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# NCSA

Bringing the Power of Advanced  
Computing  
to Science and Engineering

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QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

*University of Illinois at Urbana-Champaign*

*National Center for Supercomputing Applications*





For current status, see:

<http://www.ncsa.uiuc.edu/AboutUs/NCSABuildingWebcam.html>



**NCSA: A Cyberinfrastructure Facility**  
providing the U.S. research  
community with:

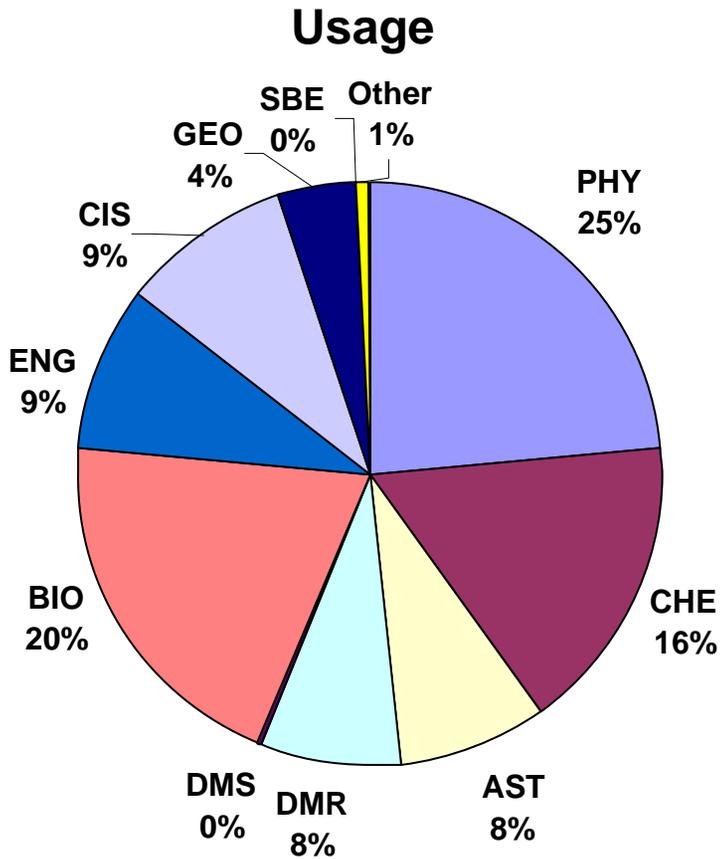
- **CyberResources**
- **CyberEnvironments**
- **Innovative Systems**

## Major NCSA Systems

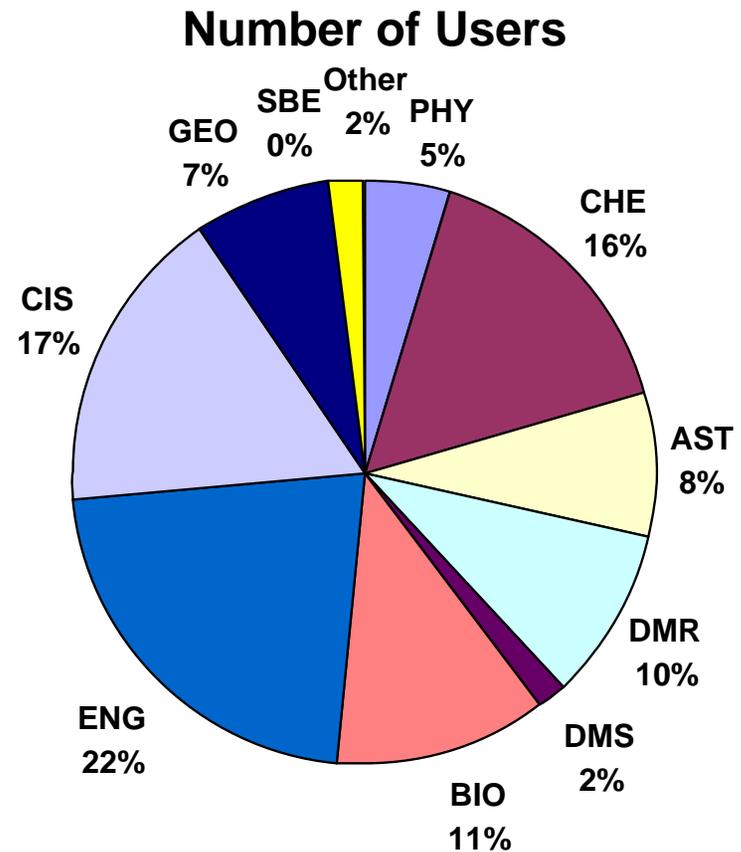
- **Distributed Memory Clusters**
  - Dell (3.2 GHz Xeon): **16 Tflops**
  - Dell (3.6 GHz EM64T): **7 Tflops**
  - IBM (1.3/1.5 GHz Itanium2): **10 Tflops**
- **Shared Memory Clusters**
  - IBM p690 (1.3 GHz Power4): **2 Tflops**
  - SGI Altix (1.5 GHz Itanium2): **6 Tflops**
- **Archival Storage System**
  - SGI/Unitree (**3 petabytes**)
- **Visualization System**
  - SGI Prism (1.6 GHz Itanium2+ GPUs)



*Cyberresources*  
**Distribution of Resources by  
 Discipline** (FY2005 through July 24, 2005)



534,000,000 NU Delivered



1,255 Users

# What are Cyberenvironments?

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- Cyberenvironments are ...
  - Integrated software environment
    - GUIs/portals appropriate for a scientific community
    - Workflow, data management, analysis, visualization, ... tools
    - Collaboration tools
    - Scientific and engineering applications
    - Middleware, web services, ...
  - Designed and built to meet the needs of a scientific community
  - Persistent, robust, and supported
- Cyberenvironments will ...
  - Dramatically reduce barrier to use of cyberinfrastructure by providing convenient “point-and-click” interface to cyberinfrastructure resources and services
  - Broaden access to and use of cyberinfrastructure

## **Advanced Computers of the Future**

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- **Faltering Terascale Technologies**
  - Increasing power and cooling demands as frequency increases
  - Uneven progress in subsystem technologies (processor, memory bandwidth and latency, communications bandwidth and latency)
  - Fall off in “Moore’s Law” gains; increasing cost of Fabs
- **Technologies for Petascale Computing**
  - Low power processors
    - Low performance – need unprecedented scalability (100,000s proc.)
    - Need ability to recover gracefully from processor loss (few per day)
  - Multicore chips
    - Need to address number of issues: scalability, memory access, ...
  - Field Programmable Gate Arrays (FPGAs)
    - Capabilities increasing rapidly – riding silicon technology curve
    - Need efficient software development tools

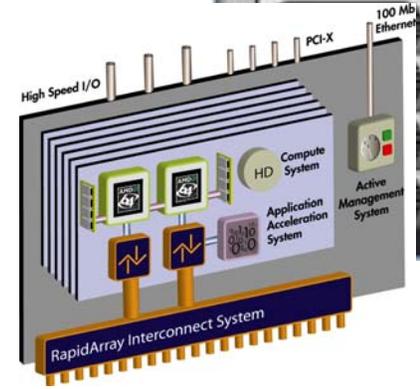
# Innovative Systems Laboratory

- **Exploratory Development Platforms**

- Cray XD1
  - Dual cores and FPGAs
- SGI Altix
  - Dual cores and FPGAs
- Other platforms: *TBD*

- **Applications Software**

- Multidisciplinary software development teams
  - Computational chemistry
  - Computational biology and bioinformatics
  - Computational materials science
  - Others: *TBD*



# NCSA Innovation to Enable Discovery

NCSA's guiding mission is to enable new discoveries by leading the way in developing and deploying an advanced cyberinfrastructure for science and engineering. The center provides the U.S. research community with:

- **Cyber-resources:** more than 40 terabytes of high-end computing power, including Linux clusters and an SGI Altix SMP system;
- **Cyberenvironments:** research environments that make all the tools, applications, and resources of an advanced cyberinfrastructure easily available from the desktop;
- **Innovative systems:** a commitment to working with experimental systems and to pushing beyond what's available now to better serve science.

## NCSA Cyber-resources

### Copper

2 teraflops peak performance  
384 IBM POWER4 1.3 GHz processors  
IBM pSeries 690 Turbo  
Gigabit Ethernet interconnect  
AIX operating system  
Entered production April 2003

### Cobalt (TeraGrid Resource)

6.55 teraflops peak performance  
1,024 Intel Itanium 2 1.6 GHz processors  
SGI Altix 3700 Bx2 system  
NUMalink interconnect  
Linux operating system  
Entered production March 2005

### TE

7.37 teraflops peak performance  
1,024 Intel Xeon EM64T 3.6 GHz processors  
Dell PowerEdge 1850  
Infiniband interconnect  
Linux operating system  
Entered production December 2004

### Mercury (TeraGrid Resource)

10.26 teraflops peak performance  
1,776 Intel Itanium 2 1.3/1.5 GHz processors  
IBM system  
Myrinet interconnect  
Linux operating system  
Entered production June 2004

### Tungsten

15.3 teraflops peak performance  
2,500 Intel Xeon 3.06 GHz processors  
Dell PowerEdge 1750  
Myrinet interconnect  
Linux operating system  
Entered production November 2003

## Computational chemistry/biology applications commonly used on NCSA systems

### Quantum Chemistry

Gaussian08, Gaussian03, ACESII, ADF2000.2, Crystal08, DMol3 4.0 GAMESS-Nov04, Jaguar4.1050, Molcas6, Molpro2002.6, NWChem 4.7, QChem 1.2, VASP, Wick2K-04

### Molecular Mechanics and Dynamics

Amber 8.0, CHARMM Harvard, CHARMMC31B2, Discover 080, COMPASS 4.0, Gromacs 3.3, Macromodel 7.0, Moldy, NAMD, OFF 4.0

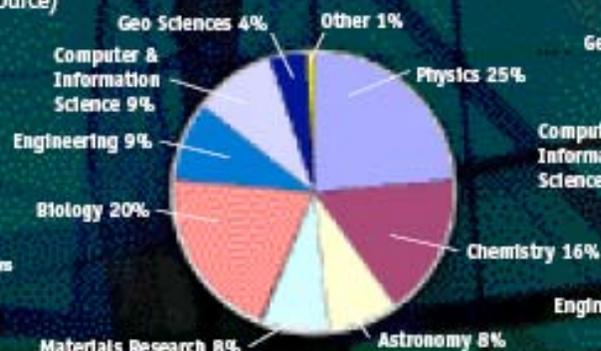
### Bioinformatics and Database

CAP3, MrBayes, Pseq, Blast, Clustalx, Hmmer, HTBlast, NCBI Blast, MPI Blast, FastDNAML, Seqs, CSD

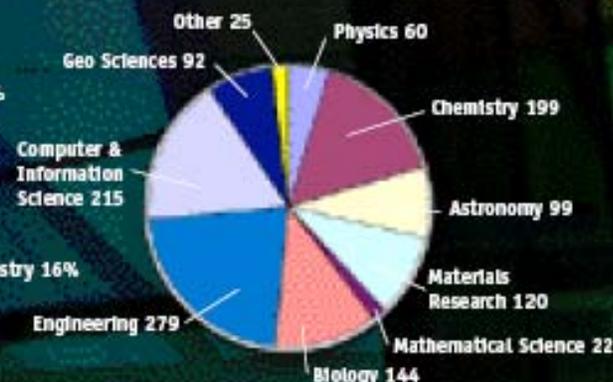
### Graphics Interface and Molecular Builder

Cerius2 4.2MS, Crystal Builder 4.0, INSIGHT-II, PolymerBuilder 4.0, Surface Builder 4.0, Molden 4.0, NCSA NanoCAD 1.0, Pymol, VMD

NCSA Resource Use by Discipline  
FY2005



NCSA Number of Users by Discipline  
FY2005



534,000,000 NU Delivered 1 NU is equivalent to 1 Cray X-MP Hour