Virtual Organizations

November 9, 2006

National Science Foundation
Directorate for Engineering

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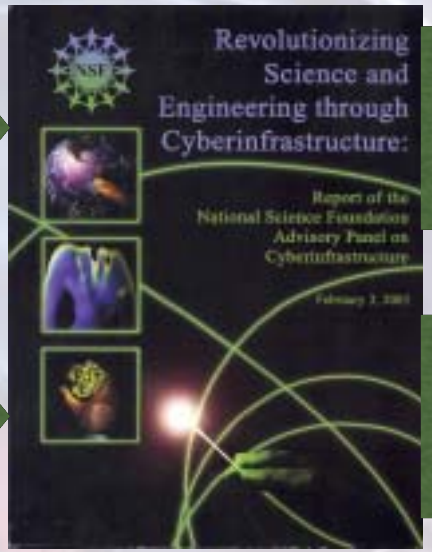
ENG Cyberinfrastructure Working Group

NSF Cyberinfrastructure Vision

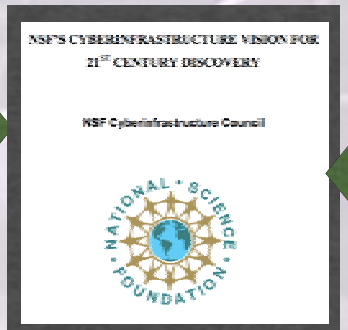
Advances in components of CI-systems for S&E R&E

Complex, multi-scale, multidisciplinary S&E research challenges



30+ disciplinary workshops on CI vision & impact

NSF internal working groups



NSB & Community Input

CI Council, Directorate/Office CI Activities, OCI, ACCI

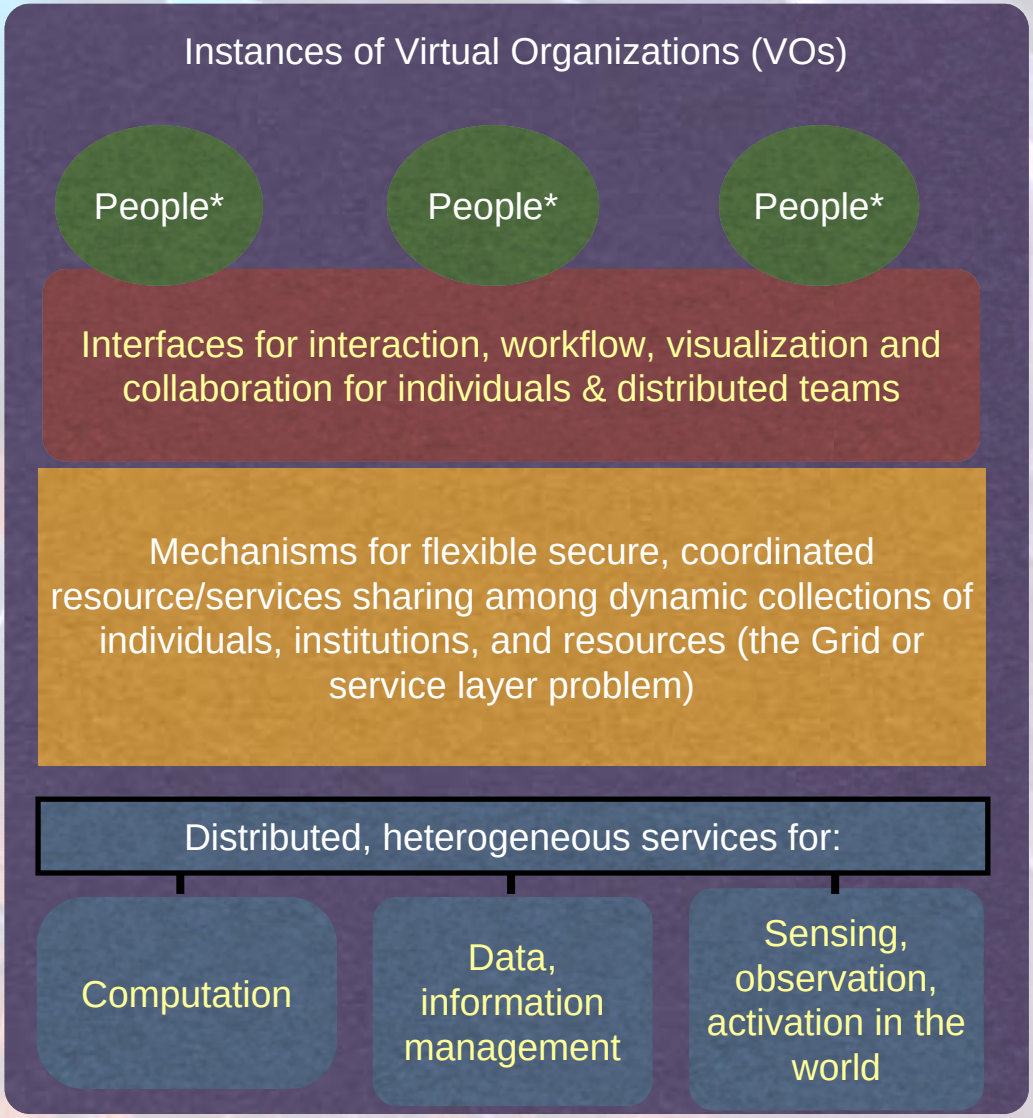
Vision Framework

- High Performance Computing
- Data, Data Analysis & Visualization
- Virtual Organizations
- Learning & Workforce Development

- *All directorates and offices support cyberinfrastructure.*
- *Science-driven partnerships between creation, provisioning and use of CI*
- *Supports integrated research and education and broadened access and participation.*

Draft available at www.nsf.gov/oci/

Virtual Organizations (VO)



- Virtual organizations offer a community of practice the opportunity to work together - sharing expertise, tools, information and facilities.

Alternate Names for VOs:

- Co-laboratory
- Collaboratory
- Grid (community)
- Network
- Portal
- Gateway
- Hub
- Virtual Research Environment
- Other?

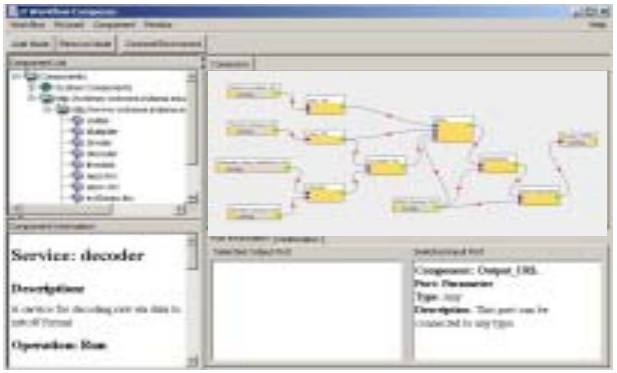
Virtual Organizations: NSF Goals

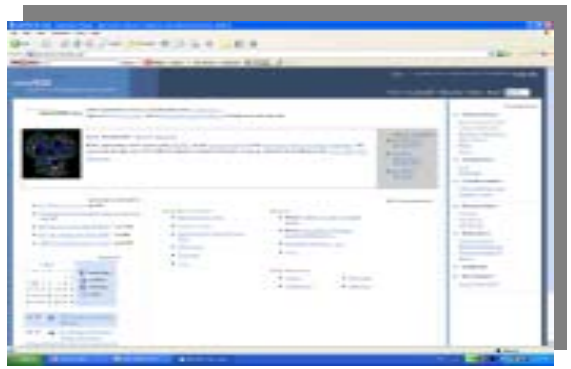
- To catalyze the development, implementation and evolution of *functionally-complete* national cyberinfrastructure …
- To promote and support the establishment of world-class VOs that are secure, efficient, reliable, accessible, usable, pervasive, persistent and interoperable …
- To support the development of common cyberinfrastructure resources, services, and tools …

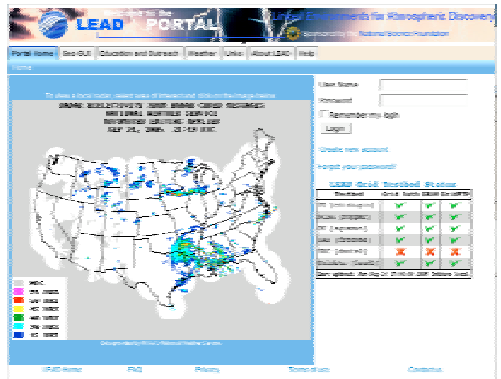
NSF'S CYBERINFRASTRUCTURE VISION FOR 21ST CENTURY DISCOVERY, www.nsf.gov/od/oci/ci-v7.pdf

TeraGrid Science Gateways

Community Interface to Grids





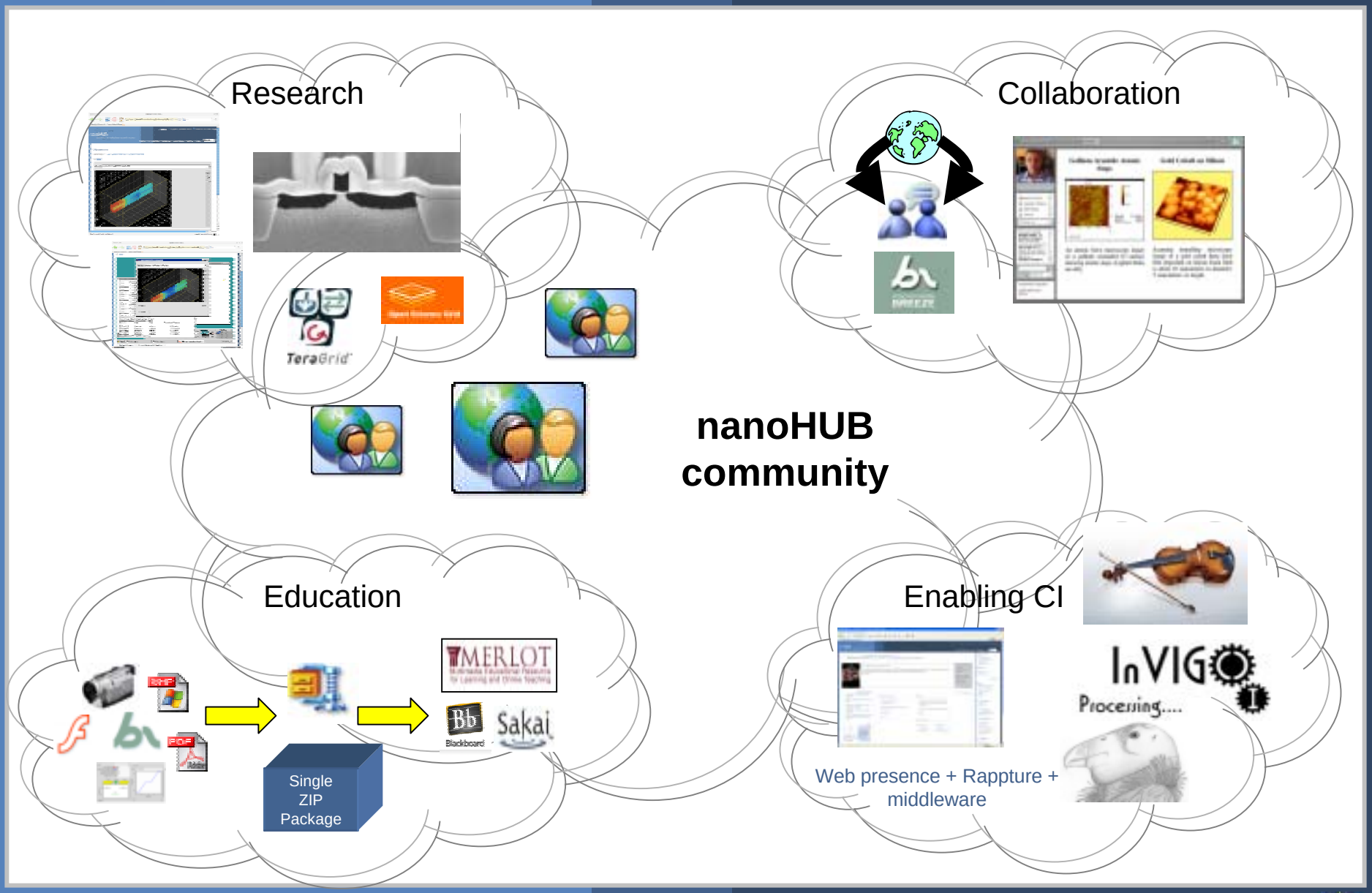


- **Type 1** — A gateway that is packaged as a web portal with users in front and TeraGrid services in back.
- **Type 2** — Grid-bridging Gateways: often communities run their own Grids devoted to their areas of science. In these cases the Science gateway is a mechanism to extend the reach of the community Grid so it may use the resources of the TeraGrid.
- **Type 3** — A gateway that involves application programs running on users' machines (i.e. workstations and desktops) and accesses services in TeraGrid (and elsewhere).

TeraGrid Science Gateway Partners

- Open Science Grid (OSG)
- Special PRiority and Urgent Computing Environment (SPRUCE, UChicago)
- National Virtual Observatory (NVO, Caltech)
- Linked Environments for Atmospheric Discovery (LEAD, Indiana)
- Computational Chemistry Grid (GridChem, NCSA)
- Computational Science and Engineering Online (CSE-Online, Utah)
- GEON(GEOsciences Network) (GEON, SDSC)
- Network for Earthquake Engineering Simulation (NEES, SDSC)
- SCEC Earthworks Project (USC)
- Astrophysical Data Repository (Cornell)
- CCR ACDC Portal (Buffalo)
- Network for Computational Nanotechnology and nanoHUB (Purdue)
- GIScience Gateway (GISolve, Iowa)
- Biology and Biomedicine Science Gateway (UNC RENCI)
- Open Life Sciences Gateway (OLSG, UChicago)
- The Telescience Project (UCSD)
- Grid Analysis Environment (GAE, Caltech)
- Neutron Science Instrument Gateway (ORNL)
- TeraGrid Visualization Gateway (ANL)
- BIRN (UCSD)
- Gridblast Bioinformatics Gateway (NCSA)
- Earth Systems Grid (NCAR)
- SID Grid (UChicago)

http://www.teragrid.org/programs/sci_gateways/

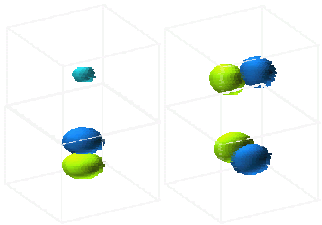

Research
TeraGrid
Collaboration
nanoHUB
community
Education
MERLOT
Bb
Sakai
Single
ZIP
Package
Enabling CI
InVIGO
Processing....
Web presence + Rappture +
middleware

Content Generation

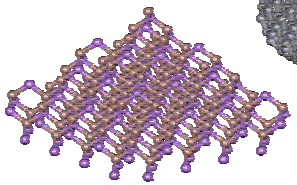
- Simulations
  - Nanoelectronics
  - Semiconductors
  - Nano-Electro-Mech Systems
  - Materials
  - Chemistry
- Educational Tools
  - Podcasts
  - Learning Modules
  - Nanotechnology 101
  - Nanotechnology 501
  - Nanocurriculum
- Collaboration
  - Research Seminars
  - Workshops
  - Publications
  - Software Projects

- CNTbands
  - Electronic band structure for carbon nanotubes
- FETToy
  - Simulate nanoscale double gate MOSFETs
- Huckel-IV
  - Conductance for a molecule between metallic contacts
- MolCToy
  - Conduction between individual molecules and two contacts
- MSL Simulator
  - Compares material properties of carbon nanotubes, nanowires, etc
- Quantum Dot Lab
  - 3-D confined states in simple quantum dot geometries
- NanoWire
  - Electronic properties of silicon nanowire transistors

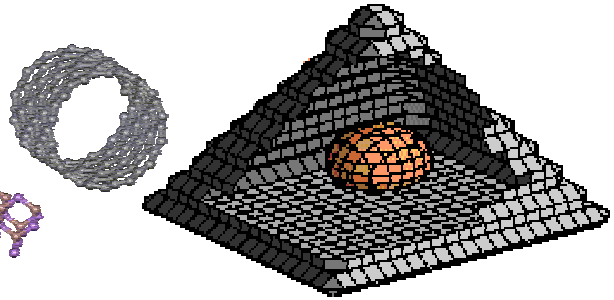
NCN Science Impact through HPC
NEMO 3-D



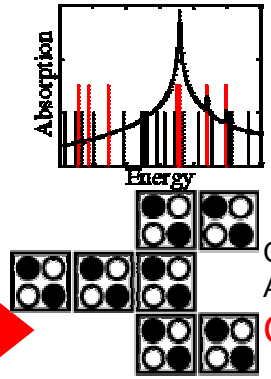
Atomic Orbitals
size: 0.2nm



Structure
Millions of atoms



Nanoscale Quantum States
(Artificial Atoms, size 20nm)

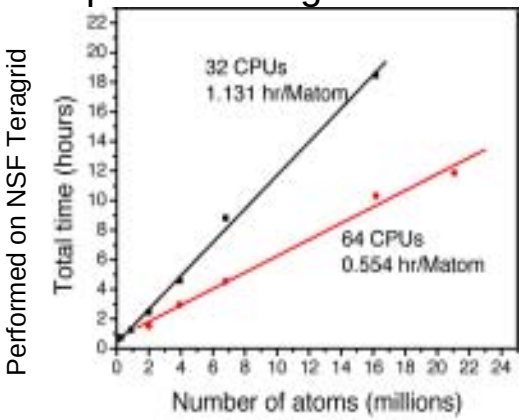


Designed
Optical
Transitions
Sensors

Quantum Dot
Arrays
Computing

Problem:

- The design space and computation is huge.
  => need a parallel design tool => NEMO 3-D

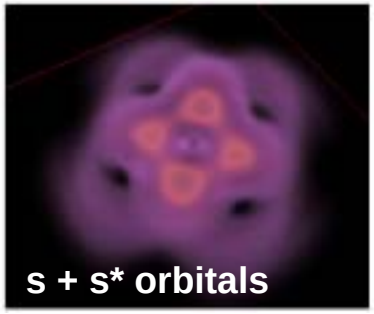


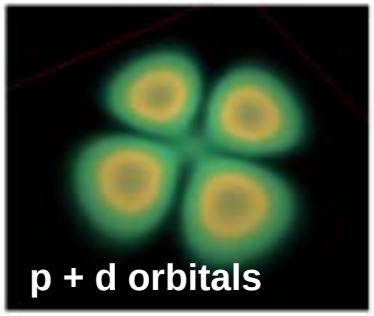
Demonstration / Capability / Impact:

- 64 million atom strain $(110nm)^3$.
- 21 million atom electronic structure $(78nm)^3$.
- Quantum dots, nanowires, quantum computing…

Visualization:

- How to visualize 21 million atoms on a zincblende lattice?
- Zincblende is not a space-filling mesh!!!
- => VolQD
- Baseline for our viz-server!





Self-Paced Interactive Learning
nanoHUB Learning Modules

Ballistic Nanotransistors

- Instructions
- Introduction
- Theory of the Ballistic MOSFET
- MOSFET IV Terminology
- FETToy
- FETToy against Experiments
- FETToy Simulation Tool
- Physics of Nanoscale MOSFETs
- Quiz
- Simple Theory of the Ballistic MOSFET

Abstract

This learning module is ... otransistors. No transistor is fully ballistic, but analy ... ing processes provides new insights into the perfor ... is learning module introduces the basic th ... urrent problems in device research. The concepts are illustrated by exercise ... of live simulations with the program, FETToy.

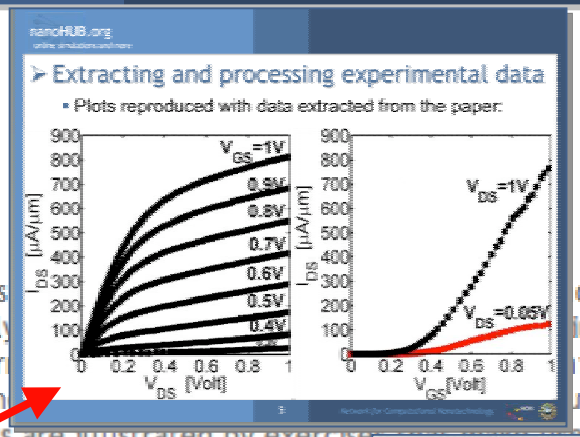
Available Downloads:

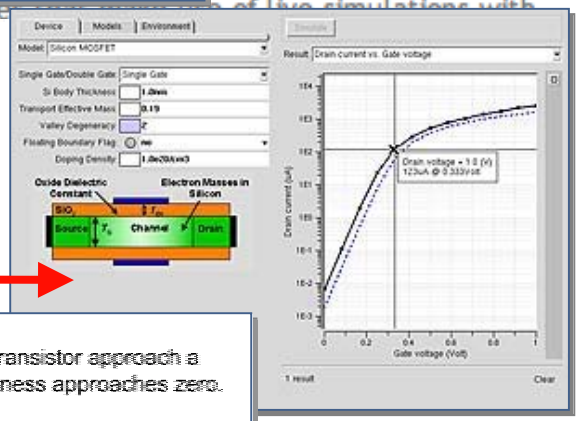
- FETToy Exercises (PDF, 205.03 Kb)
- Notes on Ballistic MOSFETs (PDF, 2.25 Mb)

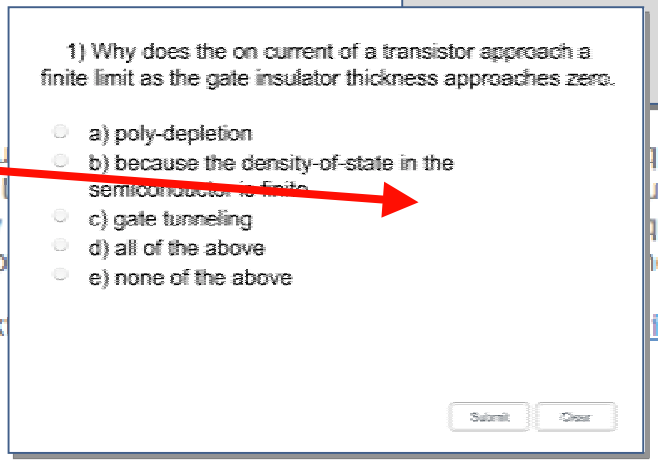
Instructions

Please use the menu ... quickly to a specific element within this l ... using this learning module, we strongly ... quentially. On subsequent visits, yo ... ost interest to you.

To view a quick walk ... ick here.







9 Learning Modules
1315 users

Content Generation

Simulations
- Nanoelectronics
- Semiconductors
- Nano-Electro-Mech Systems
- Materials
- Chemistry

Educational Tools
- Podcasts
- Learning Modules
- Nanotechnology 101
- Nanotechnology 501
- Nanocurriculum

Collaboration
- Research Seminars
- Workshops
- Publications
- Software Projects

What's new in the past 12 months?
- 247 resources
- 21 new simulators

A bottom-up community effort
- >250 contributors
- >40% outside the NCN

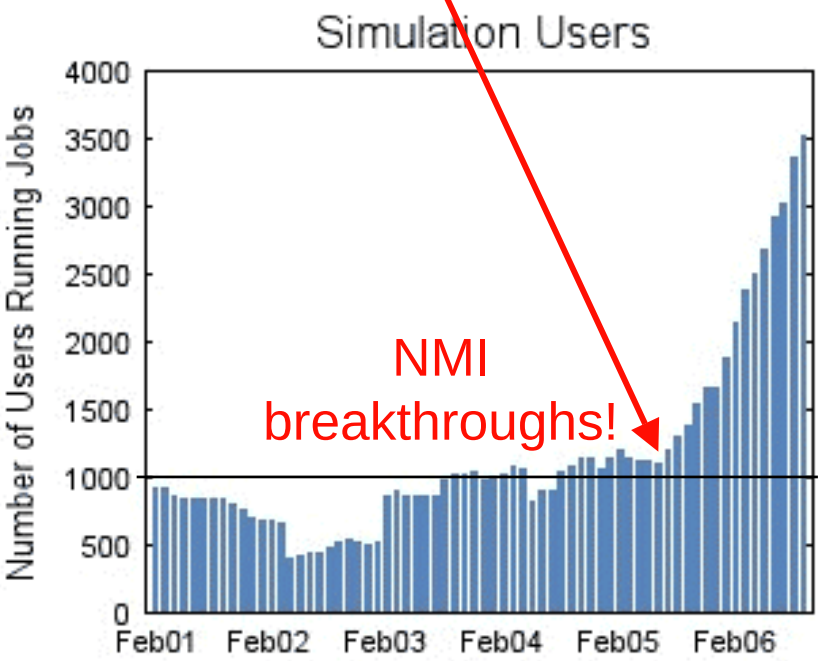
Annual nanoHUB Usage is Exploding

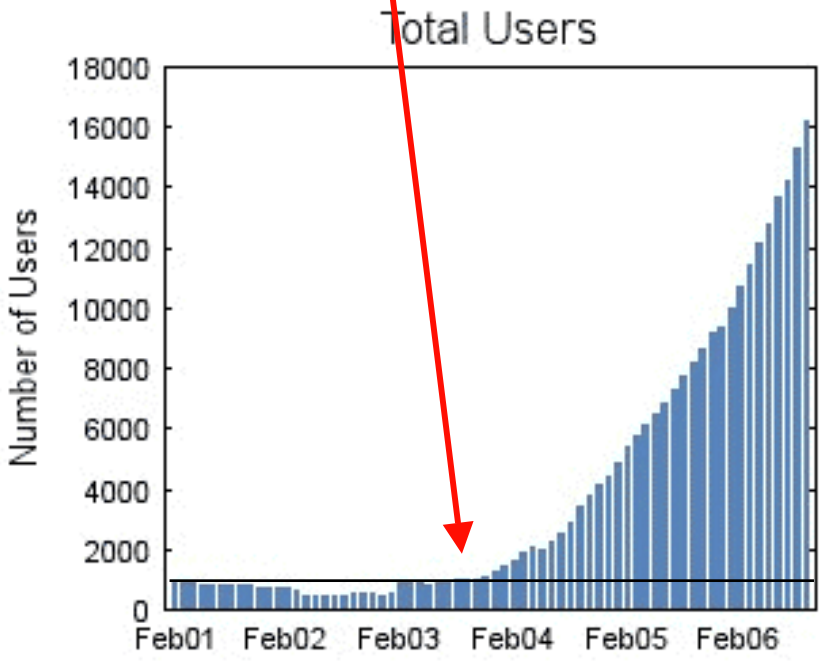
Simulation users
with at least one simulation
> 3,500 users
> 94,000 simulations (Sept. 2006)

Total users = Simulation users +
an IP with >15 minute session time
> 16,200 users
> 3.6 hrs avg session time / user

Interactive simulations introduced
in April 2005 => 3x increase

Interactive presentations introduced
in August 2003 => 16x increase





Some Open Questions

- Identifying communities ready for VO
  - Scoping a *community*
  - Attributes that measure readiness and impact
  - Seeding communities
- Approach to building VOs
  - Specific needs of each community
  - Investment level and duration required
  - Incentives for participation
  - Social and cognitive dimensions
- Sustainability of VOs
  - Evolution, enhancement and continuous improvement
  - Reuse, extensibility and transfer to other VOs
  - Long term sustainability – beyond project funding horizon

Engineering Gateway Seed Grants

Anticipated Solicitation

- Virtual organizations (VOs): Communities of researchers and educators linked by CI resources
  - Can play an important role in promoting collaboration
- Early NSF experience with gateways has been very positive
  - nanoHUB.org for nanotechnology researchers
  - NEES for earthquake engineering researchers
- NSF Engineering is considering seed grants to assist communities form VOs

Thank you