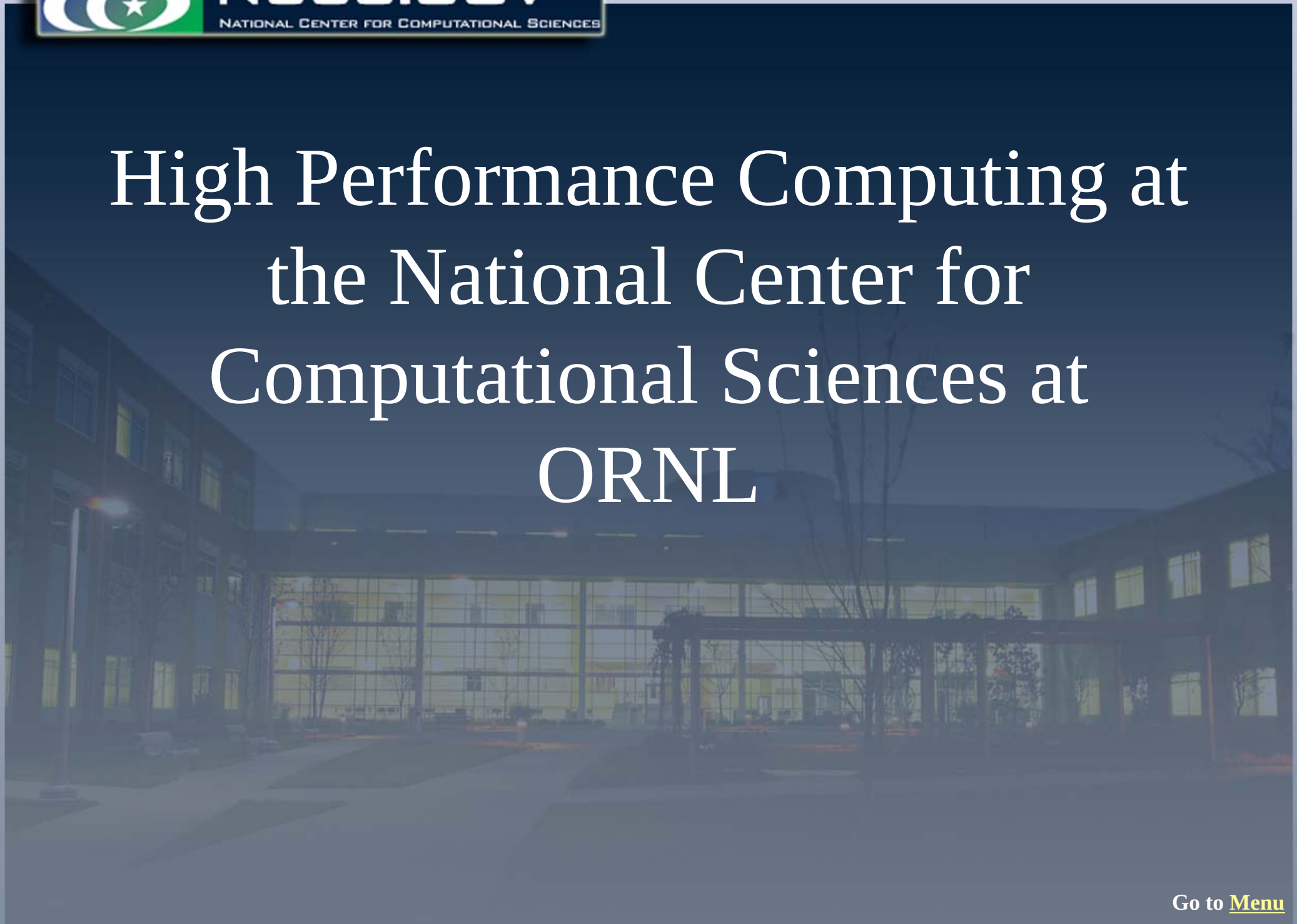
High Performance Computing at the National Center for Computational Sciences at ORNL



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Outline

- Our Mission
- Computer Systems: Present, Past, Future
- Challenges Along the Way
- Resources for Users

Our Mission

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ORNL is the U.S. Department of Energy's largest science and energy laboratory

- $1.3B budget
- 4,250 employees
- 3,900 research guests annually
- $350 million invested in modernization

- World's most powerful computing facility
- Nation's largest concentration of open source materials research

- Nation's most diverse energy portfolio
- The $1.4B Spallation Neutron Source in operation
- Managing the billion-dollar U.S. ITER project

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Computing Complex @ ORNL

$70M Operating budget to deploy and operate the computational resources required to tackle global challenges

- Providing world-leading computational resources and specialized services for the most computationally intensive problems
- Providing stable hardware/software path of increasing scale to maximize productive applications development
- Delivering transforming discoveries in materials, biology, climate, energy technologies, etc.

World's most powerful computer for open science

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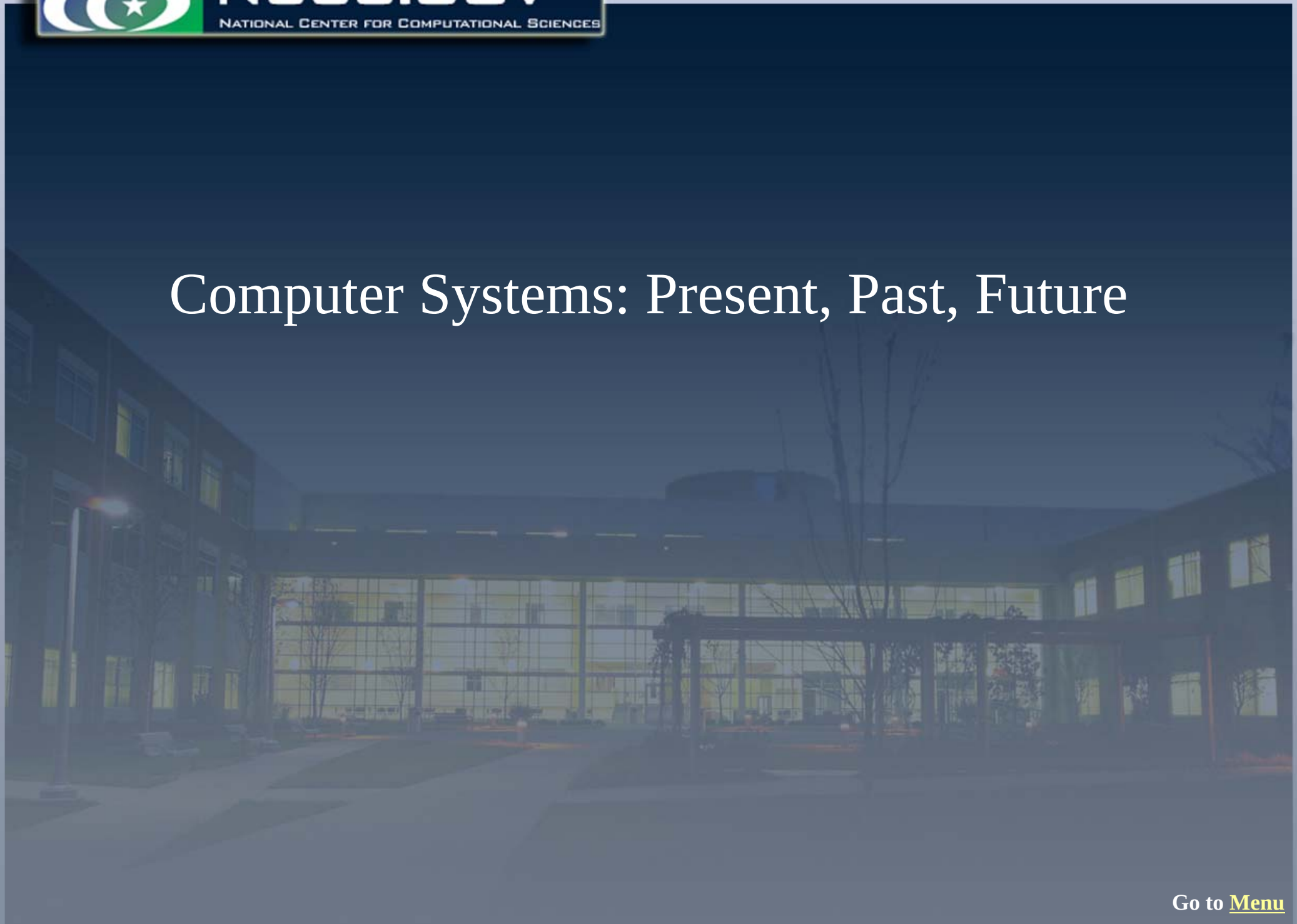
Computer Systems: Present, Past, Future



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NCCS systems, 1991–2008

1991
KSR1-64
CCS formed

1992
Paragon XP/S 35 installed

1993
PVM used to create first international grid
HPSS development begins

1994
PVM wins R&D 100

1995
Install Paragon XP/S 150-MP
Worlds fastest computer connected by fastest network–OC-12–to Sandia

First T170 climate run

1996
ORNL-SNL create first high-performance computational grid

1997

R&D 100 Award for successful development and deployment of HPSS

1998
Developed first application to sustain 1TF wins Gordon Bell prize

1999
NetSolve wins R&D 100
ATLAS wins R&D 100

Long-standing climate simulation milestone first met on CCS Compaq

2000

First OSC teraflop peak system

2001

First IBM Power4
SciDAC leadership
Human Genome Project
Jack Dongarra elected to National Academy of Engineering

2002

Partnership with Cray on X1 begins

IBM Blue Gene CRADA to develop super scalar algorithms begins

Neutron Sciences Teragrid Award

2003
GSN testing
Record TCP/IP speed
OC192 to Atlanta

2004

Leadership Computing Facility awarded to ORNL
World's largest Cray X1
ORNL provides bulk of runs of IPCC 4th assessment
OSCAR becomes world's most popular cluster management system

Robert Harrison wins Sidney Fernbach Award
World-class DOE facility

2005

EVEREST facility opens
Cray X1 upgraded to X1E
Cray XT3 installed
Largest fusion simulation using AORSA
UltraScienceNet operational
Production use of LCF

2006

XT3 upgraded to 100 TF
Breakthrough science from LCF applications

Deploy unified Lustre file system for CCS systems

·l·u·s·t·r·e·

2007
250 Tflop XT3 System

2008
1 Petaflop System

Million-fold increase in computing and data capabilities

Cray XT3
Single-core
26 TF

2004

Cray
X1
3 TF

2005

Cray XT3
Dual-core
54 TF

2006

Cray XT4
119 TF

2007

Cray XT4
Quad-core
166 TF
18TB,
0.3 PB

2008

Cray XT4
Quad-core
263 TF
62 TB,
1 PB

2008

Cray XT5
8/12-core,
dual-socket
SMP ~1 PF
100TB,
3.3 PB

2009

Jaguar
8-core,
dual-socket
SMP 1.64PF
362 TB,
10 PB

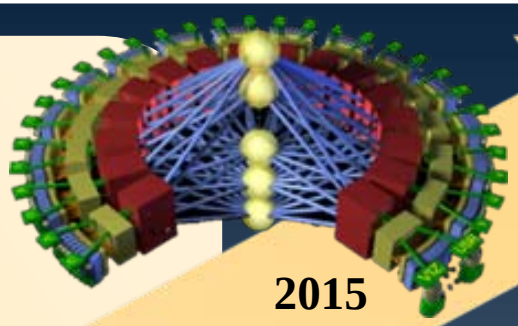
2009

Jaguar
8/12-core,
dual-socket
SMP 2.60PF
362 TB,
10 PB

2009

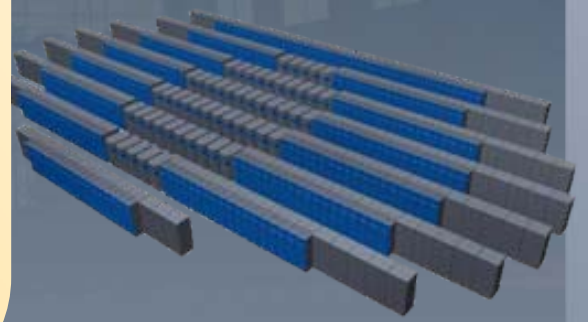
Future
system
100–250
PF

2015



Future
system
1000 PF
(1 EF)

2018



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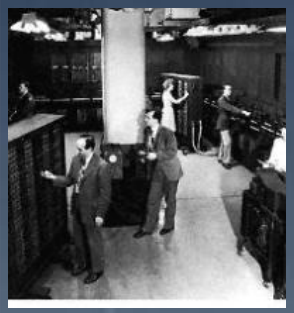
A Growth-Factor of a Billion in Performance in a Single Career





1 — 10^3 — 10^6 — 10^9 — 10^{12} — 10^{15}

One OPS — KiloOPS — MegaOPS — GigaOPS — TeraOPS — PetaOPS

1823 Babbage Difference Engine

1943 Harvard Mark 1

1949 Edsac

1951 Univac 1

1954 ORACLE

1959 IBM 7094

1964 CDC 6600

1976 Cray 1

1982 Cray XMP

1988 Cray YMP

1991 Intel Delta

1995 Intel Paragon

1996 Cray T3E

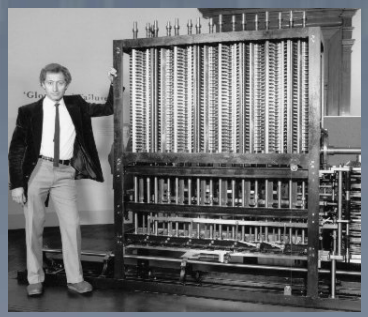
1997 ASCI Red

2001 Earth Simulator

2003 Cray X1

2005 Cray XT3

2008 Cray XT5





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NCCS.GOV
NATIONAL CENTER FOR COMPUTATIONAL SCIENCES

NCCS resources

October 2009 summary

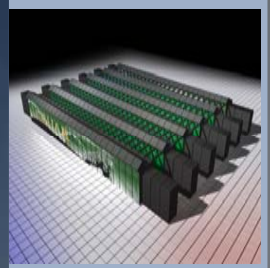
6 Systems

Supercomputers

>265,000 cores
>360 TB Memory

>2,6 PFLOPS

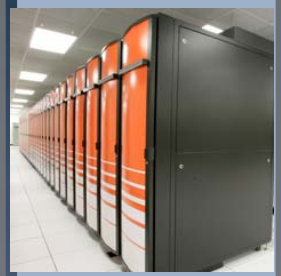
CRAY XT5
JAGUAR



(224,256)
2.6GHz
292 TB Memory

10,000 TB

CRAY XT4
JAGUAR



(31,328)
2.1GHz
61 TB Memory

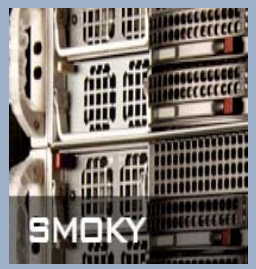
750 TB

IBM
BLUE/GENE P

(8192)
850 MHz
4 TB Memory

60 TB

LINUX CLUSTER
SMOKY



(1280)
2.4 GHz
2.5 TB

4.5 TB

LINUX CLUSTER
LENS

(128)
2.2 GHz
128 GB

9 TB

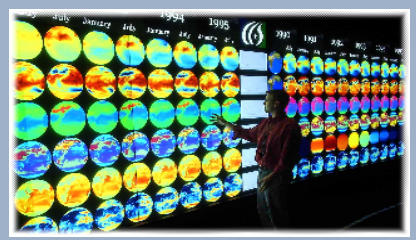
IBM
HPSS

Many storage devices supported

Max. 30 PB

Scientific visualization lab
EVEREST

27-projector PowerWall
35 million pixels



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NCCS resources: Jaguar Supercomputer

Jaguar: World's Most Powerful Computer Designed for Science from the Ground Up

	jaguar XT4	jaguarpf XT5
Peak Performance	263.16 TFLOPS	2.33 PFLOPS
System Memory	61 TB	292 TB
Disk Space	750 TB	10,000 TB
Disk Bandwidth	44 GB/s	240 GB/s
Interconnect Bandwidth	157 TB/s	374 TB/s

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NCCS resources: BG/P

- 27 TFlop System
  - 2048 850Mhz IBM quad core 450d PowerPC
  - 2 GB/node
  - 64 I/O nodes
  - 10 Terabyte GPFS parallel file system
- Available to ORNL + core university partner members

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NCCS resources: Smoky

- Resource provided to users needing system comparable to major NCCS resources for application porting, development
- 80 node Linux cluster
- Four quad-core 2.0GHz AMD Opteron processors per node
- 32 GB of memory (2GB per core)
- Gigabit Ethernet network with infiniband interconnect

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NCCS resources: Visualization Facilities

- The visualization capabilities of NCCS include:
  - visualization/data analysis cluster called Lens
  - large PowerWall display called EVEREST

- Scientists can make use of the EVEREST facility by contacting any member of the visualization team and booking a time.

NCCS resources: Lens

- Resource for data visualization
- 32 node Linux cluster dedicated to data analysis and high-end visualization
- Each node:
  - Four quad-core 2.3 GHz AMD Opteron processors
  - 64 GB memory
  - 2 NVIDIA 8800 GTX GPUs.

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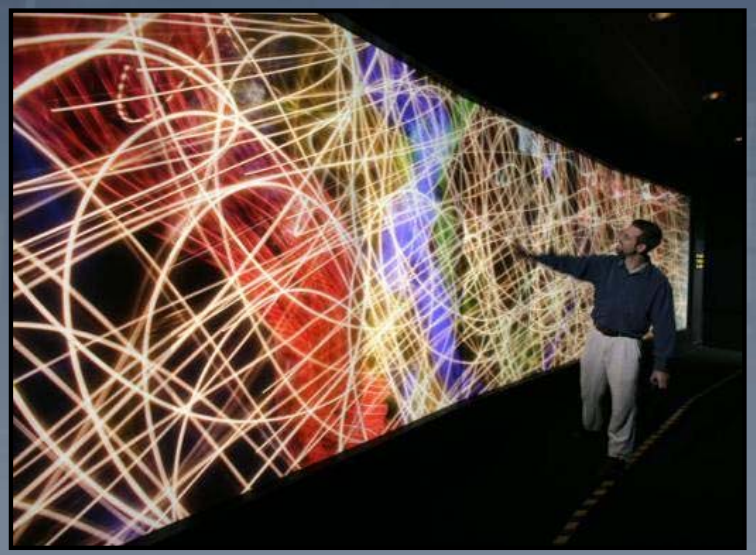
NCCS resources: Visualization PowerWall (EVEREST)

EVEREST - Exploratory Visualization Environment for REsearch in Science and Technology

- 27-projector PowerWall
- Viewing at a 30 feet by 8 feet
- 11,520 by 3,072 pixels, or a total of 35 million pixels
- The wall is integrated with the rest of the computing center, creating a high-bandwidth data path between large-scale high-performance computing and large-scale data visualization.



- EVEREST is controlled by a 14 node cluster with GPUs for remote visualization.
- Each node contains four dual-core AMD Opteron processors.
- These 14 nodes have nVidia QuadroFX 3000G graphics cards connected to the projectors, providing a very-high-throughput visualization capability.

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NCCS resources: High Performance Storage System (HPSS)

- HPSS is an archival Back-up system which consists of
  - two types of storage technology:
    - disk – “on-line” for frequently/recently accessed files
    - tape – “off-line” for very large or infrequently accessed files
  - Linux servers
  - High Performance Storage System software
- Tape storage is provided by robotic tape libraries.

- HPSS has three SL8500 tape libraries. Each can hold up to 10,000 cartridges.
- The StorageTek SL8500 libraries house a total of
  - twenty-four T10000A tape drives (500 gigabyte cartridges, uncompressed)
  - thirty-six T10000B tape drives (1 terabyte cartridges, uncompressed).
- Each drive has a bandwidth of 120 MB/s
- As of October, 2009, HPSS has 7.2 PB stored in over 16.1 million files.

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NCCS resources: Center-Wide File System (SPIDER)

"Spider" provides a shared, parallel file system for all LCF systems and based on Lustre file system

- Over 10 PB of RAID-6 Capacity
  - 13,440 1Gb SATA Drives (33 tons of discs)
  - 192 OSSs and 1344 OSTs (7 OSTs/OSS)
  - 3 Terabytes of memory
- Demonstrated bandwidth of over 200 GB/s
  - 30,000 files created per second
- Demonstrated stability on a number of LCF Systems
  - Over 26,000 lustre clients at NCCS mounting the file system and performing I/O
- Available from all systems via our high performance scalable I/O network
  - 4 InfiniBand core switches
  - Over 3,000 InfiniBand ports
  - Over 3 miles of cables

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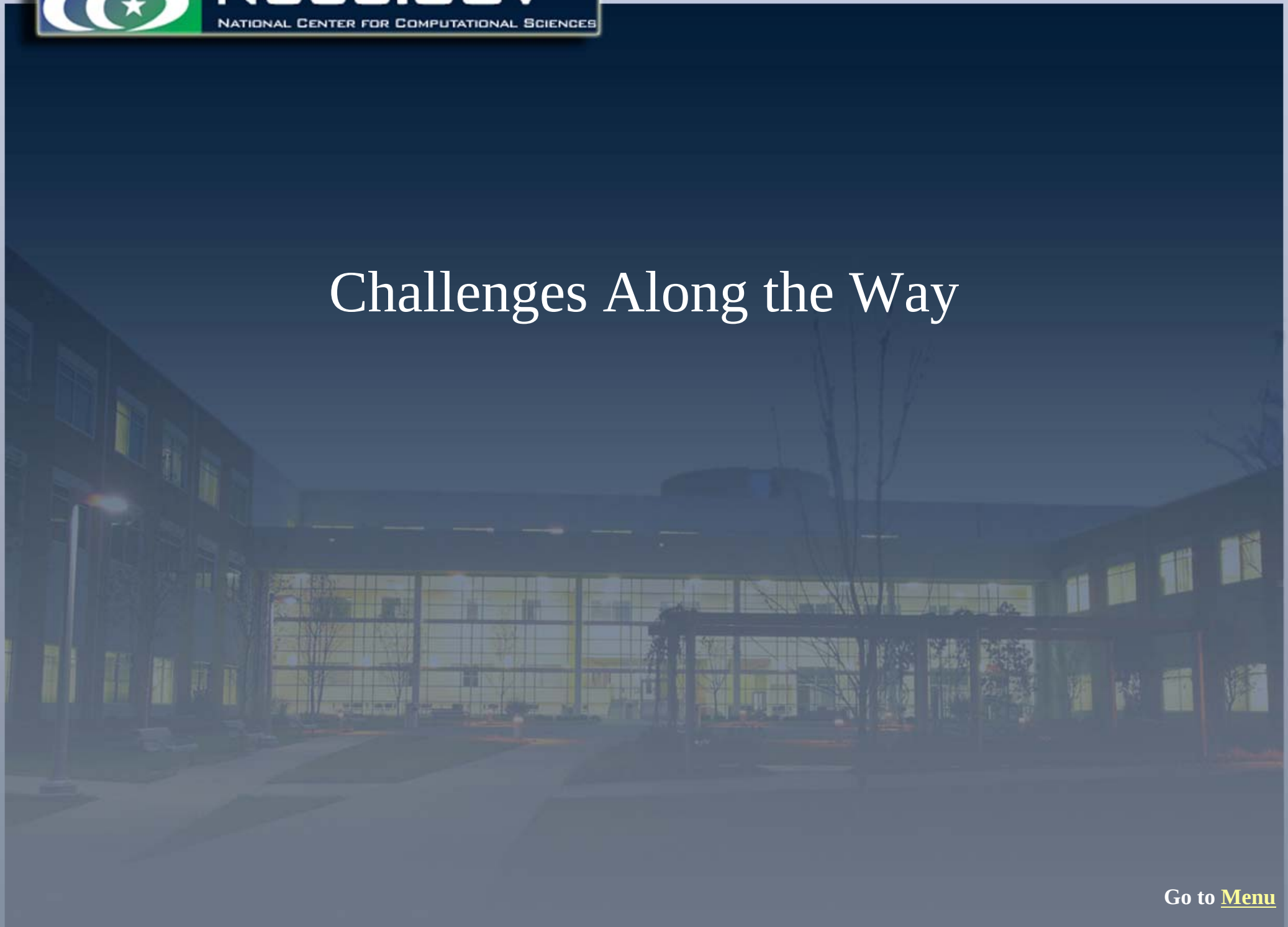
Challenges Along the Way



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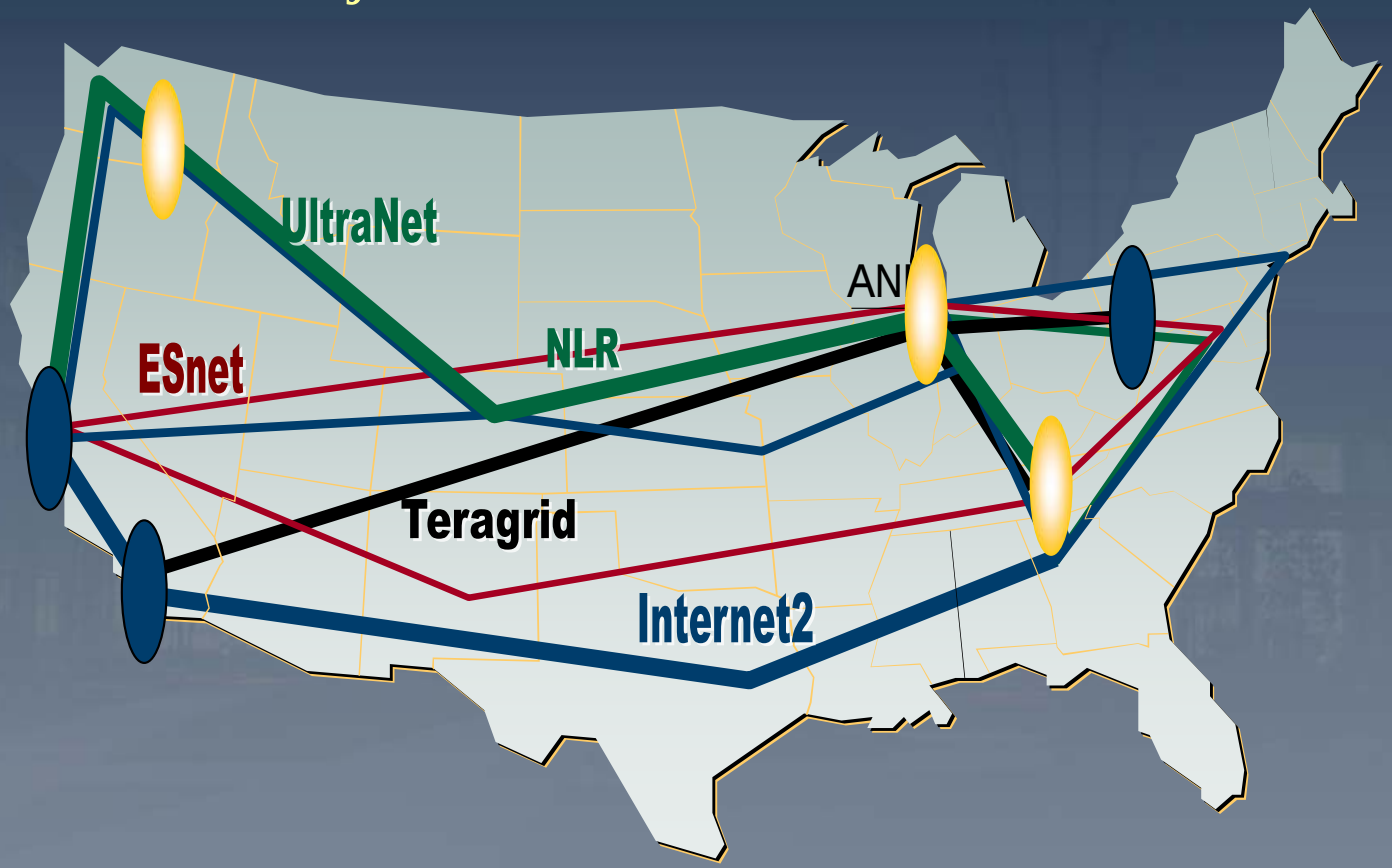
High Bandwidth Connectivity

- High Bandwidth Connectivity to NCCS Enables Efficient Remote User Access
- Connected to Major Science Networks



Target

- 100Gb/lamda (NRL+Vendor+ORNL)

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We are Addressing a Broad Range of Science Challenges

Projects	2006	2007	2008	2009
Accelerator physics	1	1	1	1
Astrophysics	3	4	5	5
Chemistry	1	1	2	4
Climate change	3	3	4	5
Combustion	1	1	2	2
Computer science	1	1	1	1
Fluid Dynamics			1	1
Fusion	4	5	3	5
Geosciences		1	1	1
High energy physics		1	1	
Life sciences	2	2	2	4
Materials science	2	3	3	4
Nuclear physics	2	2	1	2
Industry	2	3	3	3
Total Projects:	22	28	30	38
CPU Hours:	36,156,000	75,495,000	145,387,000	469,683,000

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Science Application Development & Readiness

Ensuring Application Codes Can Effectively Utilize HPC Systems on "Day One"

- Model coupling
- Hierarchical algorithms
- Solver technology and innovative solution techniques
- Accelerated time integration
- Parallel programming models
- Maintaining application libraries
- Software and algorithm strategies to mitigate high hardware latencies
- Automated diagnostics

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Resources for Users

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Resources for Users: Getting Started

- About Jaguar

  http://www.nccs.gov/computing-resources/jaguar/

- Quad Core AMD Opteron Processor Overview

  http://www.nccs.gov/wp-content/uploads/2008/04/amd_craywkshp_apr2008.pdf

- PGI Compilers for XT5

  http://www.nccs.gov/wp-content/uploads/2008/04/compilers.ppt

- NCCS Training & Education – archives of NCCS workshops and seminar series, HPC/parallel computing references

  http://www.nccs.gov/user-support/training-education/

- 2009 Cray XT5 Quad-core Workshop

  http://www.nccs.gov/user-support/training-education/workshops/2008-cray-xt5-quad-core-workshop/

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Resources for Users: Advanced Topics

- Debugging Applications Using TotalView

  http://www.nccs.gov/user-support/general-support/software/totalview

- Using Cray Performance Tools - CrayPat

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/cray-pat/

- I/O Tips for Cray XT4

  http://www.nccs.gov/computing-resources/jaguar/debugging-optimization/io-tips/

- NCCS Software

  http://www.nccs.gov/computing-resources/jaguar/software/

- Cray Documentation

  http://docs.cray.com/

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Resources for Users: More Information

- NCCS website

  http://www.nccs.gov/

- How to obtain Access to NCCS Resources

  http://www.nccs.gov/user-support/access/

- Contact us

  help@nccs.gov