



# Using I-light and the Purdue Nanohub Computing Resources to Run Computationally Intensive Codes in Nanotechnology

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Director

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Technical Director





## Vision

To help move nanoscience to nanotechnology by connecting experiment, theory, simulation, and computation in a new way **and** to become a resource to the NNI.

NNIN > NASA URETI > NCN > Ilight

## Mission

- Research
- Education
- Infrastructure



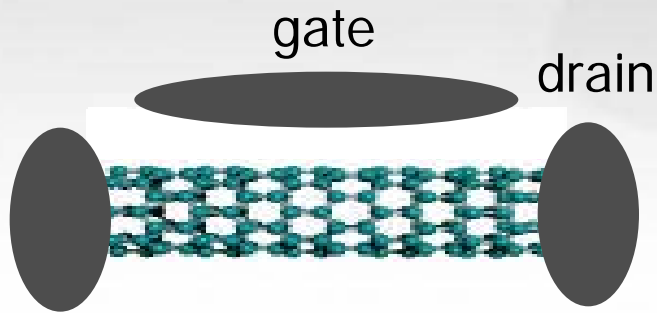
# Outline

- **The Network for Computational Nanotechnology...A research center.**
- **Building a community and providing services...A user facility.**
- **Using Ilight and Teragrid to enhance research and education...An infrastructure**



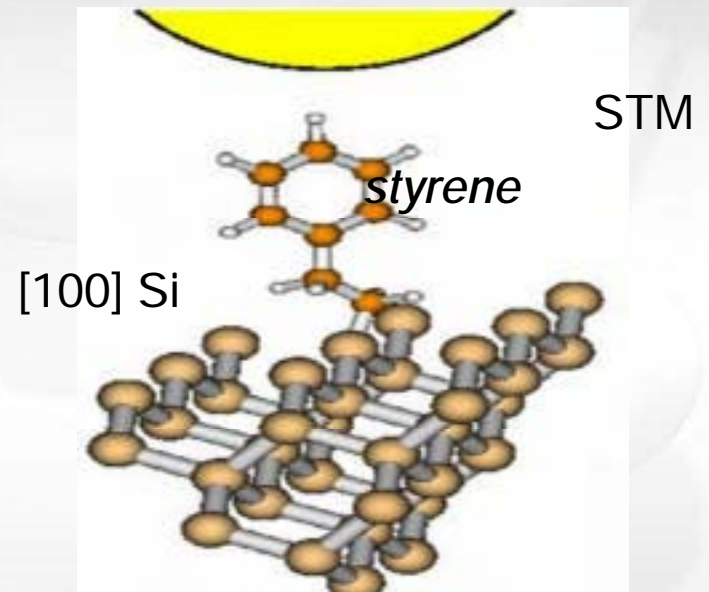
# Nanoelectronics

## carbon nanotube electronics

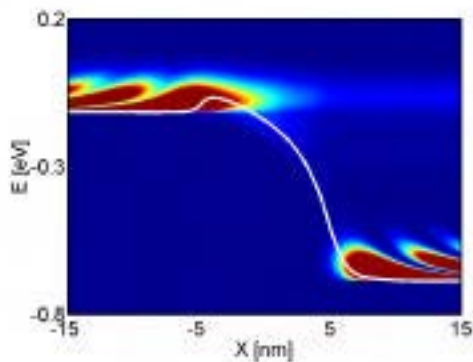


Theory: Cho, Leburton, Lundstrom, Roy  
Experiment: Dai

## molecules on silicon



## silicon nanoelectronics

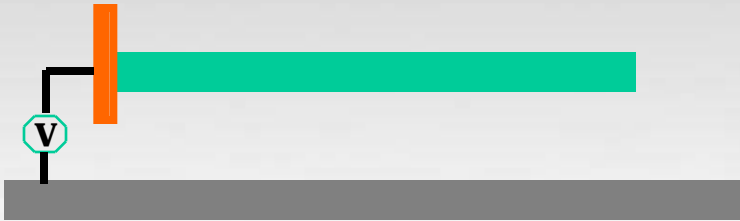


MARCO  
MSD Center

Theory: Datta, Ratner, Roy  
Experiment: Hersam  
(NASA)



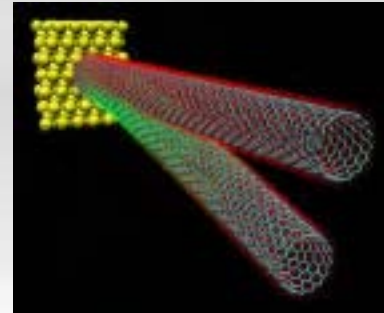
# NEMS



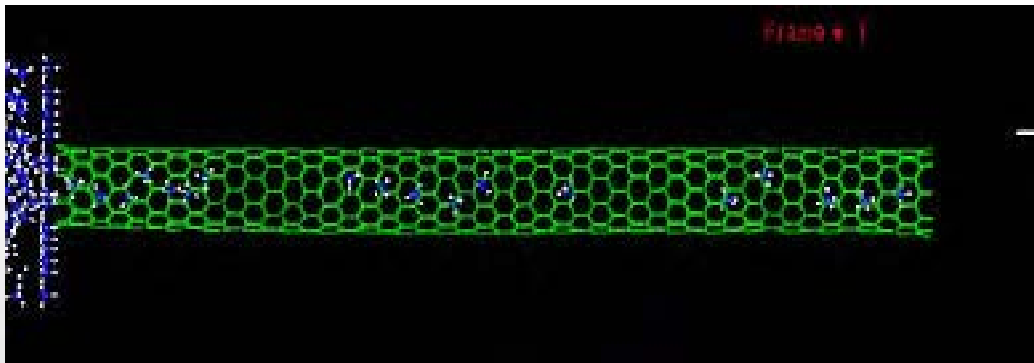
QM Models for NEM switches

Theory (Aluru, Hess, Dutton)

Experiments (Lyding, Liu)



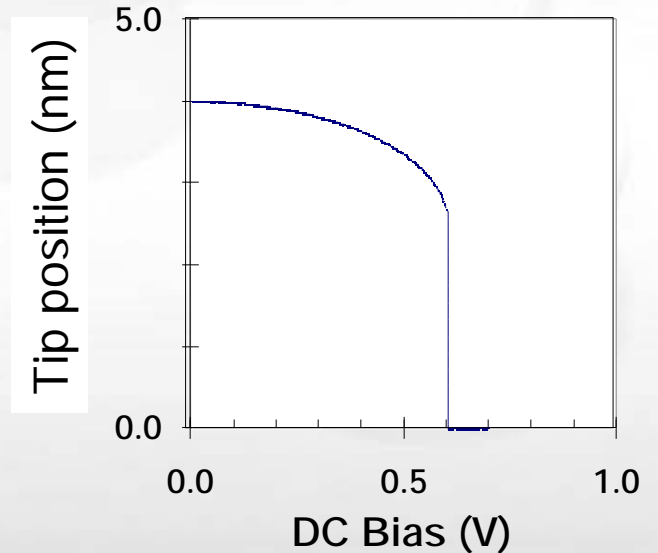
Compact models  
and circuits for  
arrays of NEMS



Fluids through nanotubes and nanopores

Theory (Sinnott, Murthy, Aluru)

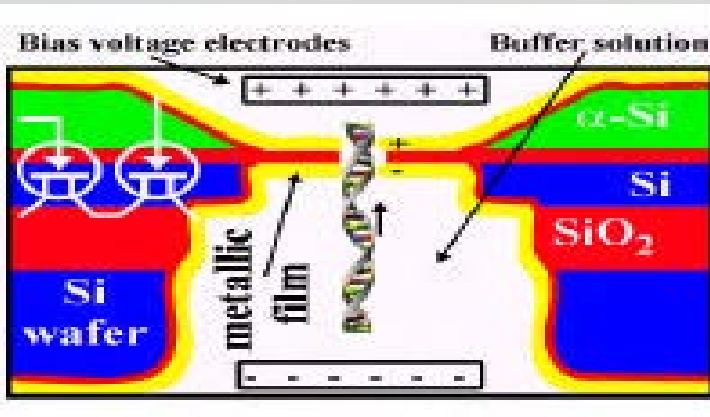
Experiments (Shannon, Bohn)



Theory (Dutton, Aluru)



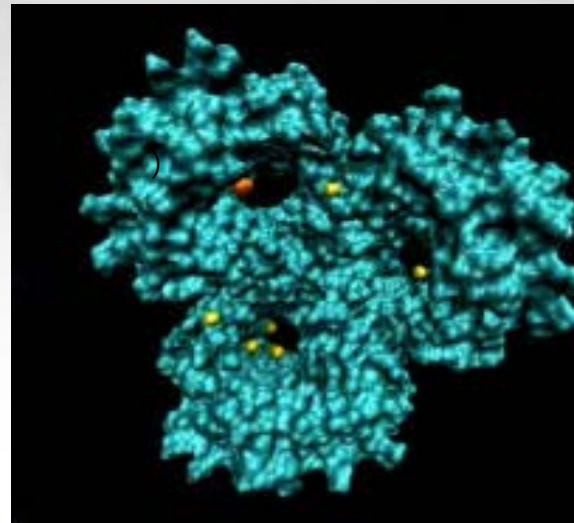
# nano-bio



DNA sequencing using artificial nanopores

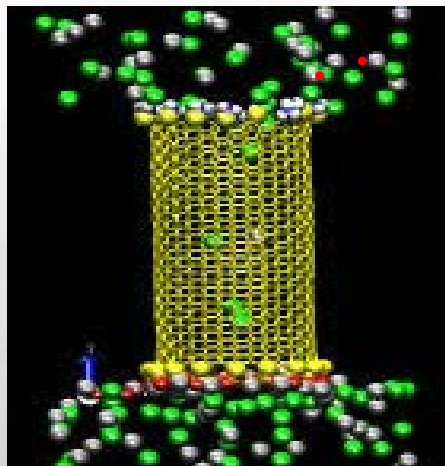
Theory (Hess, Leburton, Schulten)

Experiments (Timp)



Ion Channels in Biological Membranes

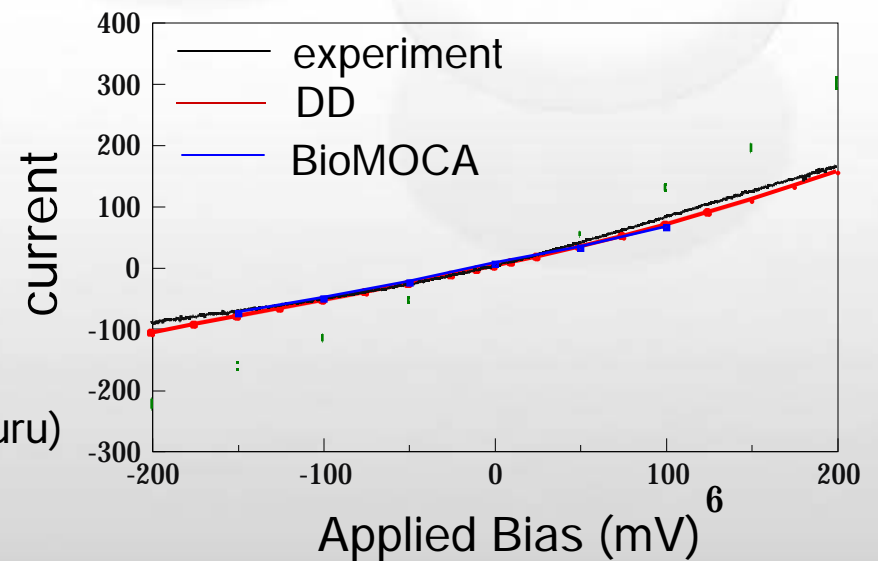
Theory (Hess, Ravaoli, Schatz)



Ion transport in artificial channels

Theory (Hess, Schatz, Aluru)

Experiments (Lyding)





## The NCN research is about

-research that makes a difference

*nanoelectronics, NEMS, nano-bio*

*tight links to experiment*

*advancing science, exploring technologies*

*new theory*

*new computational algorithms and approaches*

*open source software*

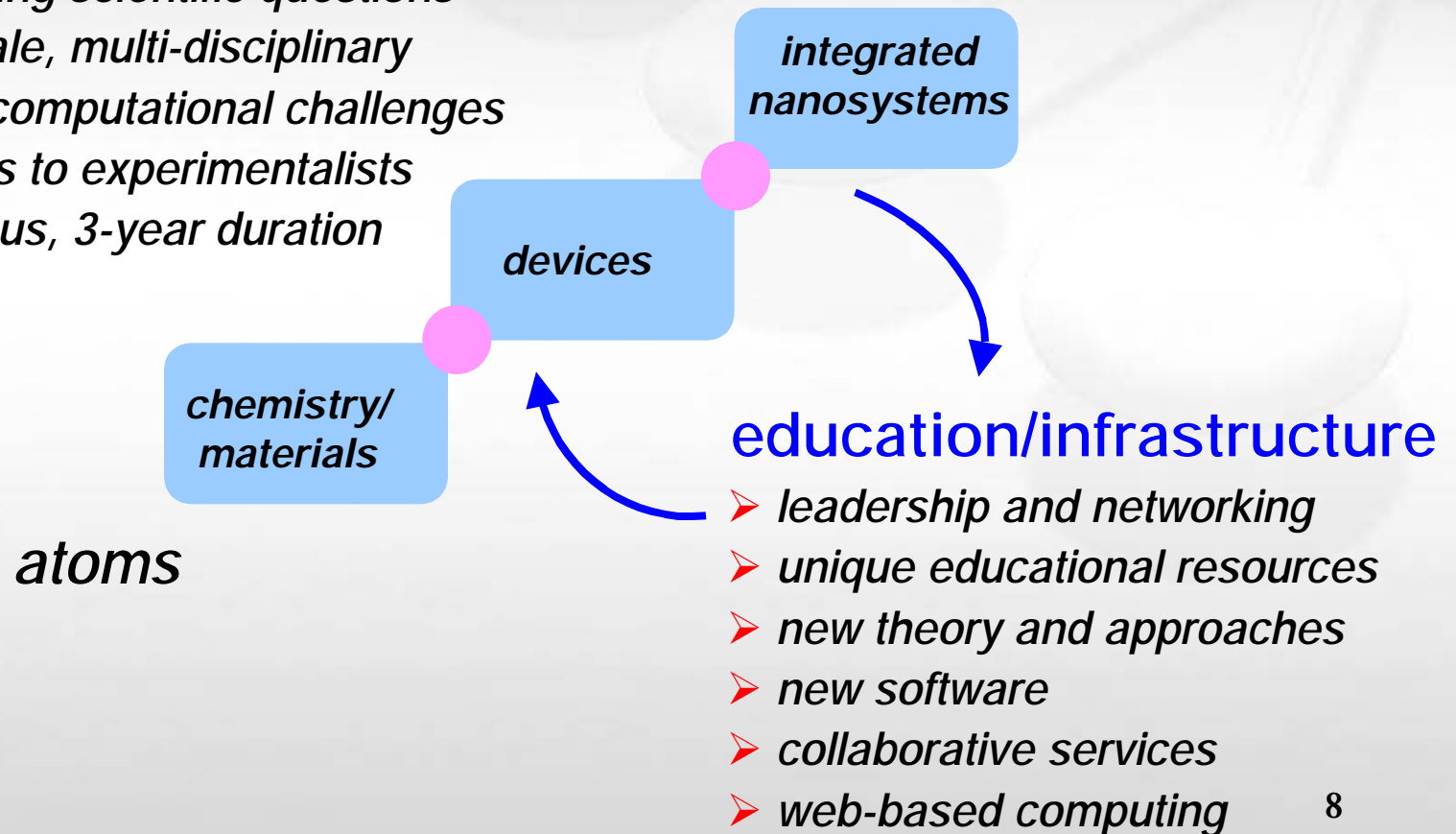


# More than Research...

## research

- *significant technological promise*
- *challenging scientific questions*
- *multi-scale, multi-disciplinary*
- *serious computational challenges*
- *tight links to experimentalists*
- *clear focus, 3-year duration*

## systems





# NCN

NETWORK for COMPUTATIONAL NANOTECHNOLOGY

# Community Building

nanohub.org - Online Simulation and More

Navigation

Research  
Courses  
Short Courses  
Seminars  
Simulation

Education  
Nano Curriculum  
Summer Institutes  
Summer Schools

Community  
Nanocomputing Debate  
Chat Rooms  
Forums

Events  
Calendar  
Workshops  
Conferences

Partners  
NASA ISAC  
CCN  
MPCO HUB

About US  
Our Mission  
Research Groups

nanohub  
Online Simulation and More  
Nano Electronic  
Nano Bio  
NEMS

an initiative led by the Network for  
Computational Nanotechnology

[www.nanohub.org](http://www.nanohub.org)

- Bringing people together
- Offering valuable content
- Fostering debates
- Sharing software and education material
- Use of new technology (Access Grid, Ilight...)
- On-line simulation



## High Value Content



“Introduction to Computational Nanotechnology”  
June 7-18, 2004 Beckman Institute, UIUC



“From Atoms to Transistors”  
Supriyo Datta

- On-line courses, streaming video and lecture notes
- On-line seminars, streaming video, slides and forums
- On-line simulation for summer school, labs and lectures on-line.

### Fundamental Limits of Digital Computation

- 1) Victor Zhirnov, SRC
- 2) Craig Lent, Notre Dame
- 3) Kostya Likharev, SUNY-SB
- 4) Vwani Roychowdhury, UCLA
- 5) ...



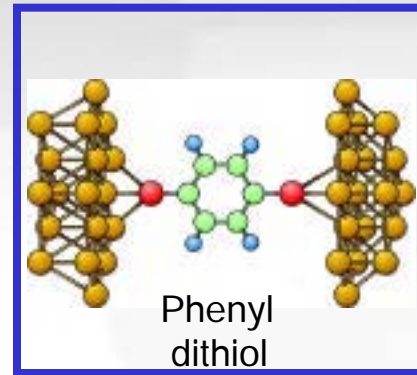
# NCN

NETWORK for COMPUTATIONAL NANOTECHNOLOGY

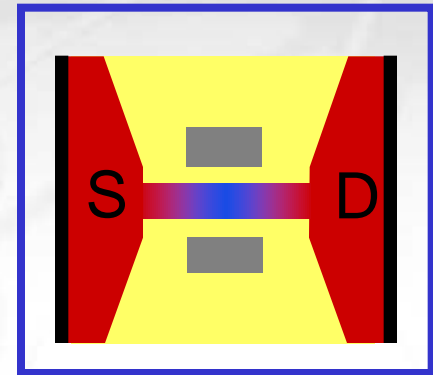
# Sharing research codes



Molecular Electronics



Si CMOS



MolcToy  
Hückel-IV 2.0  
*ab initio* DFT

FETToy  
nanoMOS 2.6

<http://nanohub.purdue.edu>

In 2003:

20 tools / 987 users / 86,152 jobs

2003: 261 on-line users (9,334 jobs)  
Total downloads: 772



# More than great content...

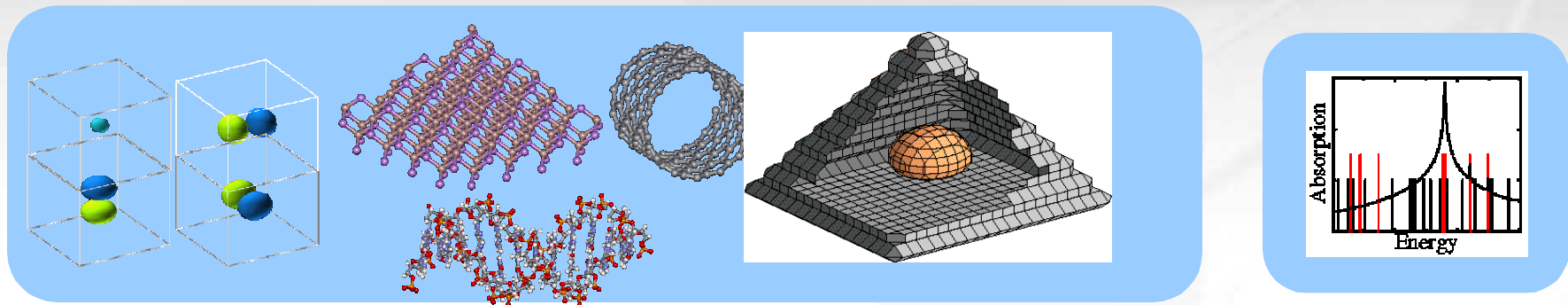
- A real user facility, [nanohub.purdue.edu](http://nanohub.purdue.edu)
- Providing on-line simulation to the nanotechnology community
- Using tomorrow's cyberinfrastructure...
  - ... Ilight and Teragrid





# Example of Application

NEMO 3D (Klimeck, et al., JPL)



Atomic Orbitals  
size: 0.2nm



Structure



Nanoscale Quantum States  
(Artificial Atoms, size 20nm)



Designed Optical  
Transitions  
**Sensors**

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**Computational Cost: 1-10 hours on 20-40 CPUs running in parallel**

- *3D quantum simulation is limited by computation*
- *We want to allow users to run these type of applications transparently*

# Infrastructure Middleware



*next-generation  
network computing*

J.A.B. Fortès  
Univ. of Florida



<http://invigo.acis.ufl.edu>

- Access to virtual machine on demand
- Shared workspace for collaboration
- Enhanced security and use of open source packages
- Grid aware, backends protocols for PBS, Condor, Globus

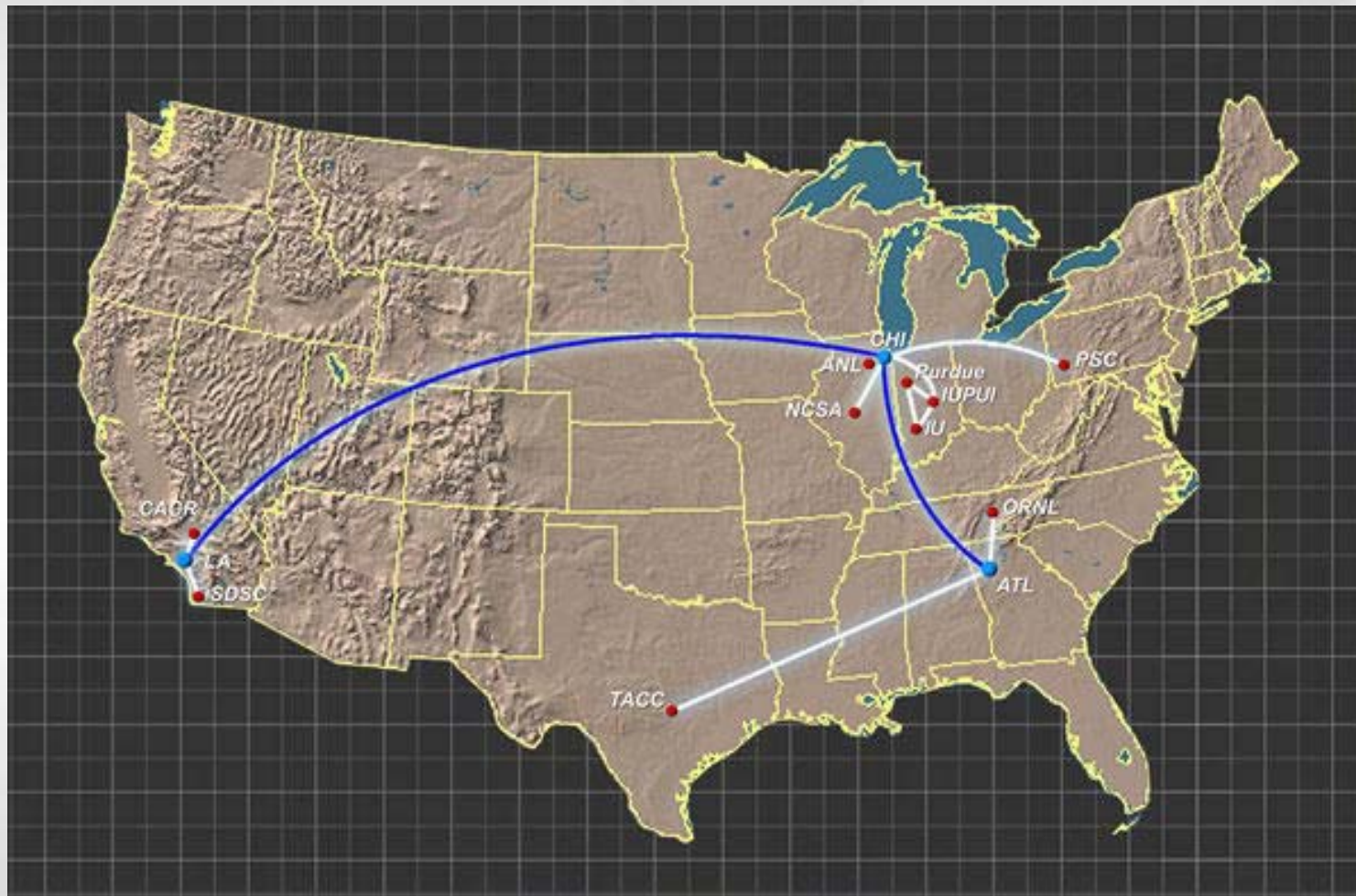


## Some Hardware...





## Some more...





## The NCN goals

- Every three years state of the art production level applications are made available on the nanohub
- Some of these are and will be computationally intensive but this should not be an issue for great research and great teaching/learning
- Significant compute cycles will be needed through the middleware infrastructure.
- 10,000 users by 2007



**NCN**

NETWORK for COMPUTATIONAL NANOTECHNOLOGY

“NCN has been designed to be the lead center of excellence for simulation at the nanoscale in the US.”

Mihail Roco

NSF Senior Advisor for Nanotechnology

