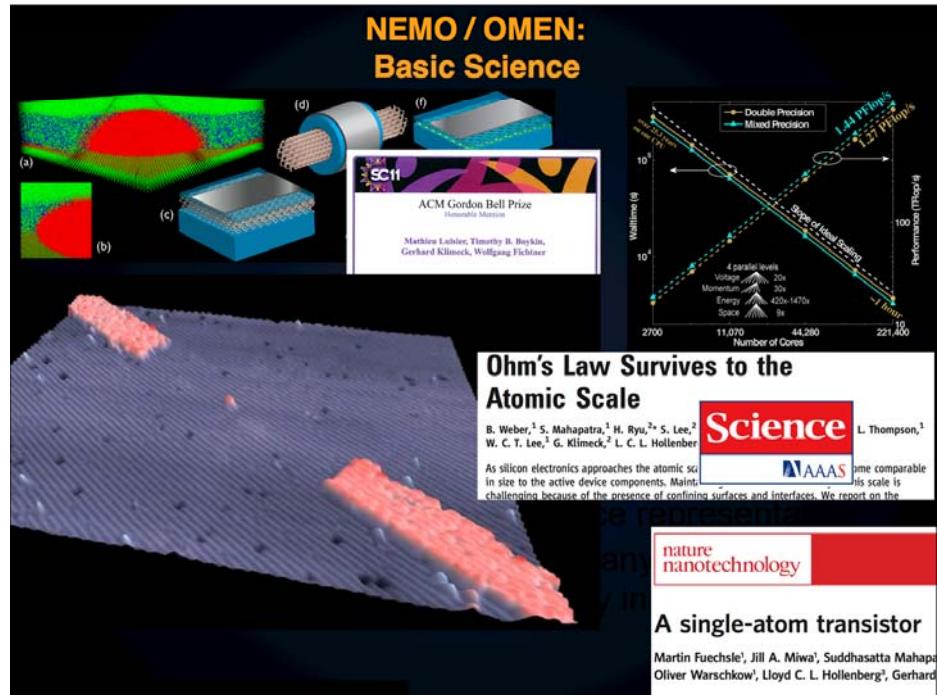
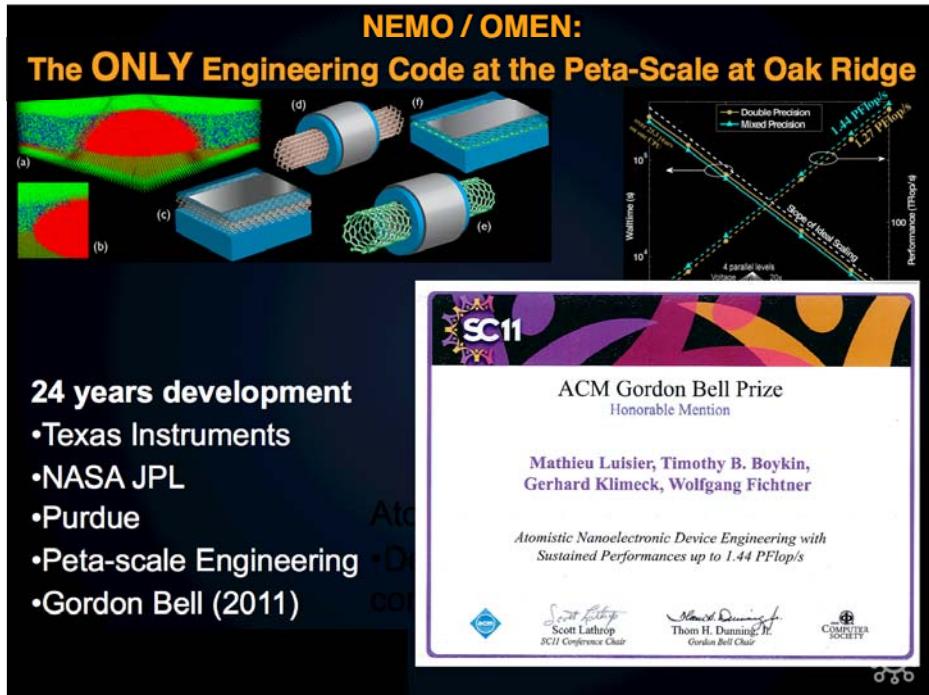


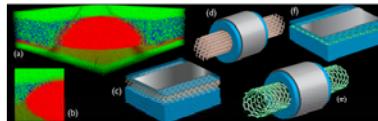
New Application Paradigm - NEMO: Bridging Basic, Industrial, Applied Research with Education



NEMO / OMEN: One of 8 Applications at the Peta-Scale at Oak Ridge







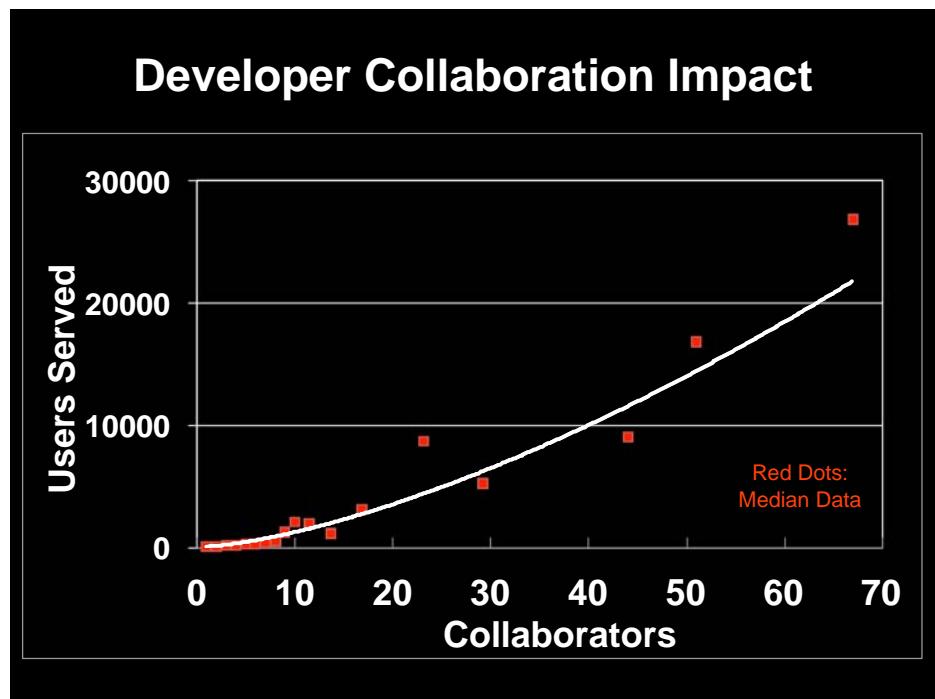
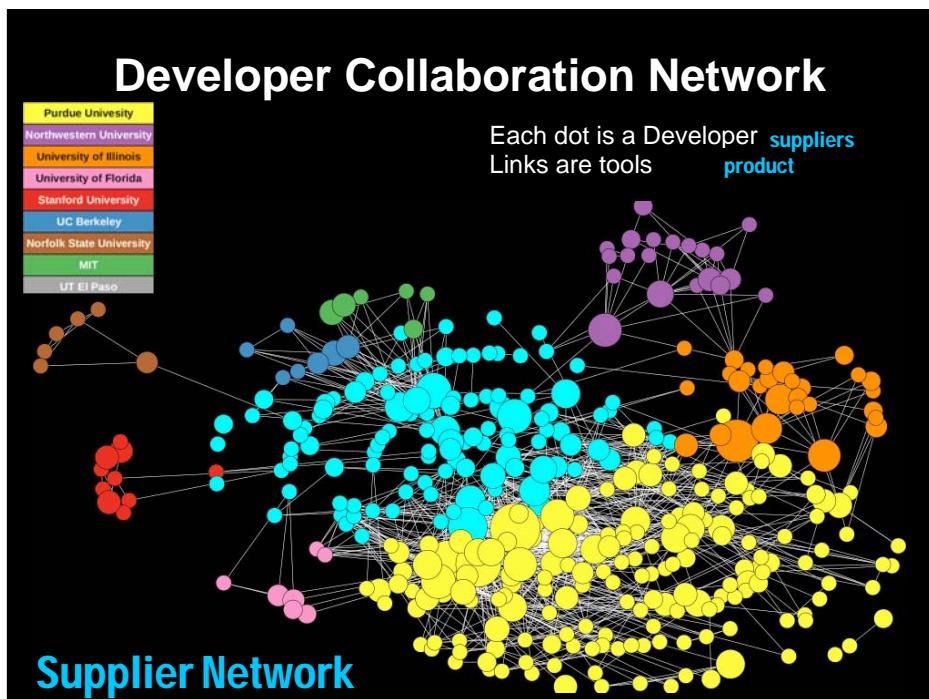
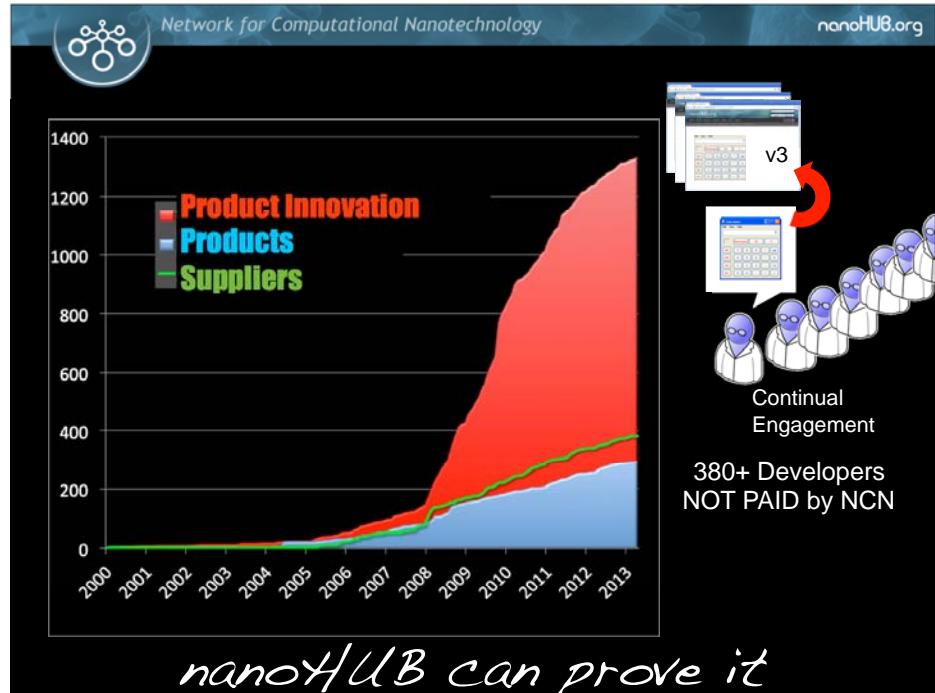
*Nano*HUB.org Network for Computational Nanotechnology

nanoHUB Process

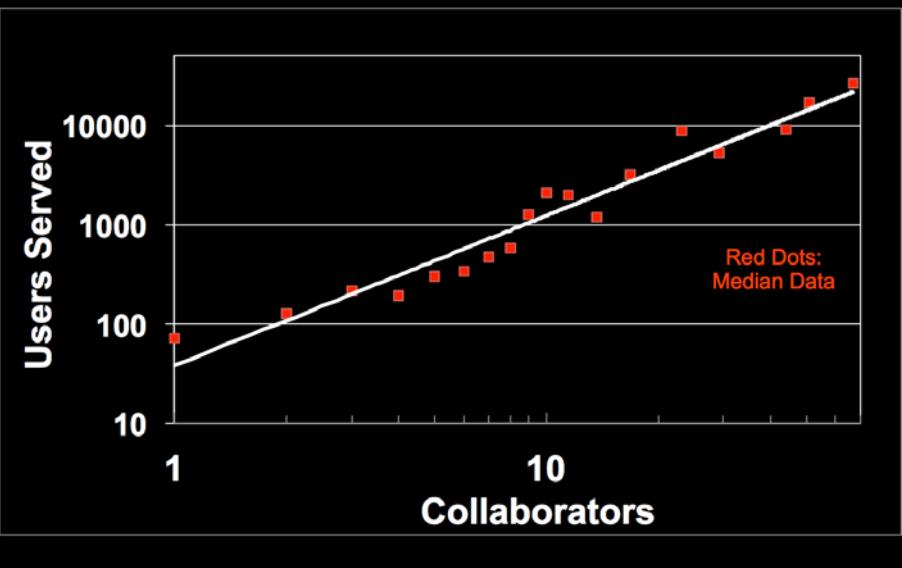
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Researcher ↔ **Sub-Contractor Consultant**

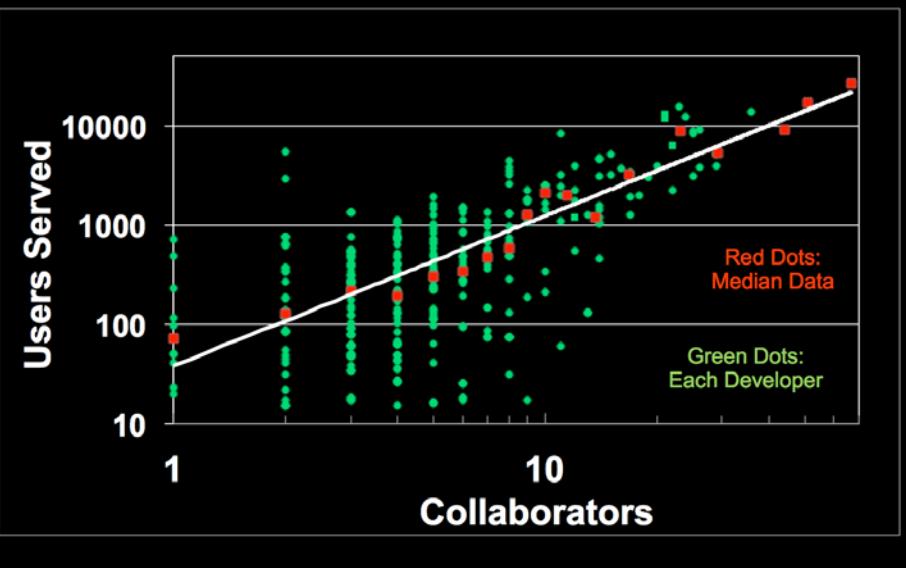
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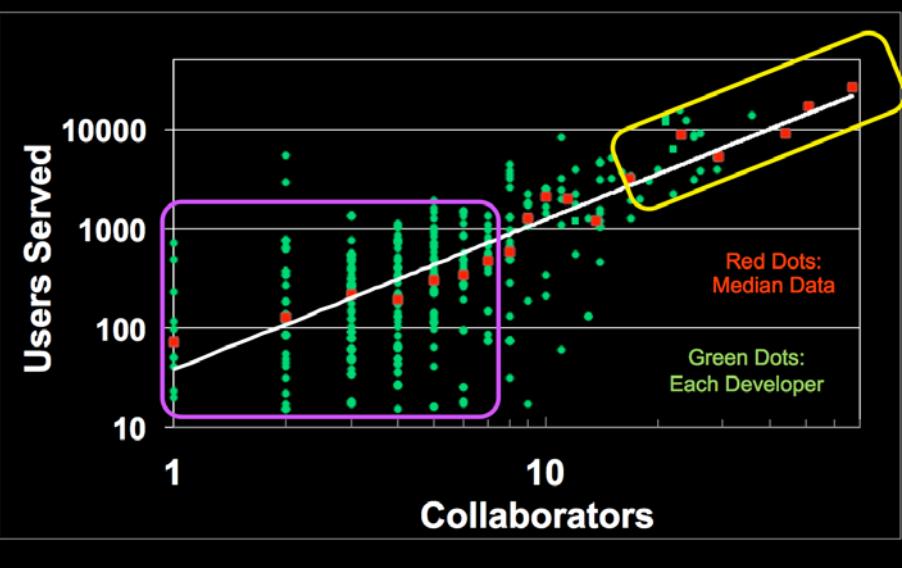
Developer Collaboration Impact



Developer Collaboration Impact

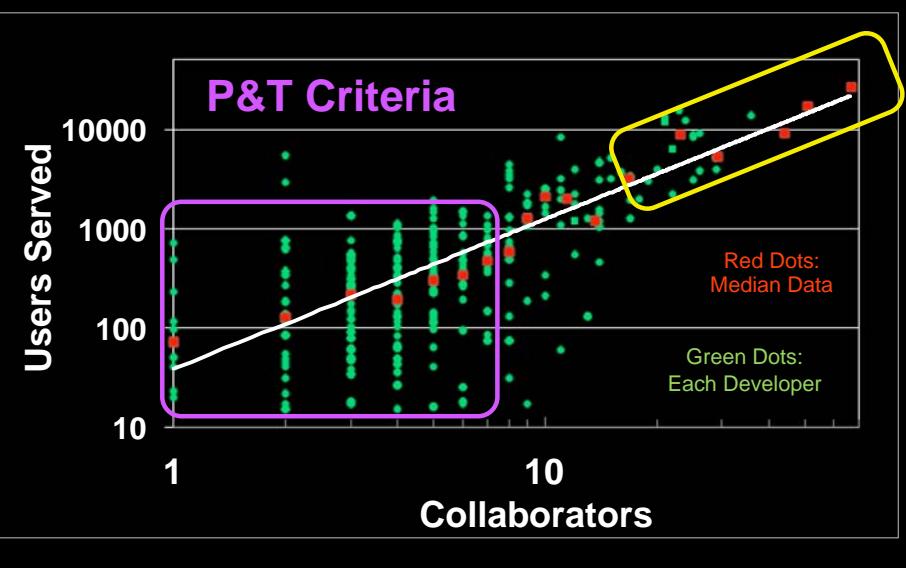


Small Collaborations: Scattered Success **Large Collaborations: Predictable Success**

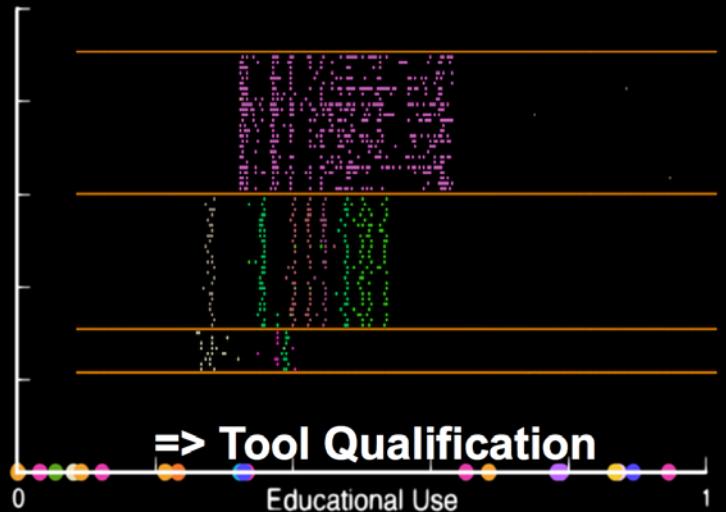


Old Approach

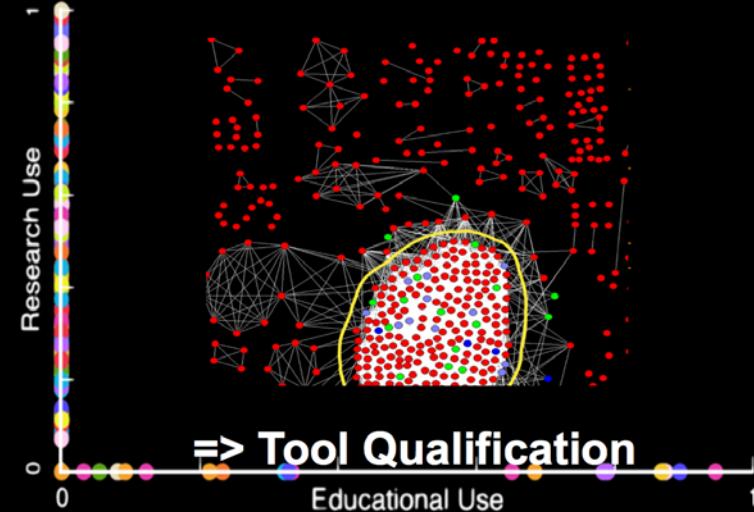
Surviving Universities



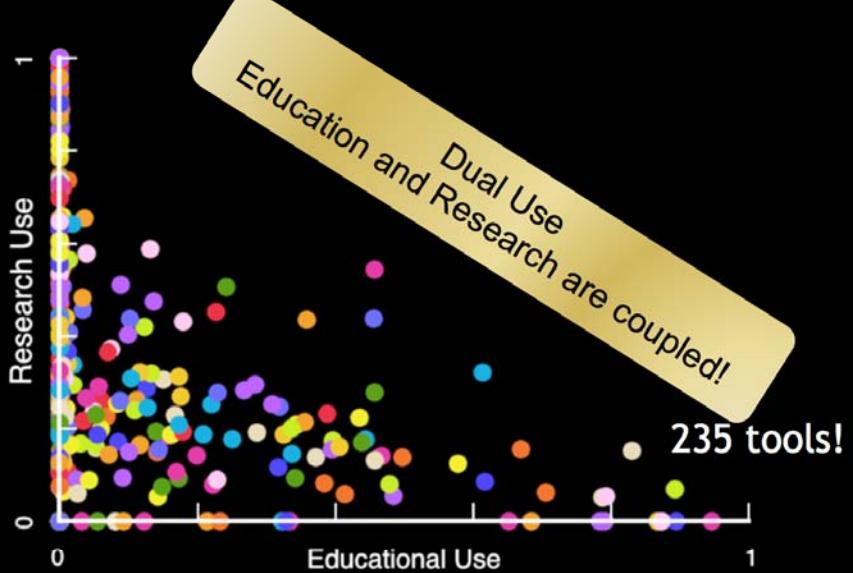
New nanoHUB Paradigm:
The fist science / engineering computing cloud
for research and education
Usage Patterns



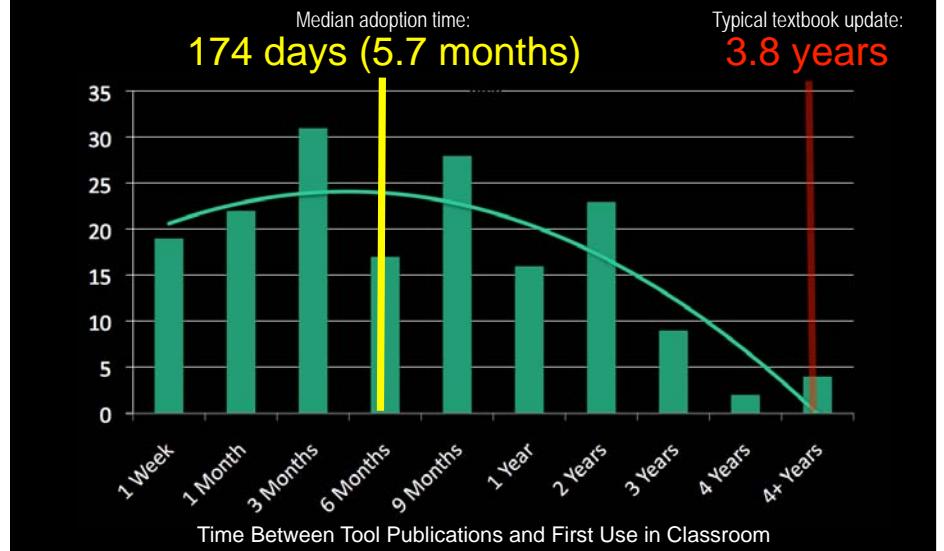
New nanoHUB Paradigm:
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Literature Citations



New nanoHUB Paradigm:
The fist science / engineering computing cloud
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Rapid Adoption of Research



nanoHUB 2018

Existence Proofs



nanoHUB 2023

Expand the Footprint Increase Impact Sustainable

Identified Gaps from Stakeholder Interactions

- End-Users:
 - Being in the day-to-day workflow
 - Personalized / customized
 - Developers / contributors
 - Being in the day-to-day workflow
 - Increase Incentives
 - Technology
 - Service based - SaaS, data access
 - Analytics driven, personalized de
 - NSF & Purdue:
 - Sustainability

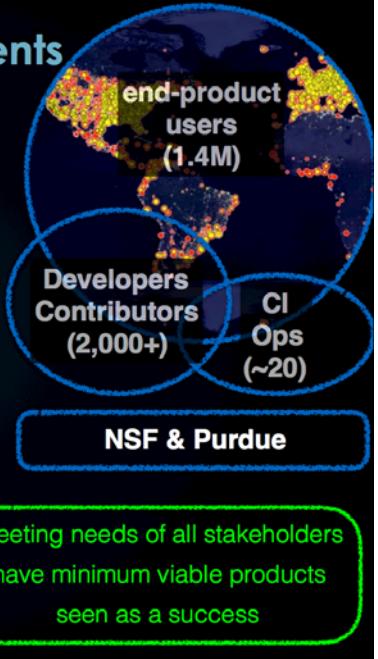
2017 user contacts:
25 workshops/tutorials, 2,300 attendees, EABs
Three Partner workshops w/ Industry, Govt. Lab

Customer Discovery => I-Corps

2018 Stakeholders & Critical Success Requirements

- End-product users
 - easy to use, no installation, compute
 - nanoHUB content developers / contributors
 - self-serve deployment
 - retain ownership and incentives (cites,use)
 - Partners (both user & developer)
 - SaaS and data
 - CI Operations
 - scalable, reliable, well managed
 - NSF & Purdue
 - Impact - Intellectual, Broad, Strategic

- meeting needs of all stakeholders
- have minimum viable products
- seen as a success



Identified Gaps from Stakeholder Interactions

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Customer Discovery => I-Corps

Partner / Center Requirements (Technical and Content)

- ATEs: content dissemination
- CEINT & Nanomaterials Registry (NR)
CEINT - have: experimental data
CEINT - need: broad exposure, integration with NR, tools
NR - have Curation process, experimental data
NR - need: broader community, visualization,
CEINT&NR: want to keep their own sites & data - link/use nanoHUB services
- OpenKIM - external database, interoperability, SaaS
- Web-of-Science: interoperable publication listing service
- GRANTA - SaaS - interoperability
- AFRL/NIST - SaaS - DaaS - interoperability



Partner workshops w/
Academia, Industry, Govt. Lab

Strategic Assessment & Alignment Funnel



nanoHUB 2023

VISION
Aspiration

Vision

Where we want to go

to accelerate innovation through
user-centric science and engineering

MISSION
Definition

Why we exist
& how we behave

Mission

to make science and engineering products
usable, discoverable, reproducible, and
easy to create
for learners, educators, researchers,
and business professionals