However:

We gladly would accept an additional grant since 2002.

**nanoHUB**
Network for Computational Nanotechnology

~ERC

SI2-S2I2

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

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

Cyberinfrastructure:
24/7 operation with 99.4% uptime

Fundamental changes in approach or underlying assumptions

=> Existence Proofs

**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

**Why is it so hard?**

Any Science Gateway’s Dream

There are worlds between...

Change...

..the...

...world
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™
Google Scholar

- 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

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

Customers / Users
• Scale back expectations
• Not research codes
• Toy applications
• Not deep research
• Maybe for education?
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

Going Beyond Specialized Capabilities

Innovative Capability Examples

- NEMO
- Abinit
- GAMESS
- LAMMPS
- Quantum Espresso
- PWsf
- Qwalk
- SeqQuest

Innovative Usability & Accessibility => Impact

nanoHUB
Innovative Capability Examples

Innovative Usability & Accessibility => Impact

NEMO
Abinit
GAMESS
LAMMPS
Quantum Espresso
PWsf
Qwalk
SeqQuest

24 years development
• Texas Instruments
• NASA JPL
• Purdue

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

24 years development
• Texas Instruments
• NASA JPL
• Purdue

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

24 years development
• Texas Instruments
• NASA JPL
• Purdue
• Peta-scale Engineering
Atomistic Device representation
• Deemed by many too computationally intensive

24 years development
• Texas Instruments
• NASA JPL
• Purdue
• Peta-scale Engineering
• Gordon Bell (2011)

NEMO / OMEN:
The ONLY Engineering Code at the Peta-Scale at Oak Ridge

NEMO / OMEN:
Basic Science

NEMO / OMEN:
Global Impact

NEMO / OMEN:
Bridging Basic, Industrial, Applied Research with Education

Industry/Government:

Industrial Partners:

Powers 9 Tools:
>27,000 Users
>530,000 Simulation Runs

>500 researchers:
source code on nanoHUB

381 classes w/ 3,756 students
94 citations

Power

New Application Paradigm - NEMO:

Ohm's Law Survives to the Atomic Scale

A single-atom transistor

Martin Fuhrer, Jill A. Mize, Sudhakar Mahapatra, Victor Worschier, Lloyd C. L. Hillebrand, Gerhard Klimeck

24 years development

Science, Nature Nano

ACM Gordon Bell Prize
Honorable Mention

Mathieu Luisset, Timothy B. Brey, Gerhard Klimeck, Wolfgang Flachert

Atomistic Nanoelectronic Device Engineering with Sustained Performance up to 1,44 PFlop/s

Industry Partners:
>500 researchers:
source code on nanoHUB

381 classes w/ 3,756 students
94 citations

Powers 9 Tools:
>27,000 Users
>530,000 Simulation Runs
**nanoHUB Process**

- 175 tools / 4 years without $88M
- Eliminate bottlenecks
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- HUBzero Ecosystem

**nanoHUB can prove it**

**Developer Collaboration Network**

Each dot is a Developer

Links are tools **suppliers**

**Supplier Network**

**Developer Collaboration Impact**

- Product Innovation
- Products
- Suppliers

<table>
<thead>
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<th>Users Served</th>
<th>Collaborators</th>
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<tr>
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<td>20</td>
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</tbody>
</table>

Red Dots: Median Data
Developer Collaboration Impact

Users Served

Collaborators

Red Dots: Median Data

Green Dots: Each Developer

Small Collaborations: Scattered Success
Large Collaborations: Predictable Success

Old Approach
Surviving Universities

P&T Criteria
New nanoHUB Paradigm:
The first science/engineering computing cloud for research and education

Usage Patterns

Education and Research are coupled!

Rapid Adoption of Research

Median adoption time:
174 days (5.7 months)

Typical textbook update:
3.8 years

Time Between Tool Publications and First Use in Classroom
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 (DaaS)
  - Analytics driven, personalized delivery
- NSF & Purdue:
  - Increase Incentives

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

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

NSF & Purdue
meeting needs of all stakeholders
have minimum viable products
seen as a success

NSF & Purdue
Sustainability

End-product users (1.4M)
Developers
Contributors (2,000+)
CI Ops (~20)

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

**Recent Prototypes / initiatives**

Partner workshops w/ Academia, Industry, Govt. Lab

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**nanoHUB 2023**

**Vision**

*to accelerate innovation through user-centric science and engineering*

**Mission**

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