

Nanotechnology Research, Education, Infrastructure, and Collaboration at Purdue University

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Discovery Park

PURDUE
UNIVERSITY



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Birck Nanotechnology Center
Purdue University, West Lafayette Campus

HDR
Architecture • Engineering • Planning

Nanotechnology Focus Areas

- Molecular Electronics
- Micro- and Nano-Mechanical Systems
- Micro- and Nano-Biotechnology
- Sensors
- Nanoscale Metrology
- Computational Nanotechnology

Mission

To address key challenges in moving the nanoscience to nanotechnology through:

- 1) **Research** that links computational scientists, experimentalists, and computer scientists in teams that address critical challenges.
- 2) **Education**, directed at students and professionals, that teaches computational methods and that uses simulations to bring abstract concepts to life.
- 3) **Infrastructure** that delivers nanotechnology simulation services and that fosters education and collaboration.

Challenges

- Developing new theory and approaches for multi-scale simulation
- Working closely with experimentalists
- Solving problems quickly, producing insight not numbers
- Computational demands
- Providing access to simulation tools and services
- Supporting and educating users

Major Grants

- NASA Institute for Nanoelectronics and Computing *~ \$15M (5 years)*
 - To lay a foundation for a new class of heterogeneous terascale systems with the intelligence, adaptability, and fault tolerance necessary for future NASA missions
- 21st Century Fund Support (contingent cost share \$2M)
 - To help Indiana companies and universities benefit from the research, expertise, and facilities of the INAC
- NSF Network for Computational Nanotechnology *\$10.5M (5 years)*
 - Conduct research that begins at the molecular level and ends at the system level and is tightly linked to experiment.
 - Deploy a cyberinfrastructure that facilitates collaborations and delivers simulation services.
 - Educate students and professionals.

Discovery Park Leveraging

•Network for Computational Nanotechnology – NSF – Lundstrom

Discovery Park Cost Sharing

–E-Enterprise Center	\$867,282
–Birck Nanotechnology Center	\$500,000
»Total	\$1,367,282

University Cost Sharing

–ECE	\$195,894
–Mechanical Engineering	\$195,894
–Schools of Engineering	\$2,293,674
–School of Science	\$423,118
–CRI	\$322,425
–ITaP	\$1,129,385
–Provost	\$337,198
–Vice Provost for Research	\$346,750
»Total	\$5,244,338

Indiana 21st Century Cost Sharing \$2,100,000

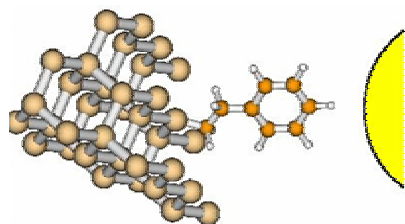
National Science Foundation \$10,500,000

Total \$19,211,620

Research

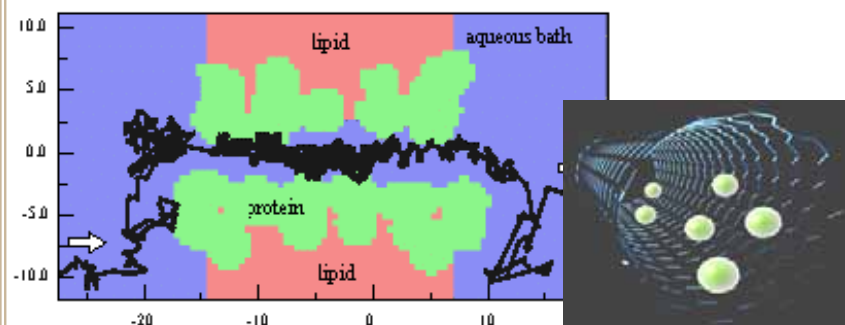
nanoelectronics

- carbon nanotube electronics
- molecules on silicon (NASA)
- silicon nanotransistors (SRC/MARCO)



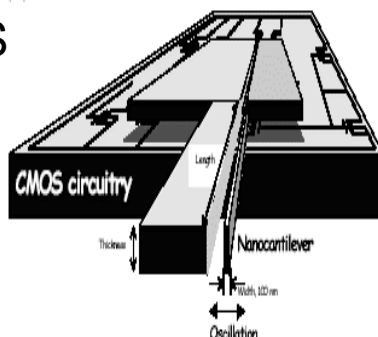
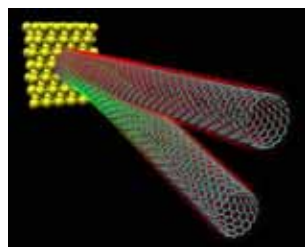
nanobioelectronics

- natural and artificial ion channels



nanoelectromechanics

- Si and CNT NEMS



partnerships / collaborations

- MEMS
- nanophotonics
- energy conversion
- nanofluidics
- catalysis
- nanomaterials
- thermal conduction
- etc.

Research - Computational Problem-Solving

- High-performance computing with Matlab
- New algorithms and parallel implementations
- Grid computing
- Visualization
- Engaging computer scientists and applied mathematicians
- Education

Purdue's ***Computing Research Institute***

nanoHUB: Interface between NCN and ITaP

NANOTOOLS
NANO/MOLECULAR
CNTbands
CNT-IV **NEW!**
Huckel-IV 2.0 **NEW!**
MolCToy **NEW!**
NanoMDS 2.0
Schred
TBGreen **NEW!**
TunProb



- software
- simulation services
- educational resources
- data bases
- ...

- on-line 24 hours/day since 1995
- >150,000 simulations since 2000
- expect ~ 1000 users in 2003

applications
install "as is"

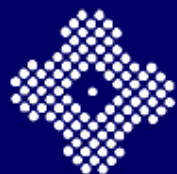
PUNCH 5.0
grid computing
middleware

resources "plug in"

www.nanohub.purdue.edu

- 1) USER selects application
- 2) PUNCH identifies available hardware
- 3) PUNCH runs application
- 4) PUNCH displays results to user





NANO HUB

[NSF Nanoscale Modeling
and Simulation Program](#)

NEWS

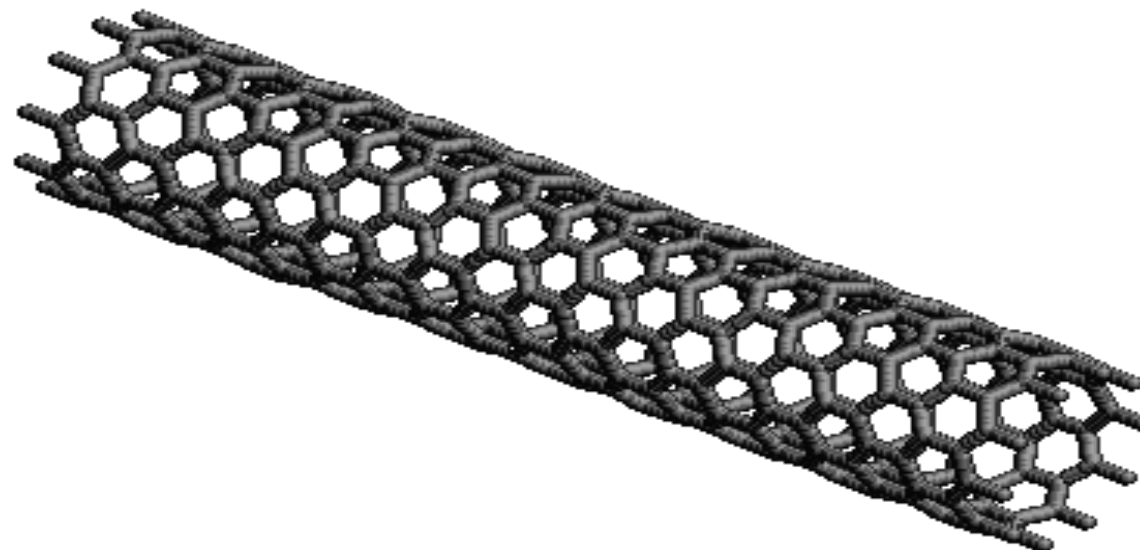
NEW!
**The Purdue
Computational
Electronics Research
Group** will be offering a
two-day, hands-on,
short course at the
University of Illinois,
Urbana-Champaign,
May 21-22!

[Details](#) and a tentative
[agenda](#) are available.

**Discussion Forums are
here!** Click the "Hub
Forums" tab to read and
post to discussion forums
on NanoHub tools. You
will need a separate forum
account to post. For
details, see the FAQ in the
forums.

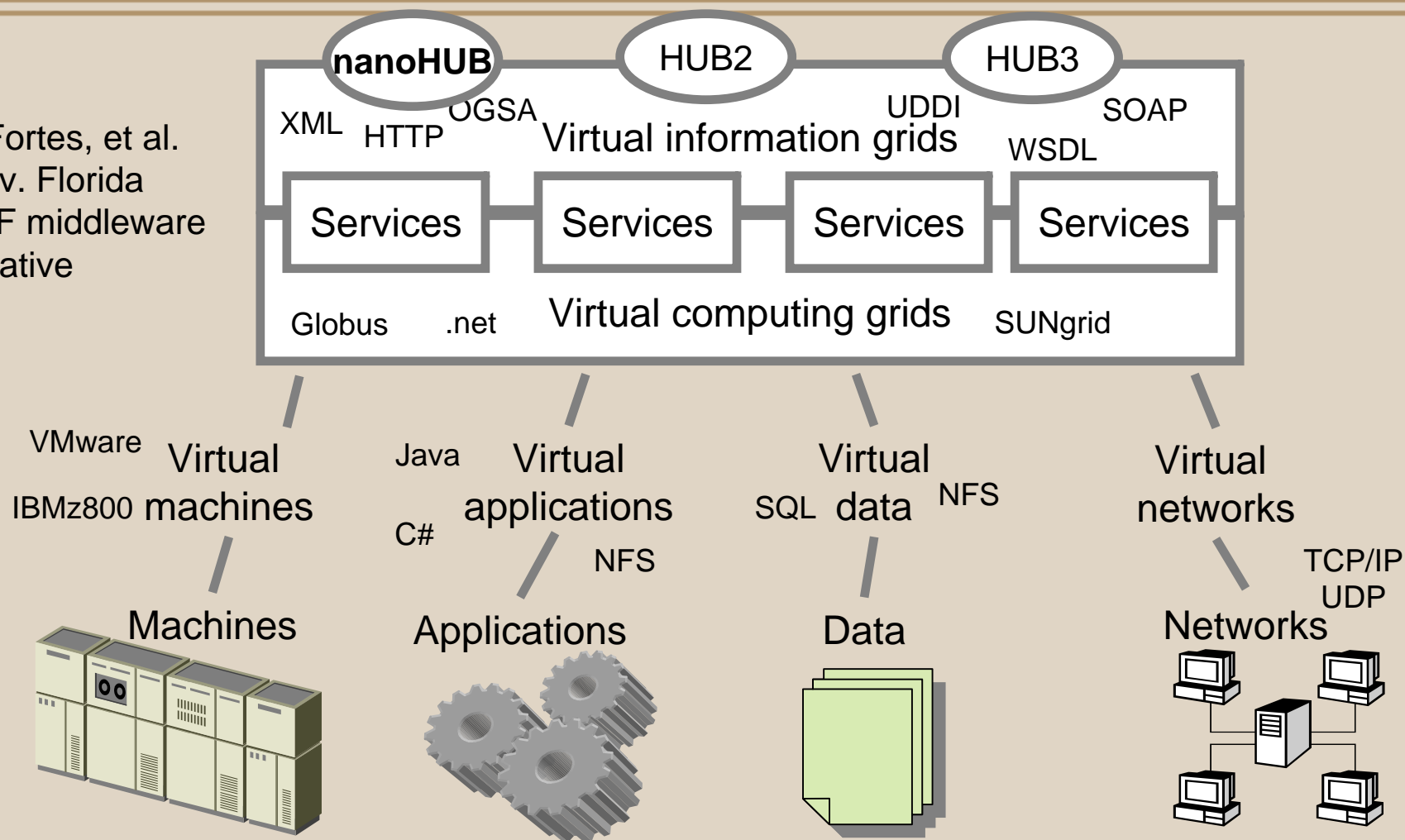
LINKS

[About nanoHub](#)
[People](#)
[Credits](#)
[Sponsors](#)
[Contact](#)
[PUNCH Hubs](#)



From PUNCH to In-VIGO*

J. Fortes, et al.
Univ. Florida
NSF middleware
initiative



**grid computing on virtualized end resources*

NCN Portal Up and Content Being Added

The screenshot shows the NCN portal in a Microsoft Internet Explorer browser window. The address bar displays `http://offcampus.purdue.edu/ncn/portal/.pcmd/changePageGroupJSPCommand`. The page features a blue header with the NCN logo and navigation links: Welcome, INAC, NCN, nanoHUB, and a Search Google button. A red circle highlights the NCN logo, and a red arrow points from it to a text box. The main content area includes a 'QUICKPLACE LOGIN' section with a 'Welcome to the NCN' message and a 'Welcome' message from Mark Lundstrom. A red circle highlights the 'Quickplace Login' section, and a red arrow points from it to another text box. The right sidebar contains a 'Director's Message' from Mark Lundstrom, 'NCN Links' (including The National Nano Initiative, Nanotechnology news, Institute for Molecular Manufacturing, Nanoworld for Kids, SENS, and European Nano Network), and 'NCN News' (including Smalltimes and The Indianapolis Star).

Portal provides access to initiatives and tools in one location

This log-in automatically spawns a Quickplace session for collaborators

Web-based Collaboration Tools in Place

Discovery Park
It will happen here.

May 13, 2003 - 12:39pm

Welcome
My Places
Select Time Zone
Help

My Places

Title	Last Modified	Size
ALS/NSCORT	5/13/03	332MB
babies		22MB
bioscience		6MB
ee659		5MB
e-enterprise		819MB
executivecommittee		9MB
grouper		89MB
iapt		47MB
icb		102MB
inac		446MB
knowledgebase		25MB
metabolite		5MB
ncn		4MB
nortal		134MB
		3MB
		20MB
		7MB
	5/13/03	18MB
	5/13/03	5MB

QuickPlace - Features

- Team Rooms – secure team based workspace
- Threaded Discussions
- Document Drop and version control
- Team calendaring
- Themes
- Forms
- Awareness & Chat
- Notification
- Browser based

Lotus Quickplace:
Project collaboration sites
aggregated in one place.

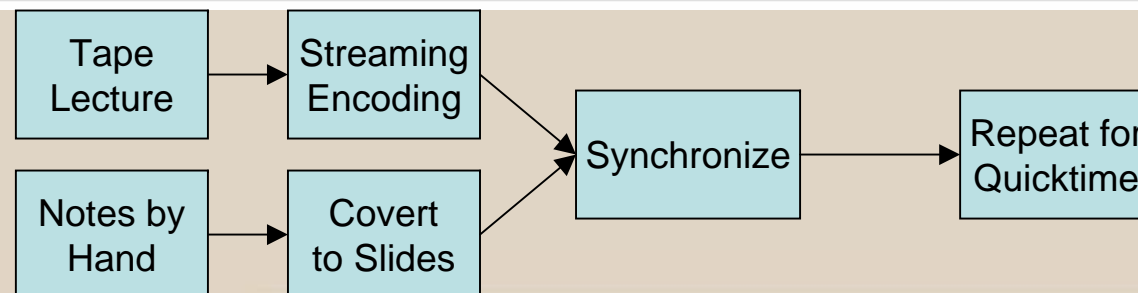
Online Course Materials

The screenshot shows a web browser window titled "Quantum Phenomena: From Atoms to Transistors - Microsoft Internet Explorer". The main content area displays a video player with a thumbnail of a professor writing on a chalkboard. To the right of the video player is a large graphic with a molecular structure background. The graphic contains the following text:

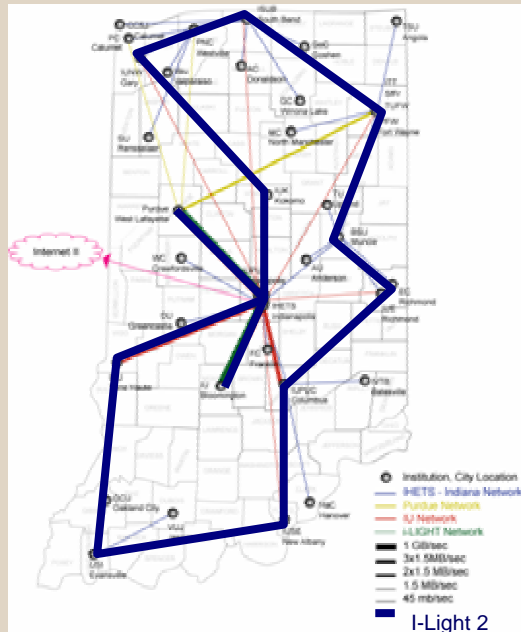
- Quantum Phenomena:** From Atoms to Transistors
- Prof. Supriyo Datta
EE 659
- Purdue University, NCN
- Feb 17, 2003
- Lecture 15:**
Basis Functions: Equilibrium Matrix II

Below the video player is a "Table of Contents" list:

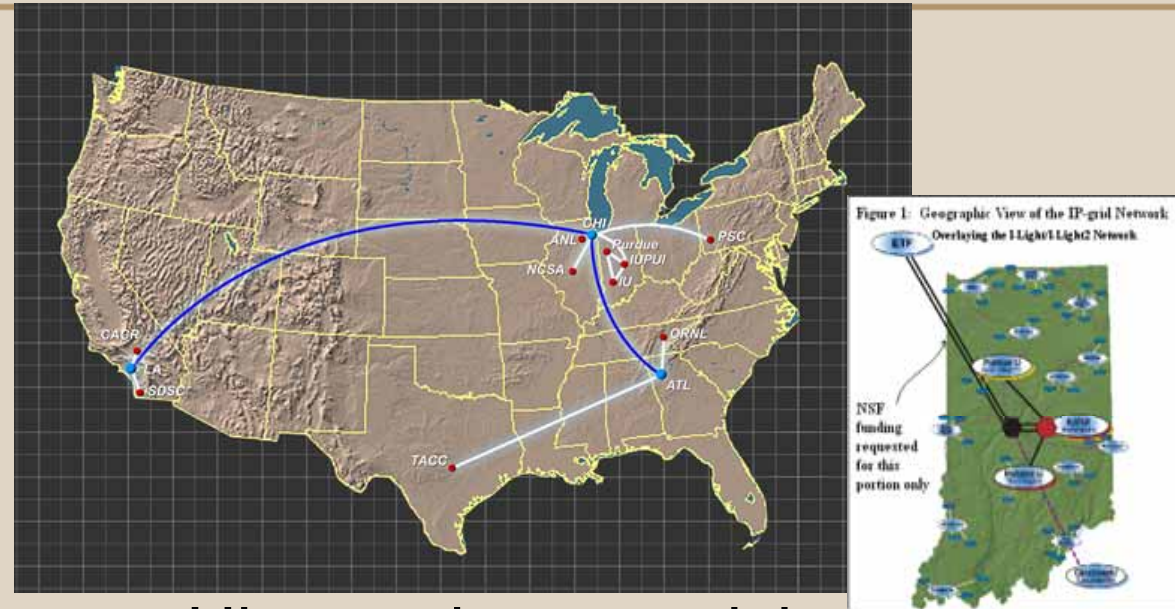
- Lecture 15: Basis Functions: Equilibrium Matrix II
- Basis Functions
- Basis with Periodic Boundary Conditions
- Function of a Matrix
- Real Space Density Matrix
- Physical Meaning of Electron Density
- Physical Meaning of Electron Density
- Physical Meaning of Electron Density
- Summary, and an Example
- Example: Current Flow
- Basis with Periodic Boundary Conditions



Intrastate and National Network Connectivity



- I-Light
 - Investment by State of Indiana to purchase optical fiber infrastructure
 - Currently at 1-2 Gigabit/sec
- New Capabilities
 - Distributed Terascale
 - “I-Light 2”



- Hi-speed connectivity:
 - Collectively provide on the order of 15 TFLOPS of computational capacity and nearly 1 Petabyte of rotating storage.
- Access to TG resources up to the percent of resources we put into the grid

Graphic Courtesy of www.teragrid.org

Rosen Center for Advanced Computing



High throughput computing
(recycled clusters, 1,000 nodes)



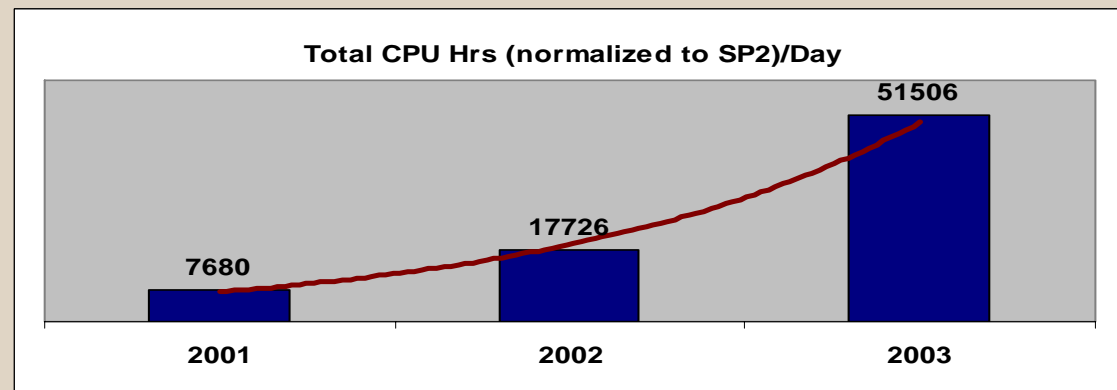
Capturing unused cycles, 2,800 desktops



Dedicated
(Life Sciences,
Nano Sciences)



MPP & large memory



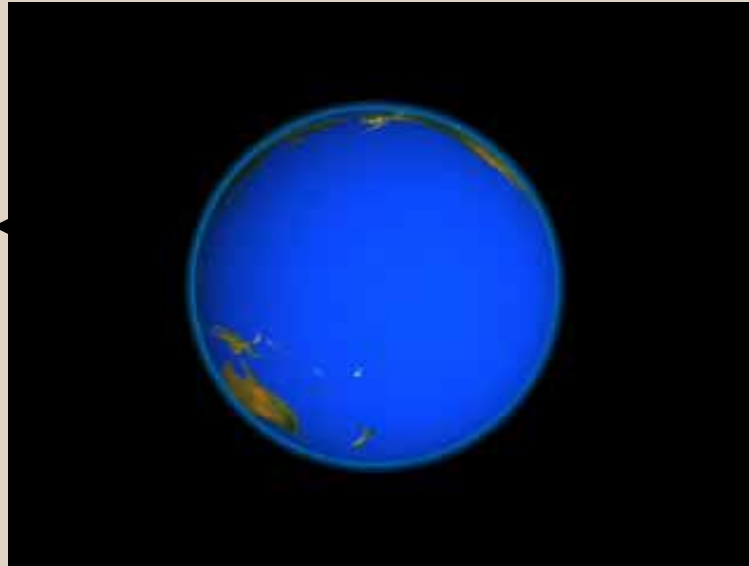
Capacity has been increased by a factor of seven
HPC roadmap outlining capability goals is under development

Purdue Terrestrial Observatory (PTO)

PURDUE
UNIVERSITY

Participating Departments

Agronomy
Ag. & Bio. Engineering
Agriculture
Agricultural Economics
Atmospheric Science
Chemistry
Civil Engineering
Computer Science
Earth & Atmospheric Sciences
Electrical & Computer Eng.
Env. Science & Engr. Inst.
Forestry & Natural Resources
ITaP
Management
Nuclear Engineering



Real-Time Remote Sensing Data

Sample Applications:

Precision Farming
Homeland Security
Disaster Intervention
Forestry & Ecology
Urban Planning
Epidemiology
Oceanography
Industrial Development
Geology & Mineralogy

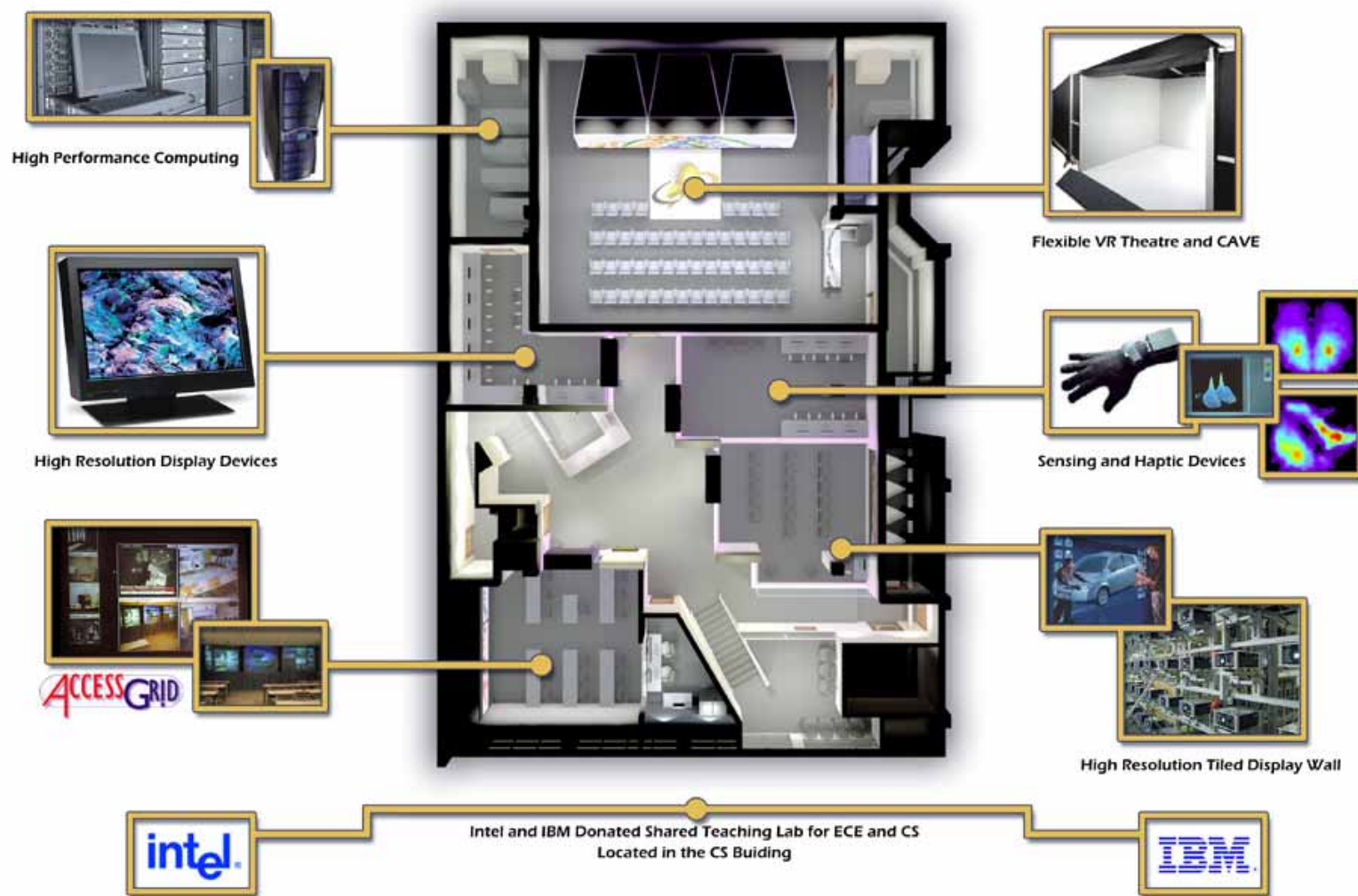


Envision Center for Data Perceptualization

- The Envision Center is administered and supported under the Office of the Vice President for Information Technology.
- Faculty driven initiative with initial funding from a \$900,000 NSF-MRI grant, Chris Hoffmann from CS was the PI.
- IBM and Intel donated hardware for the facility and a teaching lab in Computer Science to be used by all disciplines.
- Construction completed September 29?
Ready for use by December 1?



Simulation of the Pentagon 9-11 event



Cyberinfrastructure Technology Investments Relevant to NCN

- Indiana, Purdue University, Indiana University, ITaP and e-Enterprise are making significant, coordinated investments in advanced networking and middleware
 - I-Light and the IP-grid as a prototype of the NSF Extended Terascale Facility
 - Virtual Research Park
- Implementing the PUNCH concepts in an “industrial-strength” web services applications environment
 - » Applications in Climate Modeling, Systems Biology, and Agriculture
 - » Technology Transfer back to NCN as appropriate
- Data storage and retrieval technologies suited to support knowledge emergence
 - Catalysis Science, Bioinformatics, institutional databases