ORNL Computing Overview

Computing and Computational Sciences Directorate

RAMS Update

ORNL
January 21, 2009

Our vision for sustained leadership and scientific impact

- Provide the world's most powerful open resources for capability computing and data analytics
- Follow a well-defined path for maintaining world leadership in these critical areas
- Attract the brightest talent and partnerships from all over the world
- Deliver cutting-edge science relevant to the missions of DOE and key federal and state agencies
- Invest in cross-cutting partnerships with industry
- Provide unique opportunity for innovation based on multi-agency collaboration
- Invest in education and training

We are achieving national objectives through interagency partnerships

Applications

Superconductivity | Chemistry | Fission | Climate change | Bioinformatics

Materials | Combustion | Fusion | Geosciences | Biology

Nanoscience | Energy | Molecular dynamics | Groundwater | Biophysics

Institute for Advanced Architecture and Algorithms
DOE-SC and NNSA

Extreme Scale Software Center
DOE-SC and DOD

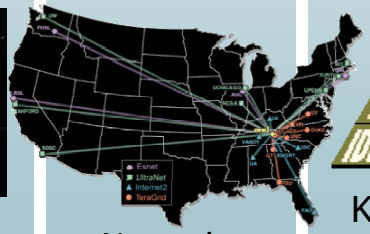
HPC experience and operations

Facilities and infrastructure

Data storage and file systems

Computer systems

Visualization



Networks

Knowledge discovery

Recipe for Leadership in Scientific Computing (Outline)

- **Scalable infrastructure**
  - **Space, power, cooling, cybersecure network, etc**
- **An ultrascale computing strategy and a complementary strategy for data**
  - **Partnership with Intel, Cray and IBM**
  - **DARPA HPCS**
- **Excellence in Systems Engineering, Administration, and Operations.**
  - **Experienced operational and engineering staff comprised of groups in HPC operations, technology integration, user services, and scientific computing**
  - **staffed 24 hours a day, 365 days a year to provide for continuous operation of the center and for immediate problem resolution**
- **CS tools, libraries, programming models and frameworks and complementary math algorithms that scale**
  - **IAA and ESSC**
- **Integrated simulation systems of scalable computational science models and software to deliver on the science and technology innovation missions**

ORNL's Current and Planned Data Centers

Infrastructure

Computational Sciences Building (40K ft^2)

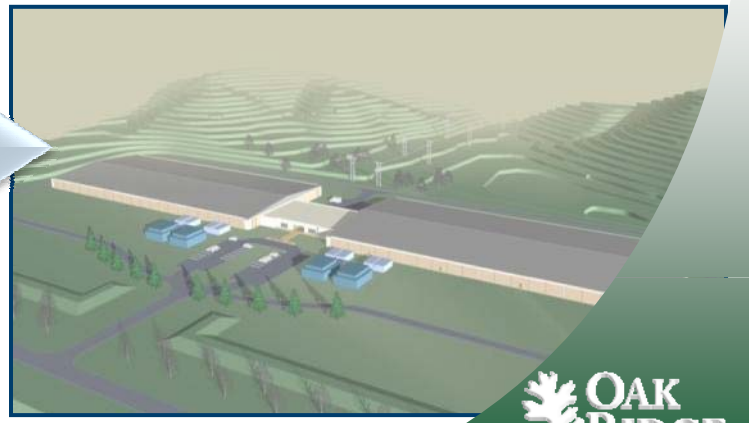
- Upgraded building power to 25 MW
- Deployed a 6,600 ton chiller plant
- Tripled UPS and generator capability

Multiprogram Research Facility (32K ft^2)

- Capability computing for national defense
- Expanded to 25 MW of power and 8,000 ton chiller

Multiprogram Data Center (260K ft^2)

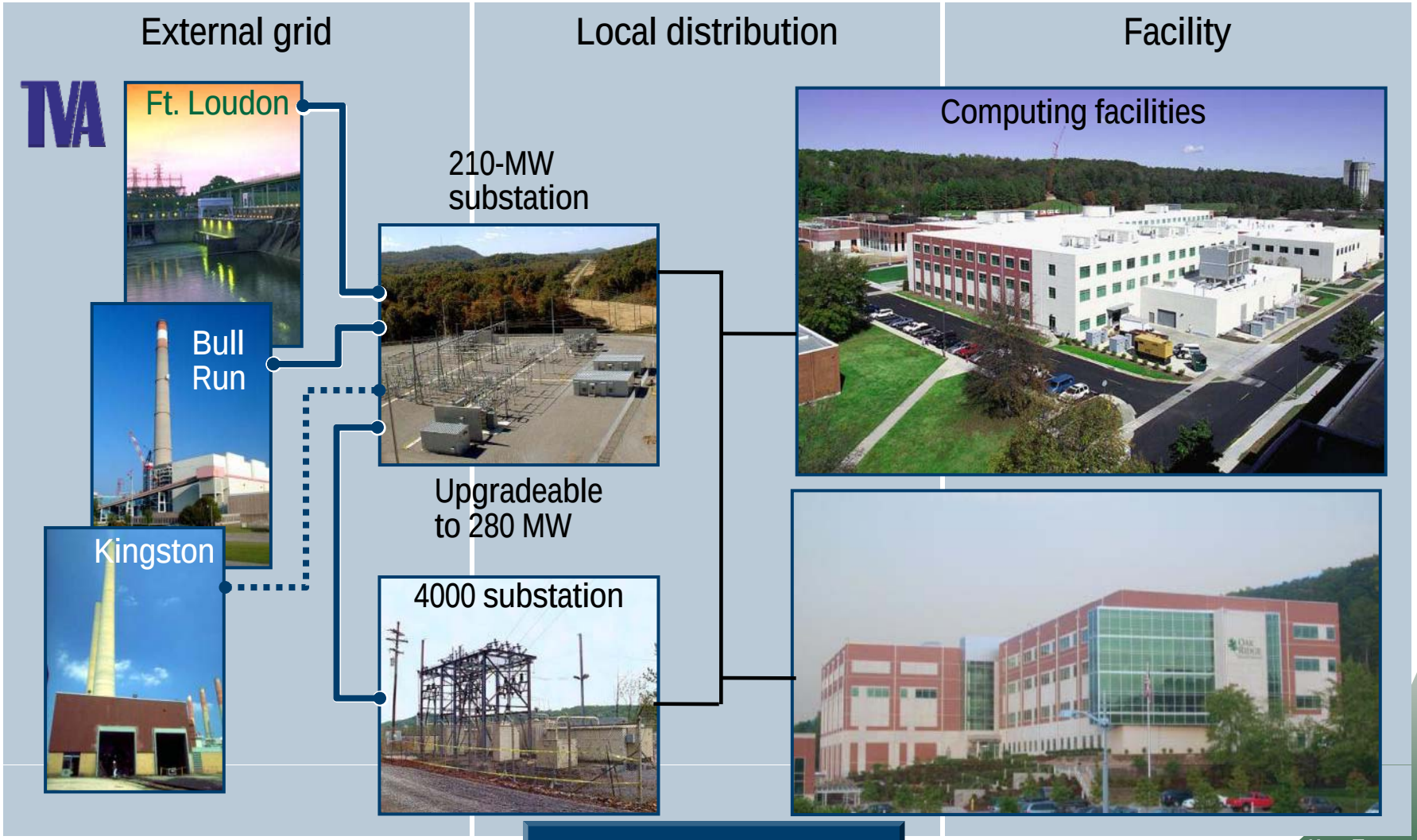
- 110K ft^2 classified; 110K ft^2 unclassified
- Shared mechanical & electrical infrastructure
- Build out 25K ft^2 on each side as needed
- Lights out facility



OAK RIDGE National Laboratory

State-of-the-art facility with ample, highly reliable, low-cost power

Infrastructure



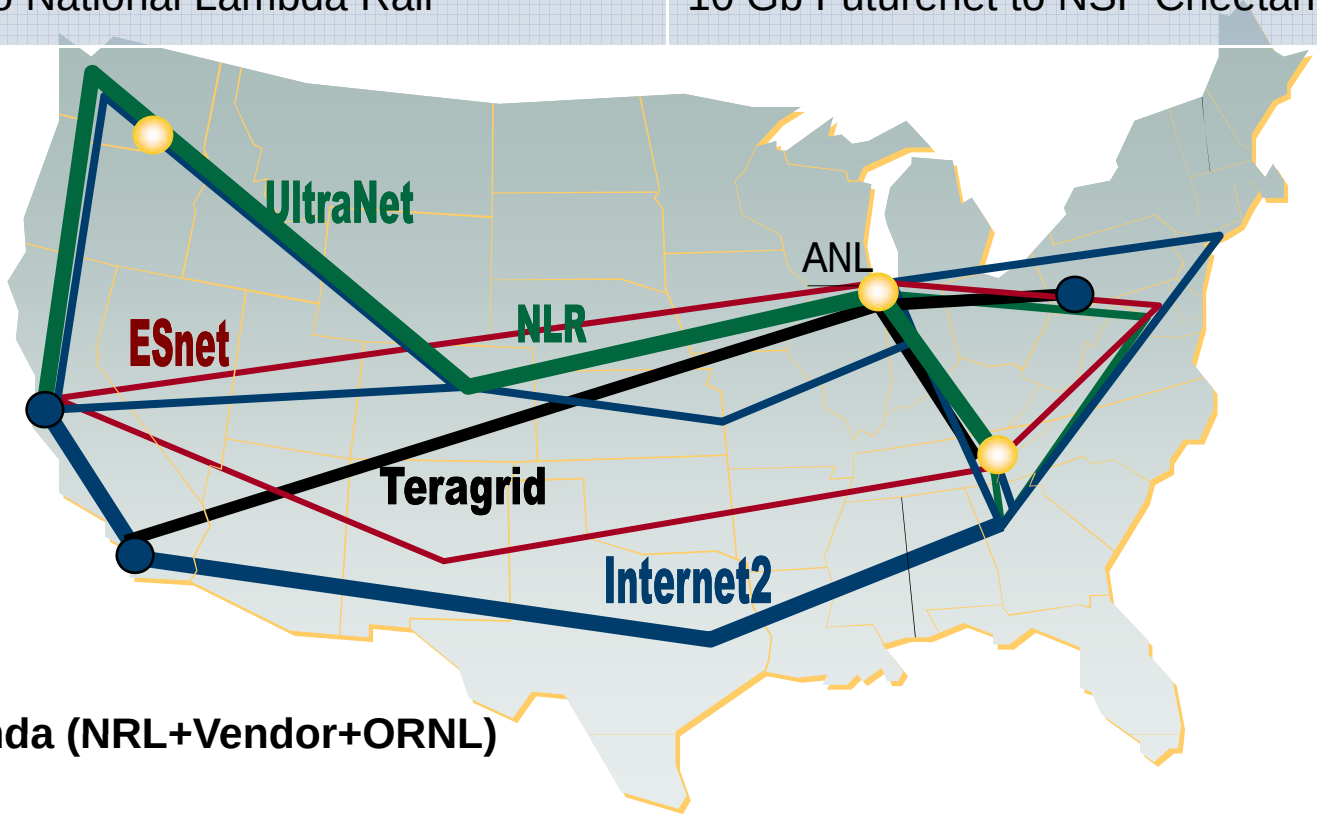
Estimated 50 MW

OAK RIDGE National Laboratory

High Bandwidth Connectivity to NCCS Enables Efficient Remote User Access

Infrastructure

Connected to Major Science Networks	
OC192 to ESNET with backup OC48	1 - 4 x 10 Gb to NSF Teragrid
10 Gb to Internet2	2 x 10 Gb UltraScienceNet
4 x 10 Gb to National Lambda Rail	10 Gb Futurenet to NSF Cheetah net



Target

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

National Center for Computational Sciences
Oak Ridge National Laboratory

Infrastructure

Mission: 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
- Deliver transforming discoveries in materials, biology, climate, energy technologies, etc.
- Ability to investigate otherwise inaccessible systems, from supernovae to energy grid dynamics

Jaguar – 1.64 PF Cray XT: 45,376 Quad-Core Processors, 362 TB memory

National Institute for Computational Sciences

A UT/ORNL PARTNERSHIP
NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES
NICS

Infrastructure

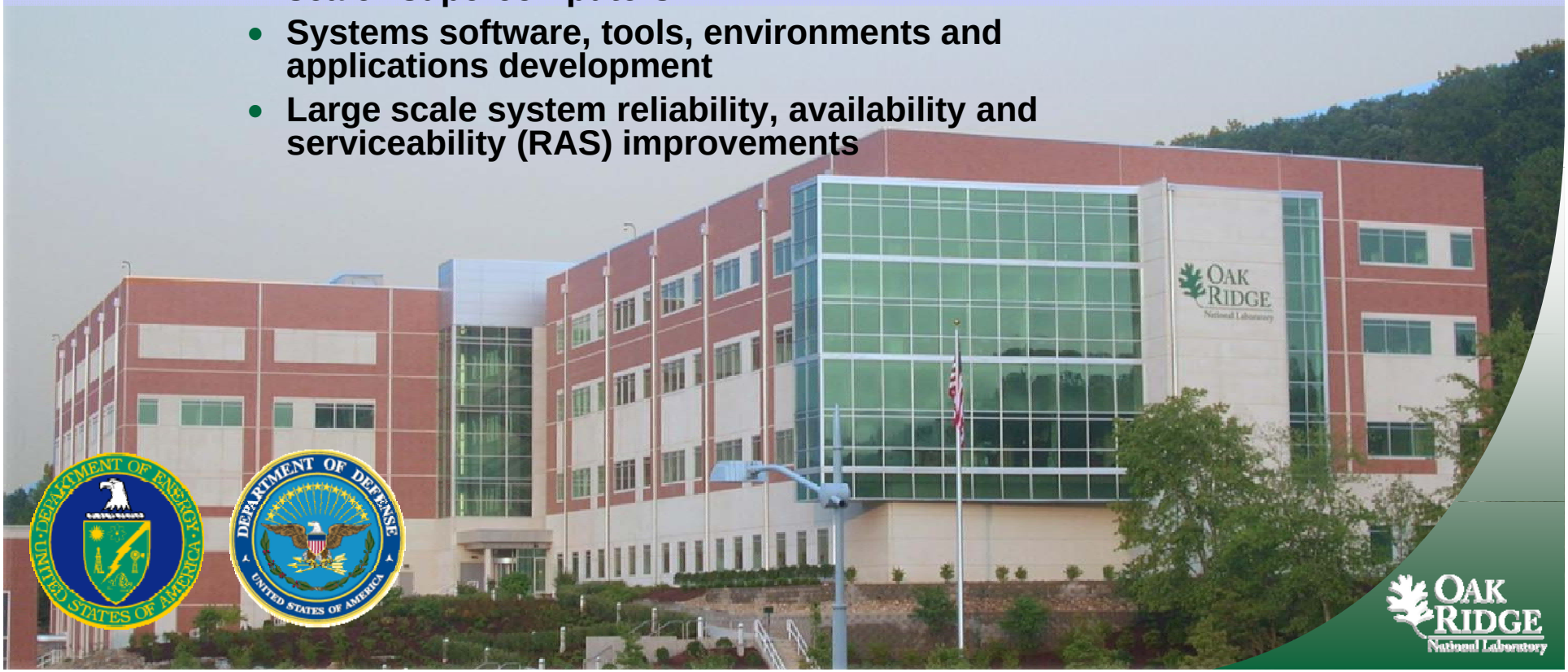
- **Awarded a $65M NSF grant to deploy and operate the world's most powerful academic supercomputer for the US research community**
- **NICS is a collaboration between the University of Tennessee and ORNL with facilities located on the ORNL campus**

ORNL / DOD HPC Collaborations

- **Peta/Exa-scale HPC Technology Collaborations in support of national security**
  - **System design, performance and benchmark studies**
  - **Wide-area network investigations**
  - **Extreme Scale Software Center**
    - **Focused on widening the usage and improving productivity the next generation of "extreme-scale" supercomputers**
    - **Systems software, tools, environments and applications development**
    - **Large scale system reliability, availability and serviceability (RAS) improvements**

Infrastructure

25 MW Power
8,000 Tons cooling
32,000 ft^2 raised floor



Current partnership with NOAA

Infrastructure

FY 2007

- Port existing models to ORNL LCF environment
- Benchmark computational performance

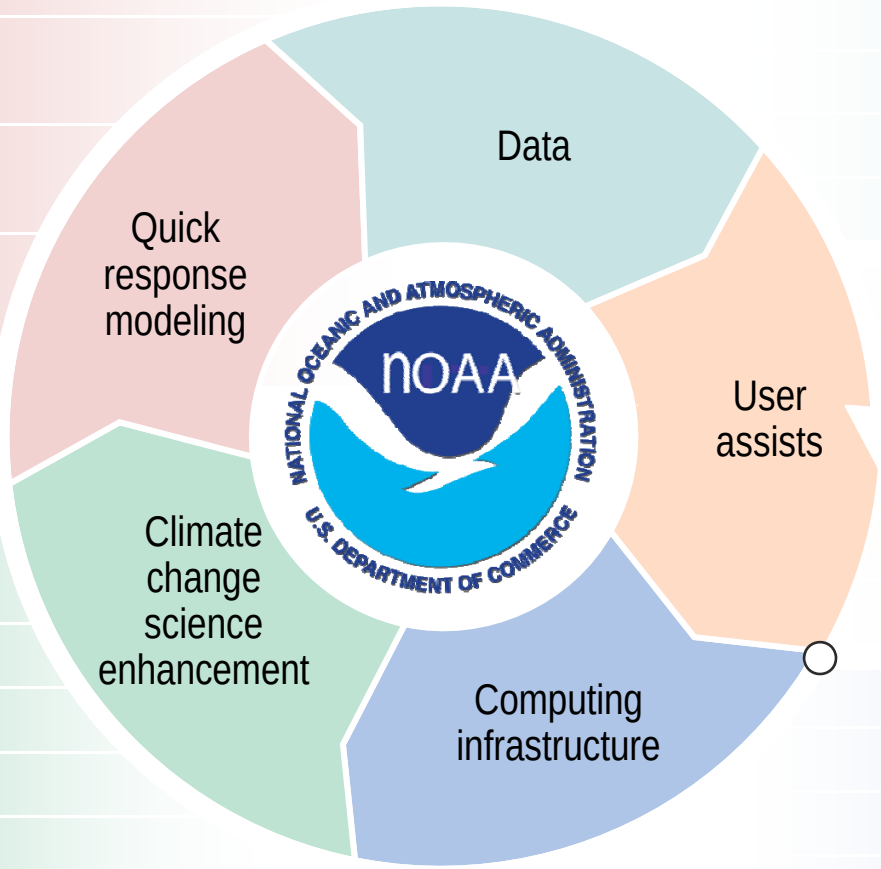
FY 2008

- System/software engineering to improve computational performance
- Evaluate potential for forecast (1–7 day) improvement from high-resolution models
  - Evaluate forecast performance
  - Evaluate computing strategy
  - Evaluate HPC requirement
- Evaluate potential for forecasting (8–60 day) hurricane genesis
- Evaluate potential for on-demand (surge) computing to support generation of high-resolution forecast guidance
  - Operations concept
  - Identify operational needs and requirements
  - Identify technical needs and requirements

We are positioning ourselves to be the lead computing lab for NOAA

Climate change	Scenario, topic, time period, location
Impacts	Topic, system, climate sensitivity
Adaptation	Topic, potentials, limits
Mitigation	Emissions, technologies, policies

Modeling and simulation	Climate change
	Impacts, adaptation
	Mitigation
Improving decision-related science	Uncertainties
	Thresholds
	Feedbacks
	Model coupling
	Integrating observations/ experiments with models



Infrastructure

- Regional climate projections
- Climate impacts
- GHG emissions (CDIAC)
- Adaptation possibilities
- ARM archive

- Visualization tools
- Expert system shells
- Semantic web searches
- Simplified models
- Climate End Station
- Scientific liaison to project

- Petascale computers
- Data analysis systems and tools
- 24x7 system and facility support
- Expert assistance with applications
- Gigabit to terabit per second networks
- Petabyte file systems and data archives

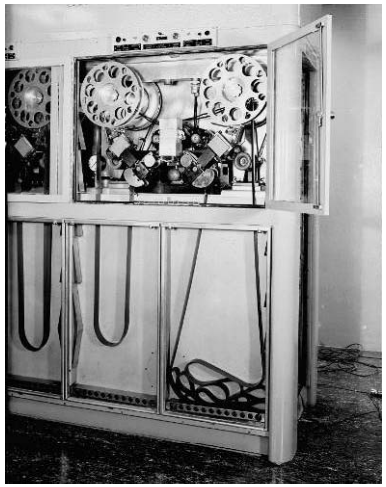
Oak Ridge Science and Technology Park:

New ways to work with our partners

- Establishing the first S&T park at a national laboratory
  - On-site presence: Universities, industry, other agencies
  - Construction of two ~100,000-ft^2 facilities is expected to begin during 2008
  - Lease rate of ~$20/sf + utilities
- Creating a 21st century research environment
- Leveraging an extensive set of partnerships
  - More than 600 industry partnerships, including TVA and Walden Reserve
  - More than 200 university partnerships, including NSF Track 2 computer
  - Leadership in local and regional economic development organizations, including Innovation Valley Inc.
- Building an entrepreneurial culture
- Providing access to venture capital

ORACLE: Oak Ridge Automatic Computer and Logical Engine (1954)

- System is a large scale and general purpose computer (*multiplied 12-digit numbers in less than 0.0005 seconds, and added the numbers in 0.00000005 sec*)
- Research and development tool for numerical analysis, programming techniques, and problems in physics, chemistry, engineering and biology
- Methods have been developed for solving linear equations, matrix inversions, computing eigenvalues and vectors of matrices, solution of reactor problems involving ordinary and partial differential equations
- Monte Carlo techniques have been designed and applied to problems in health physics and shielding
- Many "one of a kind" problems are solved which involve methods mentioned above as well as function evaluation, interpolation and statistical analysis
- In the last few years much effort has gone into data processing, data handling and reduction.



The building engineer had to warn the computer operators to save information to magnetic tape before he started up the air conditioning system, otherwise the power surge would wipe out the memory

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

computing

1 — One OPS

10^3 — KiloOPS

10^6 — MegaOPS

10^9 — GigaOPS

10^{12} — TeraOPS

10^{15} — 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

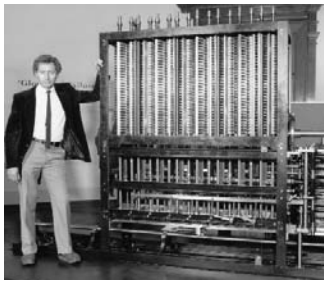
1997 ASCI Red

2001 Earth Simulator

2003 Cray X1

2005 Cray XT3

2008 Cray XT5



Million-fold increase in computing and data capabilities in the last 5 years!

computing

2004

Cray X1
3 TF

2005

Cray XT3
Single-core
26 TF

2006

Cray XT3
Dual-core
54 TF

2007

Cray XT4
119 TF

2008

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

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

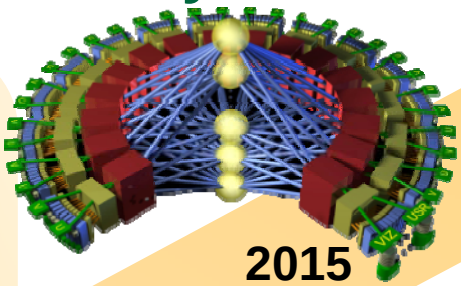
2009

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

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

2011

DARPA
HPCS
20 PF

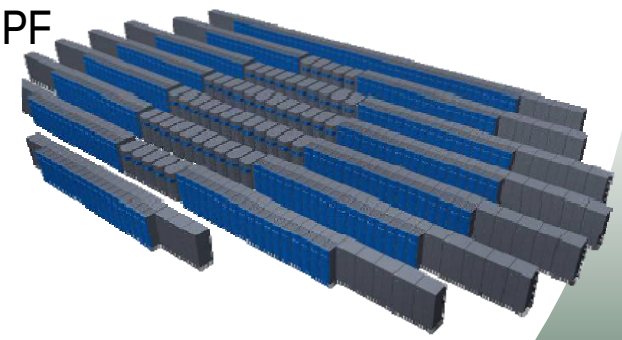


2015

Future
system
100–250 PF

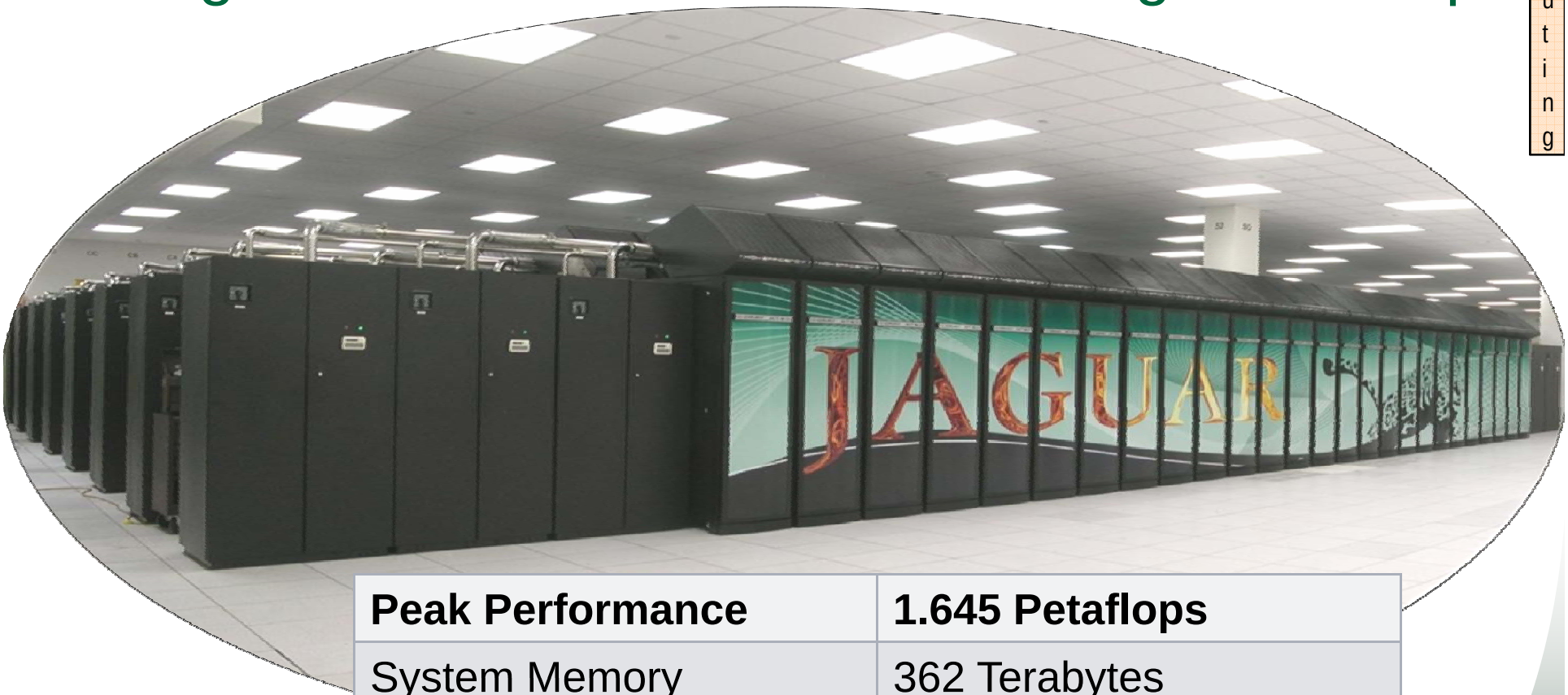
2018

Future
system
1000 PF
(1 EF)



Jaguar: World's most powerful computer. Designed for science from the ground up

computing



Peak Performance	**1.645 Petaflops**
System Memory	362 Terabytes
Disk Space	10.7 Petabytes
Disk Bandwidth	240+ Gigabytes/second
Interconnect Bandwidth	532 Terabytes/second

OAK RIDGE National Laboratory

High Performance Linpack Benchmark

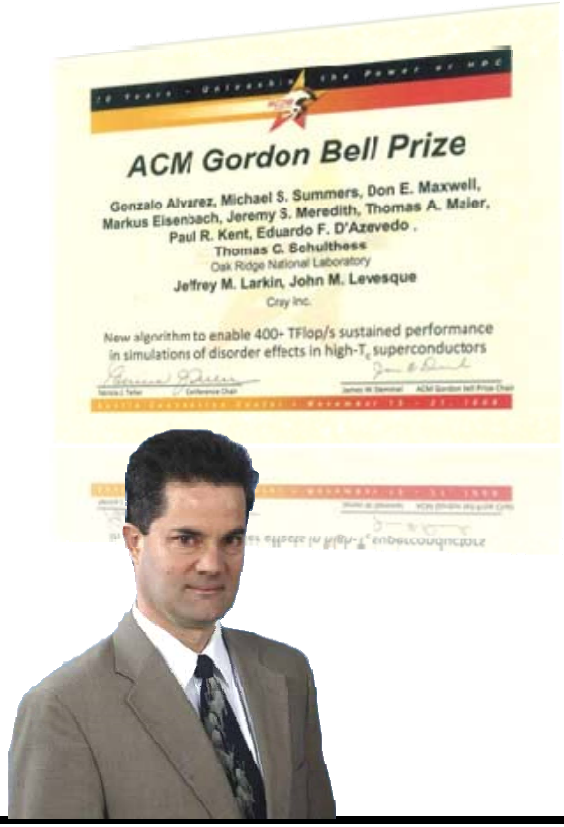
- **#2 on November 2008 list**
- **1059 TeraFLOPS (76.7% of peak)**
- **Ran on 150,152 cores**
- **Largest HPL run ever, by a huge margin**
- **Ran on the XT5 portion of the machine *41 days after delivery of a 200 cabinet system!!!***
- ***Ran for 18.3 hours without a failure!!!!***

```
T/V                N    NB     P     Q               Time             Gflops
--------------------------------------------------------------------------------
WR03R3C1     4712799   200   274   548           65884.80           1.059e+06
--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV--VVV-
Max aggregated wall time rfact . . . :              13.67
+ Max aggregated wall time pfact . . :              10.99
+ Max aggregated wall time mxswp . . :              10.84
Max aggregated wall time pbcast  . . :            6131.91
Max aggregated wall time update  . . :           63744.72
+ Max aggregated wall time laswp . . :            7431.52
Max aggregated wall time up tr sv  . :              16.98
--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=        0.0006162 ...... PASSED
================================================================================
```

Gordon Bell prize awarded to ORNL team

Materials simulation breaks 1.3 petaflops

- A team led by ORNL's Thomas Schulthess received the prestigious 2008 Association for Computing Machinery (ACM) Gordon Bell Prize at SC08
- The award was given to the team for attaining the fastest performance ever in a scientific supercomputing application
- The team achieved 1.352 petaflops on ORNL's Cray XT Jaguar supercomputer with a simulation of superconductors
- By modifying the algorithms and software design of the DCA++ code, the team was able to boost its performance tenfold



HPC Challenge Benchmarks

Four "Class 1" benchmarks:

• **HPL**	**902 TFLOPS**	**#1**
• **G-Streams**	**330**	**#1**
• **G-Random Access**	**16.6 GUPS**	**#1 Baseline**
• **G-FFTE**	**2773**	**#3**

Working on further optimizations, but just ran out of time.

A balanced, high performance supercomputer.

Early Science Applications

Science Area	Code	Contact	Cores	% of Peak	Total Perf	Notes	Scaling
Materials	DCA++	Schulthess	150,144	97%	1.3 PF*	Gordon Bell Winner	Weak
Materials	LSMS/WL	ORNL	149,580	76.40%	1.05 PF	64 bit	Weak
Seismology	SPECFEM3D	UCSD	149,784	12.60%	165 TF	Gordon Bell Finalist	Weak
Weather	WRF	Michalakes	150,000	5.60%	50 TF	Size of Data	Strong
Climate	POP	Jones	18,000		20 sim yrs/ CPU day	Size of Data	Strong
Combustion	S3D	Chen	144,000	6.00%	83 TF		Weak
Fusion	GTC	PPPL	102,000		20 billion Particles / sec	Code Limit	Weak
Materials	LS3DF	Lin-Wang Wang	147,456	32%	442 TF	Gordon Bell Winner	Weak

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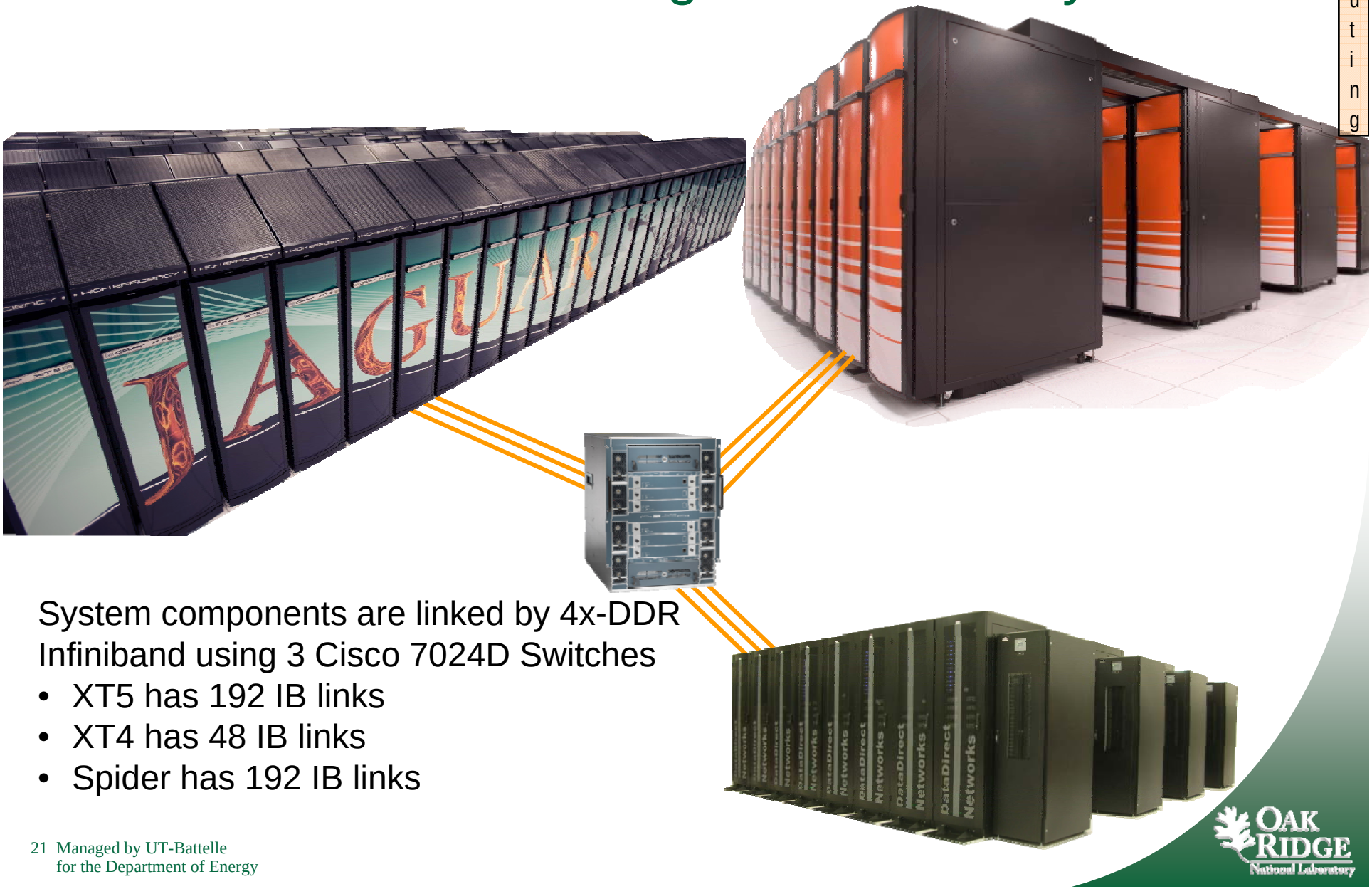
Jaguar combines a new 1.38 PF Cray XT5 with the existing 263 TF Cray XT4



System components are linked by 4x-DDR Infiniband using 3 Cisco 7024D Switches

- XT5 has 192 IB links
- XT4 has 48 IB links
- Spider has 192 IB links

Kraken

A UT/ORNL PARTNERSHIP
NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES
NICS

computing

Initial Delivery: April 2008

- **4,512 Opteron quad-core processors**
- **18 TeraBytes of memory**
- **166 TeraFLOPs**

TOP500® SUPERCOMPUTER SITES

#15
Nov. 2008

OAK RIDGE National Laboratory

Kraken Upgrade
World's Most Powerful Academic Supercomputer

A UT/ORNL PARTNERSHIP
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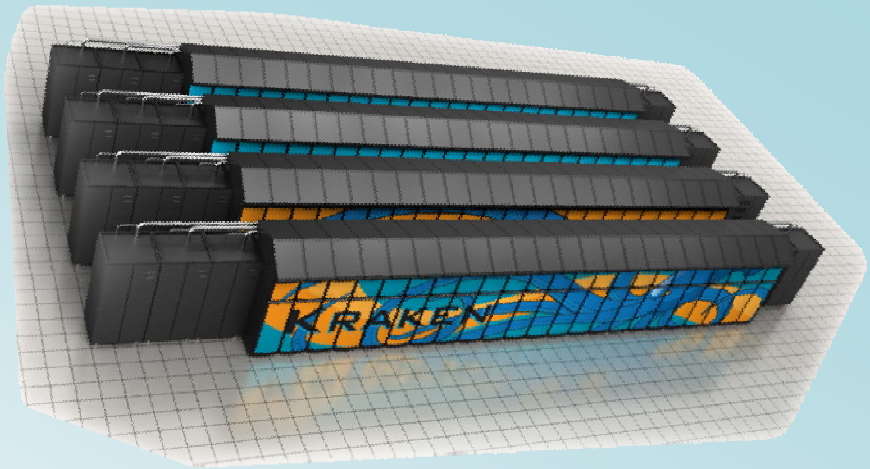
NICS

computing

Cray XT5 system - Kraken

- **In acceptance testing**
- **88 cabinets**
- **8,256 dual-socket nodes**
- **16,512 quad-core Opterons**
- **66,048 cores**
- **100 TB memory**
- **SeaStar2+ interconnect**
- **30 GB/s disk bandwidth**
- **3.3 PB disk (2.6 formatted)**
- **600+ peak TFLOPS**
- **Plan to upgrade to 6-core chips in 2009**



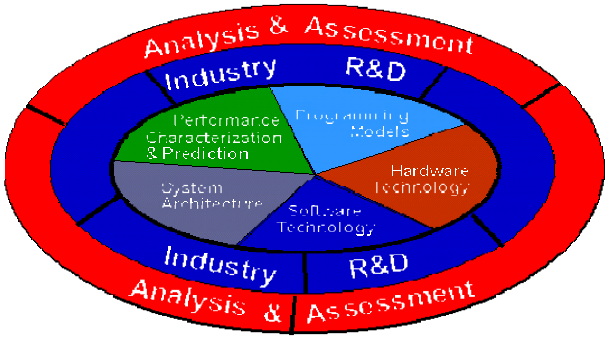
OAK RIDGE National Laboratory

We are partners in the $250M DARPA HPCS program

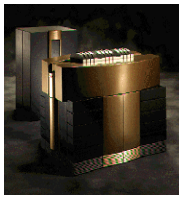
Prototype Cray system to be deployed at ORNL

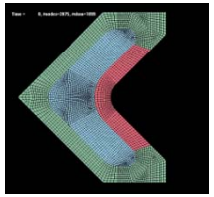
Impact:

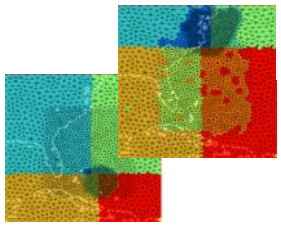
- **Performance** (time-to-solution): Speed up critical national security applications by a factor of 10× to 40×
- **Programmability** (idea-to-first-solution): Reduce cost and time of developing application solutions
- **Portability** (transparency): Insulate research and operational application software from system
- **Robustness** (reliability): Apply all known techniques to **protect against outside attacks**, hardware faults, and programming errors

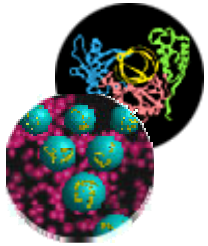


HPCS program focus areas









Applications:

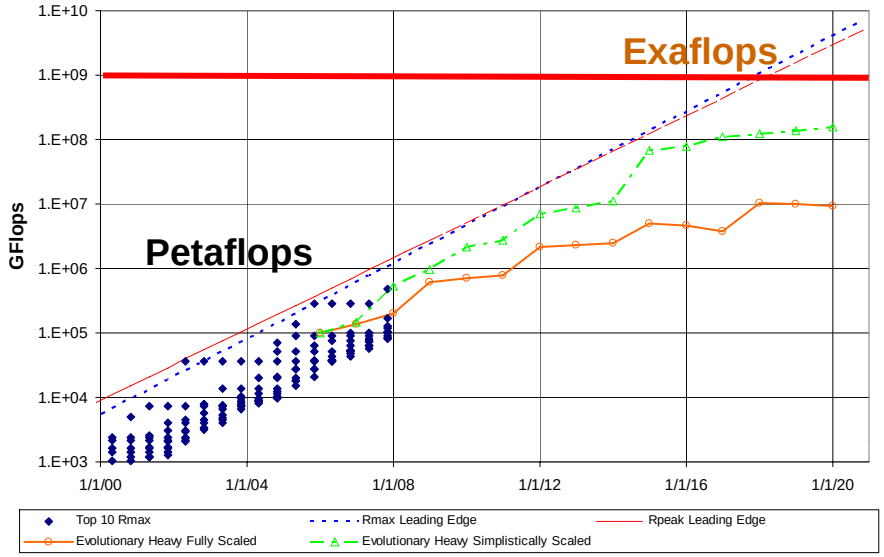
- Intelligence/surveillance, reconnaissance, cryptanalysis, weapons analysis, airborne contaminant modeling, and biotechnology

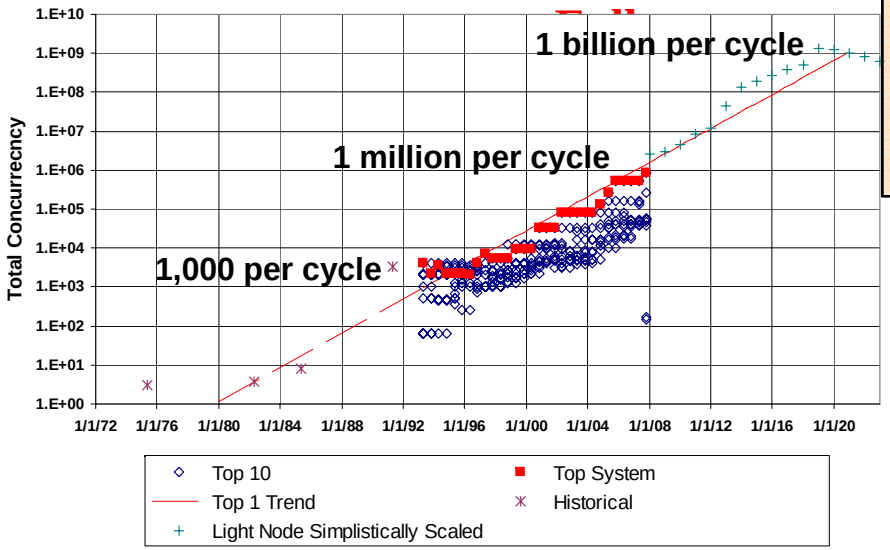
Fill the Critical Technology and Capability Gap
Today (late 80s HPC technology) ➔ Future (Quantum/Bio Computing)

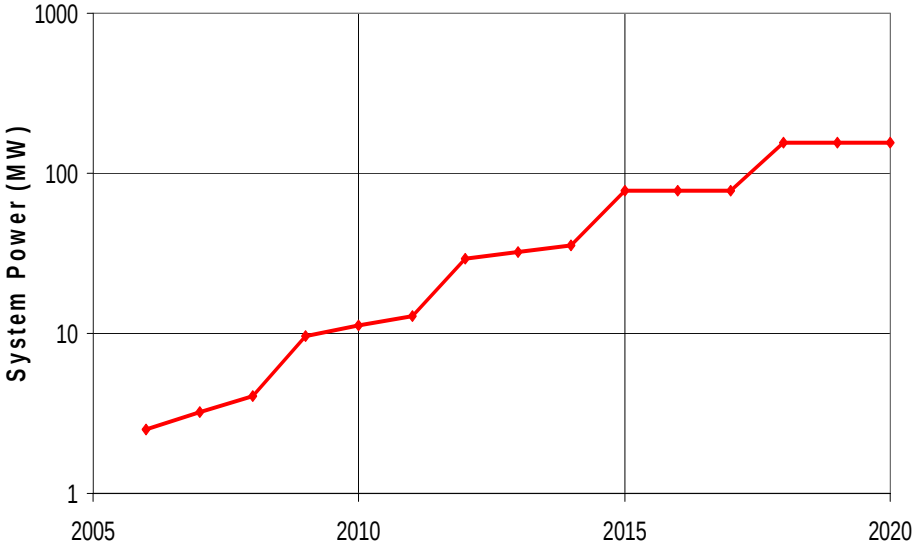
Slide courtesy of DARPA

What do we have to look forward to?

Possible System/Power Models Beyond DARPA HPCS







- **Developing these systems will be really challenging in any time frame**
- **4 key challenge areas**
  - **Power: (75MW to 250MW)**
  - **Water**
  - **Concurrency: Billion fold (software)**
  - **Memory Capacity**
  - **Resiliency**
- **Will require sustained, coordinated, multi-agency collaborations**
  - **Especially in software**

Exponential growth in data at ORNL

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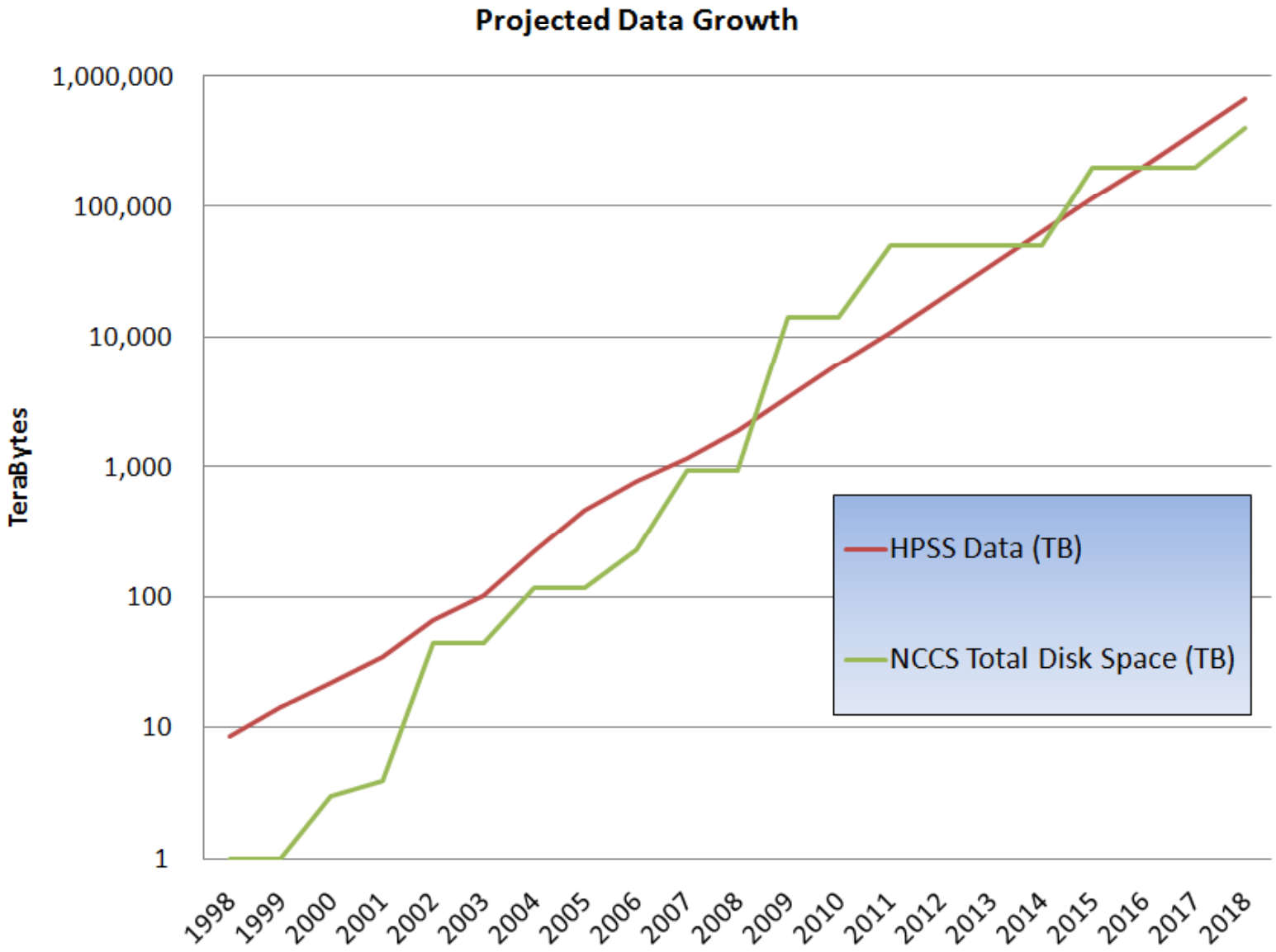

Storage for an avalanche of data

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Center wide shared file systems

- **"Spider" will be available later this year to provide a shared, parallel file system for all LCF systems**
  - **Based on Lustre file system**

Planned bandwidth of over 200 GB/s with multi-petabytes (10 PB) of capacity

- **HPSS provides archival storage for all system**
- **HPSS has been upgraded with two additional tape libraries to add additional capacity and bandwidth**

OAK RIDGE National Laboratory

Visualization and Data Analytics

d a t a

Visualization

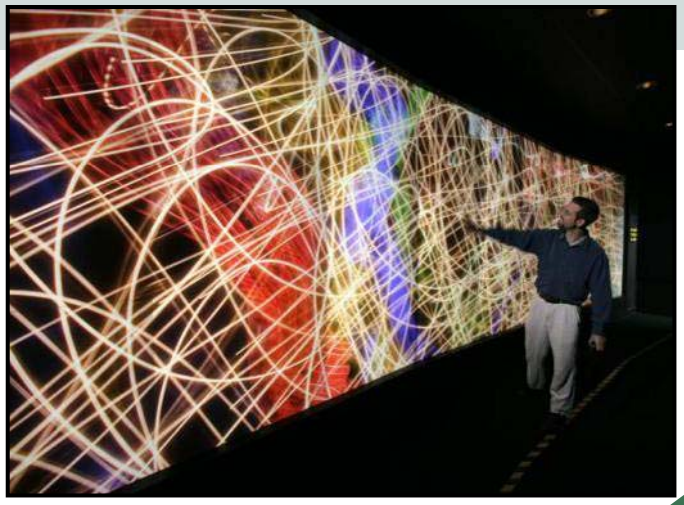
Once users have completed their runs, the Visualization task group helps them make sense of the sometimes overwhelming amount of information they generate.

- Viewing at a 30'x8' PowerWall
- Upgraded cluster with GPUs for remote visualization

End-to-End Solutions

Researchers must analyze, organize, and transfer an enormous quantity of data. The End-to-End task group streamlines the work flow for system users so that their time is not eaten up by slow and repetitive chores.

- Automate routine activities, ex. job monitoring at multiple sites
- Data Analysis



We are leveraging expertise in knowledge discovery for national security

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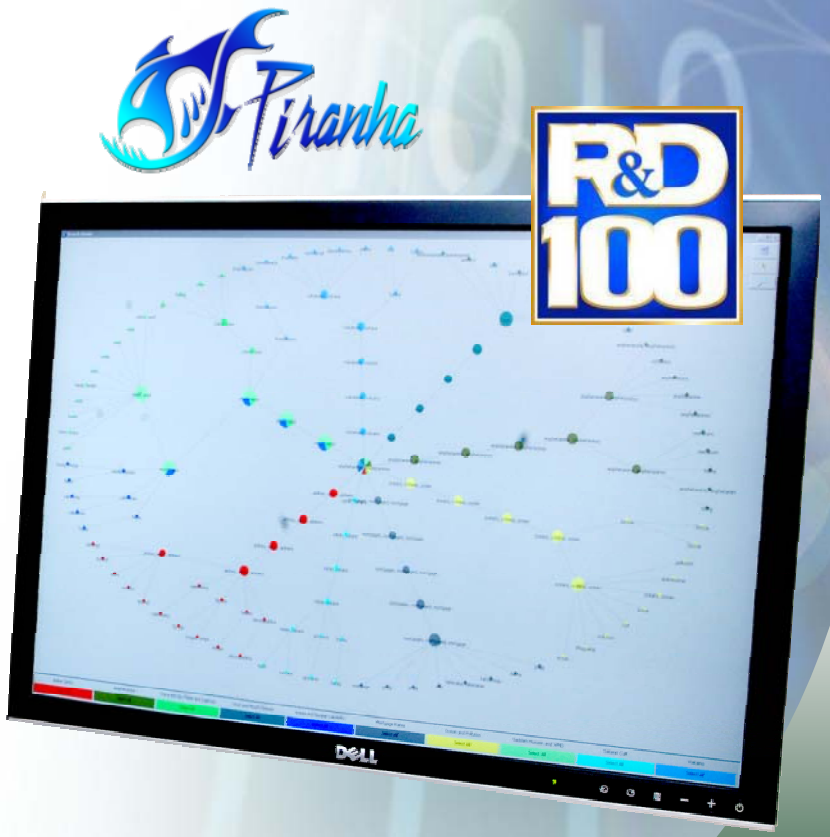
KD Focus

- Actionable insights from massive, dynamic, disparate data sources
- Ability to ask more complex questions and detect more complex processes using increasingly higher data resolution

Targeted KD Research

- High-speed analysis of text, video, audio, digital, and sensor data
- Geospatial science and technology
- Data-driven modeling and simulation to discover underlying social and physical processes
- Quantum information science
- Data quality, provenance, and security
- Hypothesis generation, deception detection, and threat anticipation



Data science strategy

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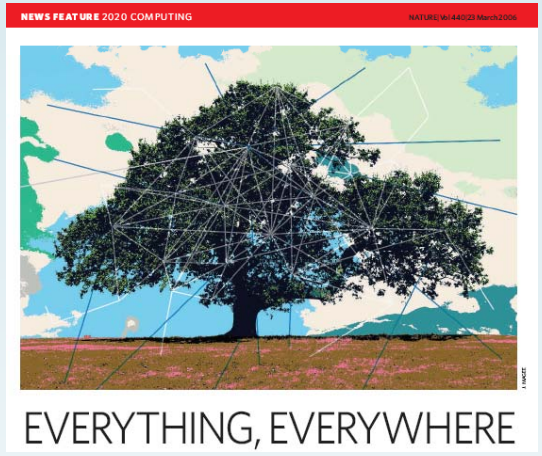
Opportunity:

- Leverage our strong Knowledge Discovery presence within the scientific community and national security applications
- Impact scientific discoveries in national security, energy, basic sciences, and biomedical sciences



ORNL resources:

- Distributed data systems testbed from SensorNet
- Experimental data from SNS, HFIR, etc
- High-speed data storage systems for HPC simulation results
- Data visualization platforms – EVEREST, etc
- Classified data systems and networks
- Key recent hires in:
  - Data fusion
  - Remote imaging mining
  - Extreme value predictions
  - High-performance data clustering
  - Data streaming analysis
  - Complex disparate data

Strategy:

- Expand KD thrust beyond national security applications
- Build world-class distributed systems testbed
- Expand our data storage systems capabilities
- Proactive collaboration with NSF
- Continue key hires

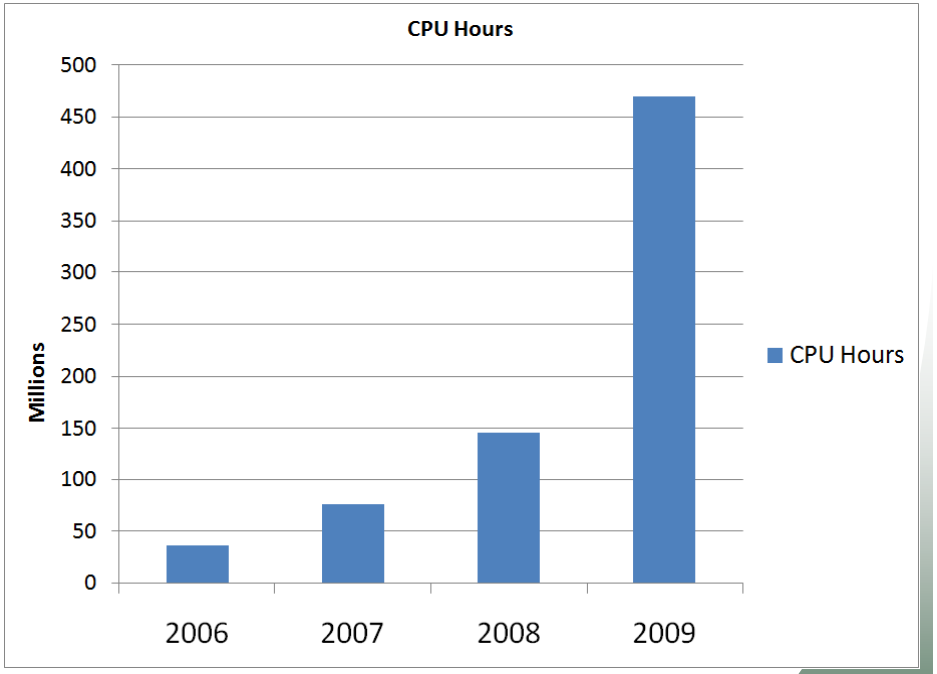
Outcome: ORNL recognized as leader in data sciences

DOE's INCITE Program

operations

- **The INCITE program grants large blocks of time to a few nationally important projects.**
- **Projects are selected through scientific peer review**
- **Call for proposals open to academic, industry, and government researchers**
- **NCCS also provides discretionary allocations for scientists and engineers who want to port, scale, and use their applications codes for cutting-edge research**
  - **For INCITE preparation, industrial collaboration, and strategic partnerships**

Office of Science
U.S. DEPARTMENT OF ENERGY
INCITE
Advancing America's Science and Industrial Competitiveness



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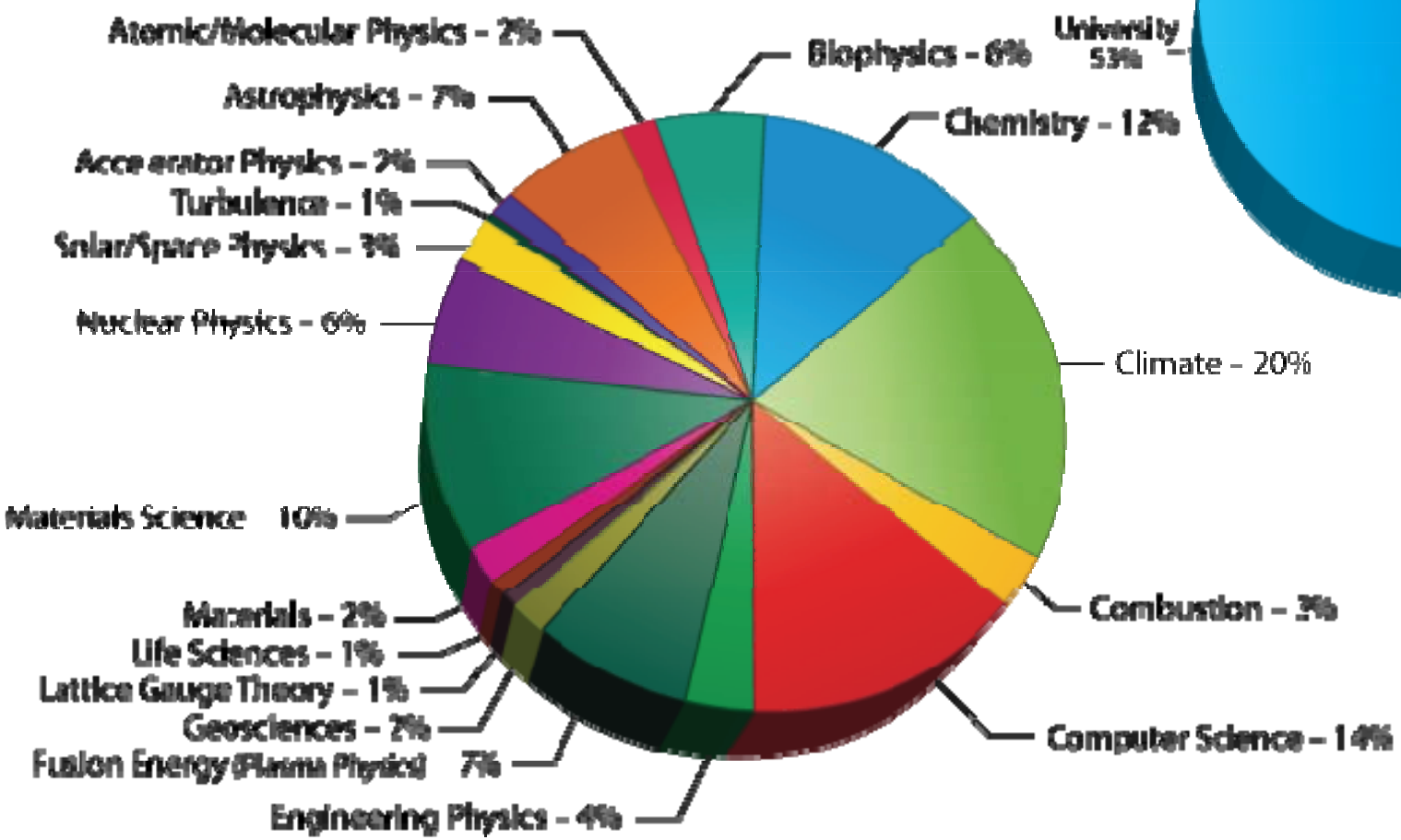
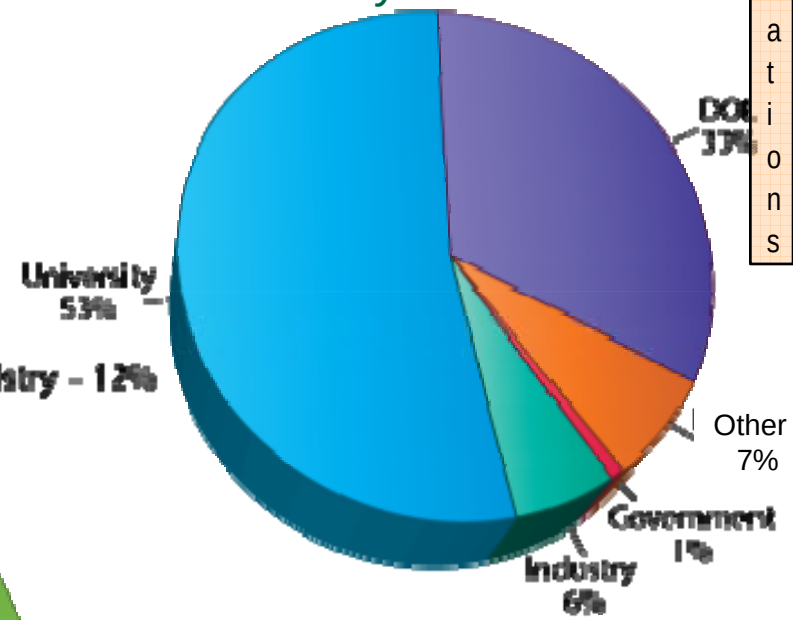
NCCS 2008 INCITE Program

NCCS Allocations by Discipline



Active NCCS Users by affiliation



operations

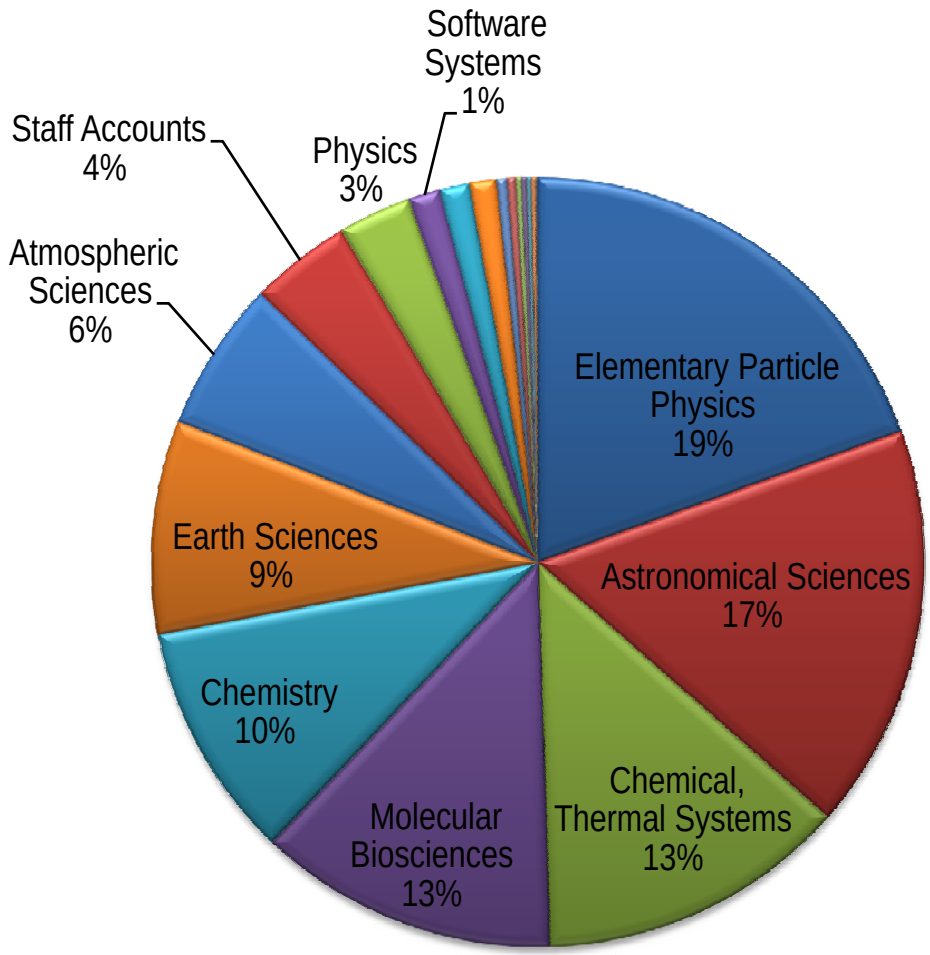
NICS system: Access and allocations

operations

- **Primarily NSF-funded**
  - **80% allocable via the TeraGrid (national allocation)**
- **Hosted and supported by UT-ORNL JICS**
  - **8% at PI's discretion for regional institutions, from R1s to JuCos, nonprofit research institutions, or state or local agencies**
  - **Excellent EOT opportunities**
- **Fosters academic/industry collaborations and tech transfer**
  - **5% at PI's discretion for industrial collaborations**
- **Fosters discovery and innovation**
  - **5% at PI's discretion to further research or education in the national science and engineering community and to broaden participation in high-performance computing**
  - **2% at PI's discretion to broaden participation of MEIs**

Kraken is over-requested by 2:1

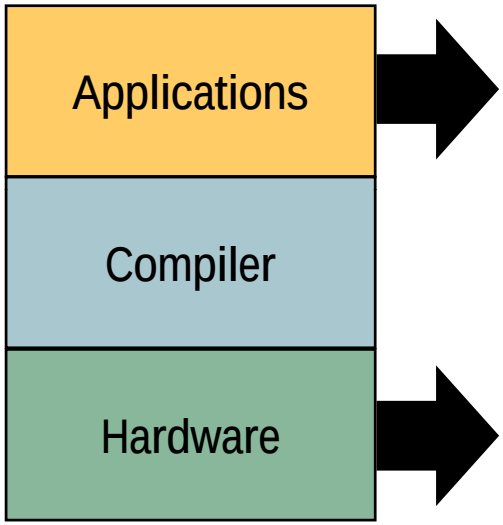
- Over 26.8M hours delivered from August through December 2008
- Over 600 users and 100 projects

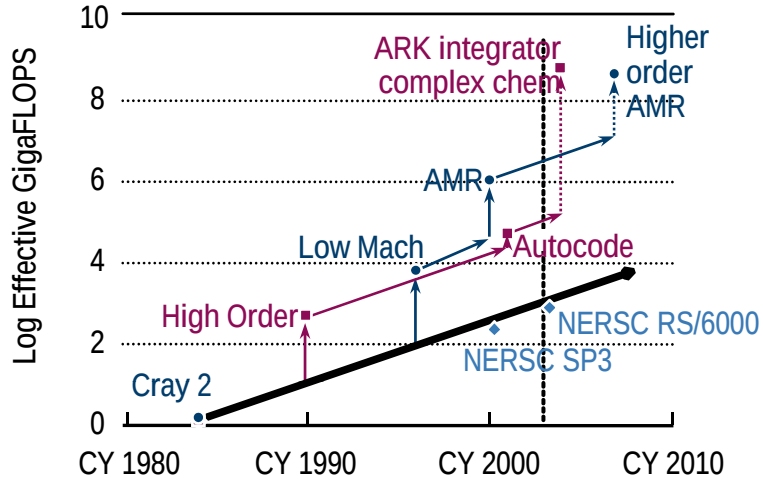


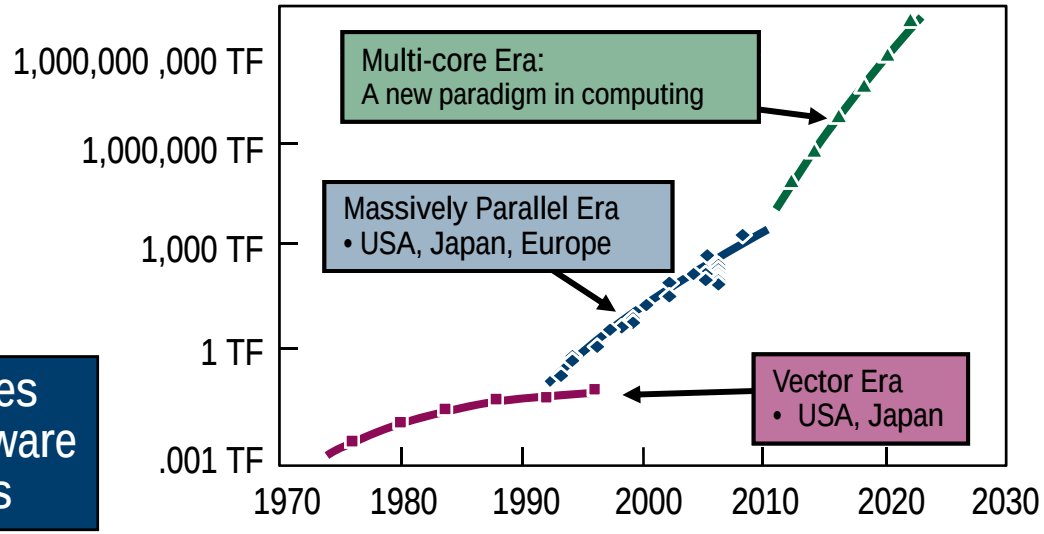
- Elementary Particle Physics
- Astronomical Sciences
- Chemical, Thermal Systems
- Molecular Biosciences
- Chemistry
- Earth Sciences
- Atmospheric Sciences
- Staff Accounts
- Physics
- Software Systems
- Advanced Scientific Computing
- Materials Research
- Computer and Computation Research
- Cross-Disciplinary Activities
- Mechanical and Structural Systems
- Electrical and Communication Systems
- Environmental Biology
- Microelectronic Information Processing Systems
- Integrative Biology and Neuroscience
- Design and Manufacturing Systems

operations

Understanding the hardware and the applications are equally important

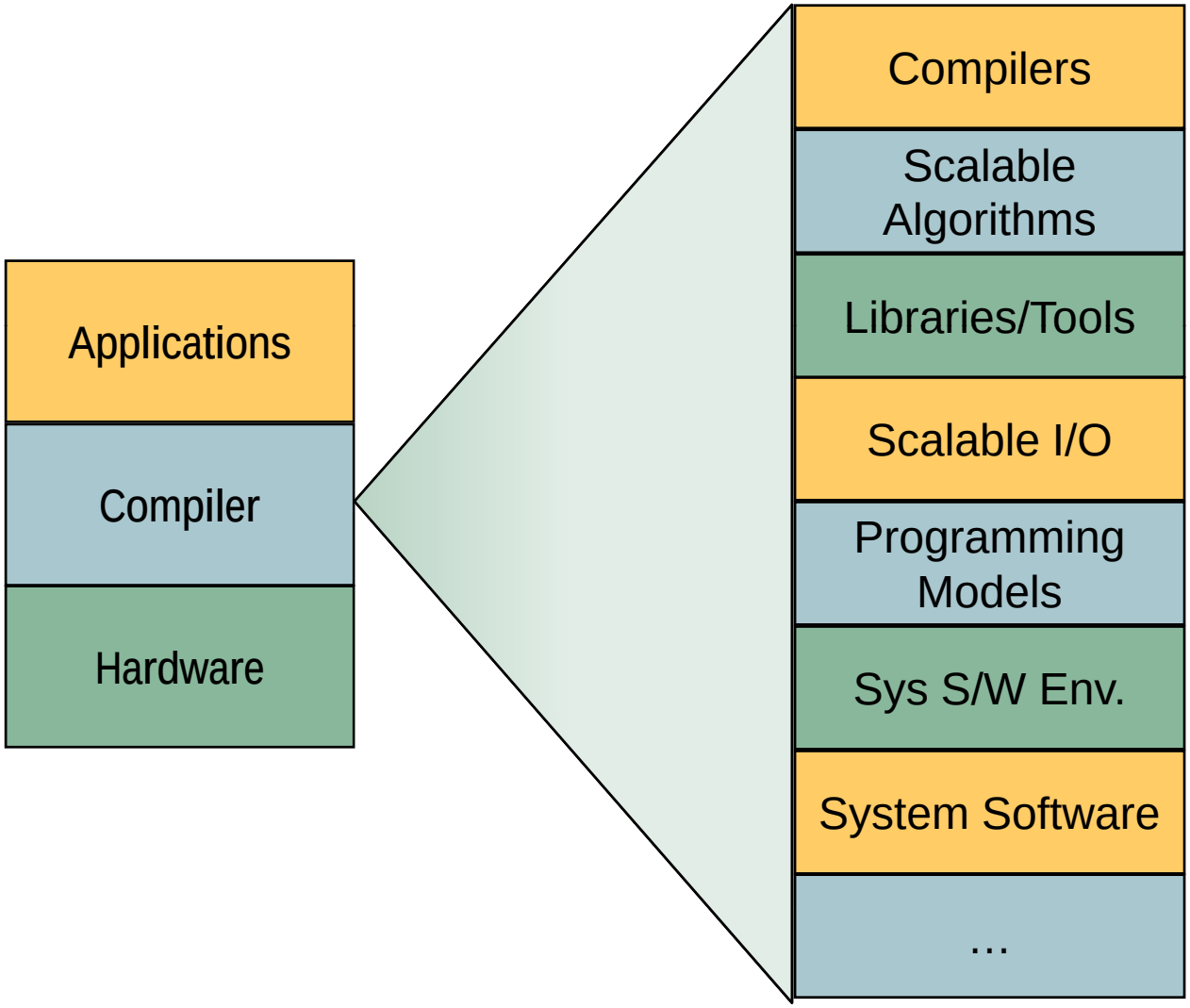






"Effective speed" increases came from both faster hardware and improved algorithms

Understanding and Developing "Middleware" is Key to Delivering Scalable Efficiency



Institute for Advanced Architectures and Algorithms

- **Jointly with SNL**
- **DOD is a member of the governing board**
- **Architectures and applications co-designed to create synergy in their respective evolutions**
- **Focused R&D on key impediments to high performance in partnership with industry and academia**
- **Foster the integrated co-design of architectures and algorithms to enable more efficient and timely solutions to mission critical problems**
- **Partner with other agencies (e.g., DARPA, DoD …) to leverage our R&D and broaden our impact**
- **Deploy prototypes to prove the technologies that allow application developers to explore these architectures and to foster greater algorithmic richness**

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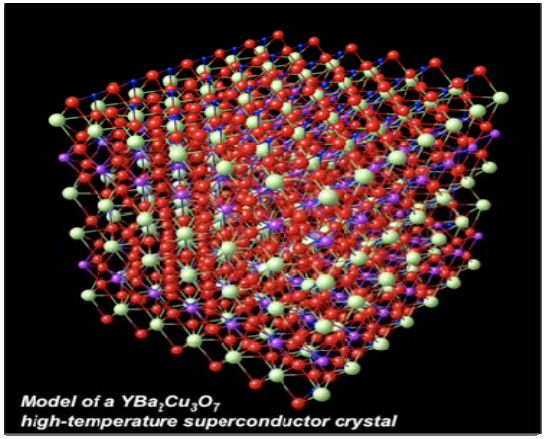
Extreme Scale Software Center (ESSC)

C S & M a t h

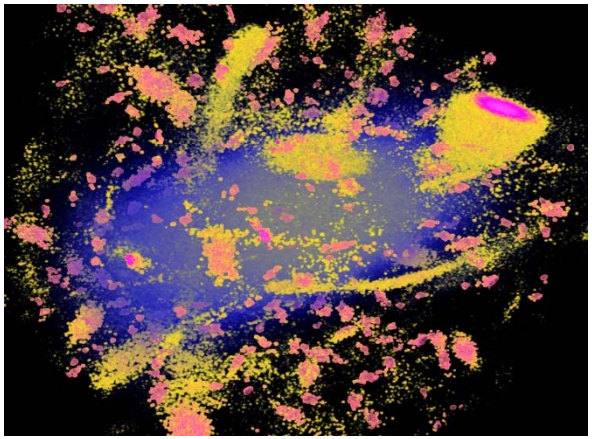
Application Performance Studies	• Modeling and Analysis of applications and kernels on large SMP's, large Clusters, SPD's – Selected kernels are supplied by DOD • Database Analysis (Analytics repository, Data base analysis of sensor data from extreme scale systems to improve resilience of these systems) • Languages (HPCS (X10, Chapel, Fortress), UPC, OpenSHMEM) – Productivity/programmability (all apps/kernels are converted to new languages)
Networking and I/O Analysis and Deployment (WAN, LAN, Interconnect, Sensors)	• 100 Gb/Lambda Long Haul (Development) • USN is a "dark fiber" ORNL controls end-to-end technology (unlimited scenarios) • Cyber Security , Dynamic performance analysis
System Software Tools	• Development Environments (Compiler analysis, Common Software Infrastructure…) • Resource Manager/Job Schedulers (Graph Analytics, Optimization, Analytics, Topology and power aware…)
RAS at Scale (Reliability, Availability, Serviceability)	• System, I/O, Network, Applications, Environment (Power, Space and Cooling and Analytics) • Power Management, Analysis, Modeling and Prediction (Optimization and Graph Analytics) • Power/location aware computing (Sensors, Analytics, Databases…)
Advanced Technologies / Architectures (NOT Cloud Computing)	• SPD's, Sensor Fusion, Analytics, Hybrid Computing, C64, memory technologies, disruptive technologies, Special Projects

Advancing scientific discovery

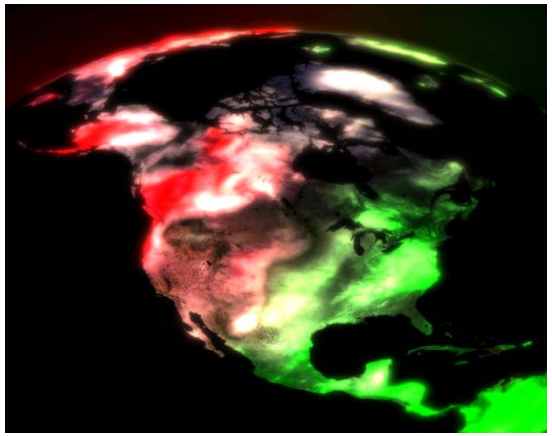
5 of top 10 ASCR science accomplishments in the past 18 months used LCF resources and staff



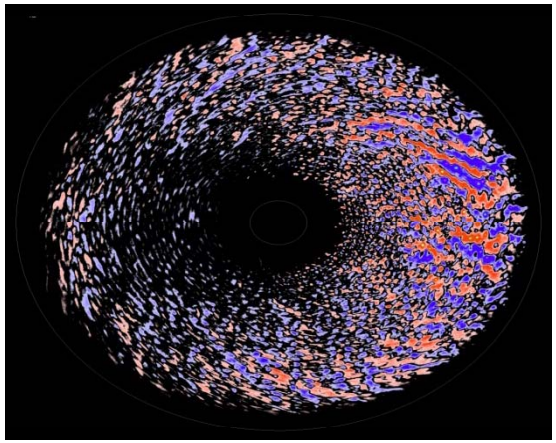
Electron pairing in HTSC cuprates
PRL (2007, 2008)



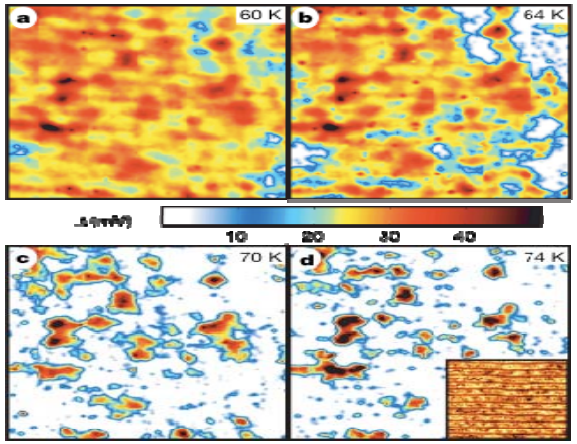
Shining a light on dark matter
Nature 454, 735 (2008)



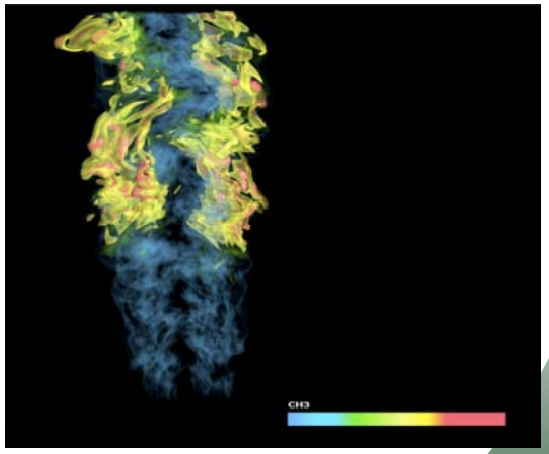
Modeling the full earth system



Fusion: Taming turbulent heat loss
PRL 99, *Phys. Plasmas* 14



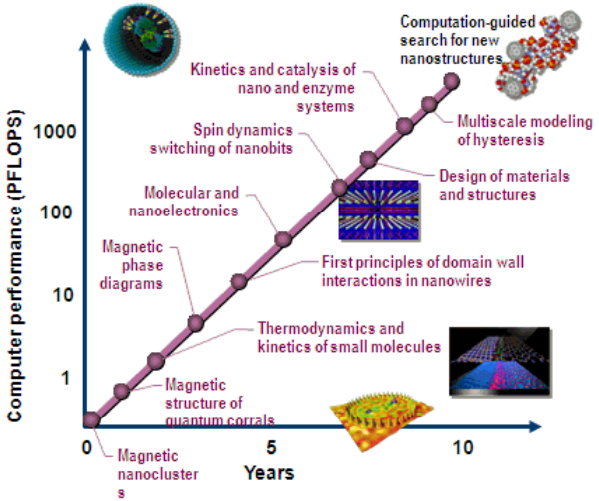
Nanoscale nonhomogeneities in high-temperature superconductors
Candidate for Gordon Bell prize



Stabilizing a lifted flame
Combust. Flame (2008)

Scalable Applications

Science Roadmaps



Nanoscience

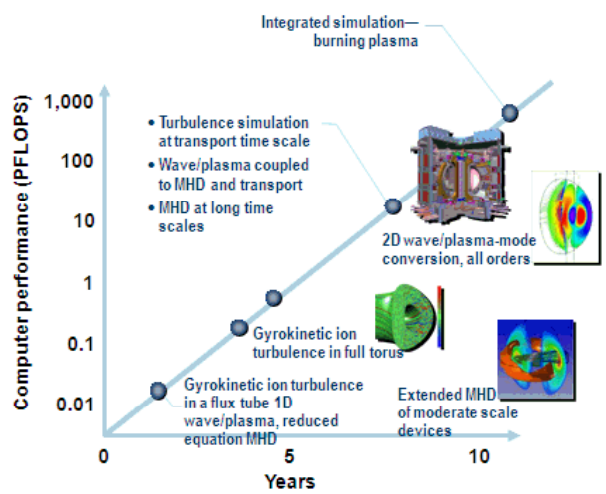
Expected outcomes

5 years

- Realistic simulation of self-assembly and single-molecule electron transport
- Finite-temperature properties of nanoparticles/quantum corrals

10 years

- Multiscale modeling of molecular electronic devices
- Computation-guided search for new materials and nanostructures



Fusion

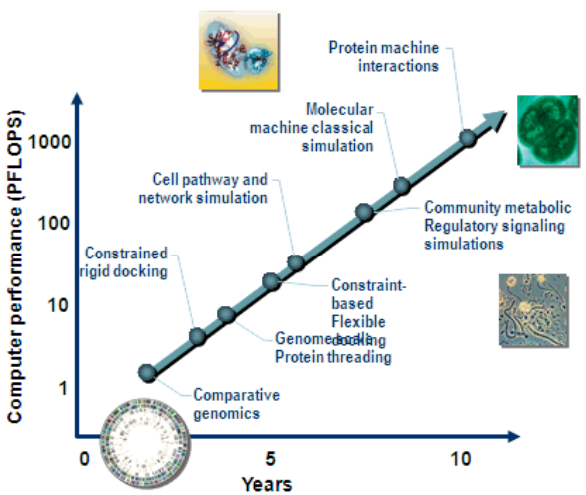
Expected outcomes

5 Years

- Full-torus, electromagnetic simulation of turbulent transport with kinetic electrons for simulation times approaching transport time-scale
- Develop understanding of internal reconnection events in extended MHD, with assessment of RF heating and current drive techniques for mitigation

10 years

- Develop quantitative, predictive understanding of disruption events in large tokamaks
- Begin integrated simulation of burning plasma devices –



Biology

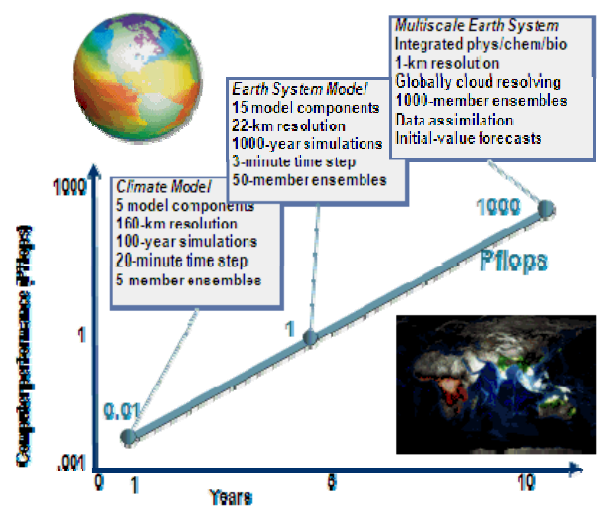
Expected outcomes

5 years

- Metabolic flux modeling for hydrogen and carbon fixation pathways
- Constrained flexible docking simulations of interacting proteins

10 years

- Multiscale stochastic simulations of microbial metabolic, regulatory, and protein interaction networks
- Dynamic simulations of complex molecular machines



Climate

Expected outcomes

5 years

- Fully coupled carbon-climate simulation
- Fully coupled sulfur-atmospheric chemistry simulation

10 years

- Cloud-resolving 1-km spatial resolution atmosphere
- Fully coupled, physics, chemistry, biology earth system model

Scalable Applications

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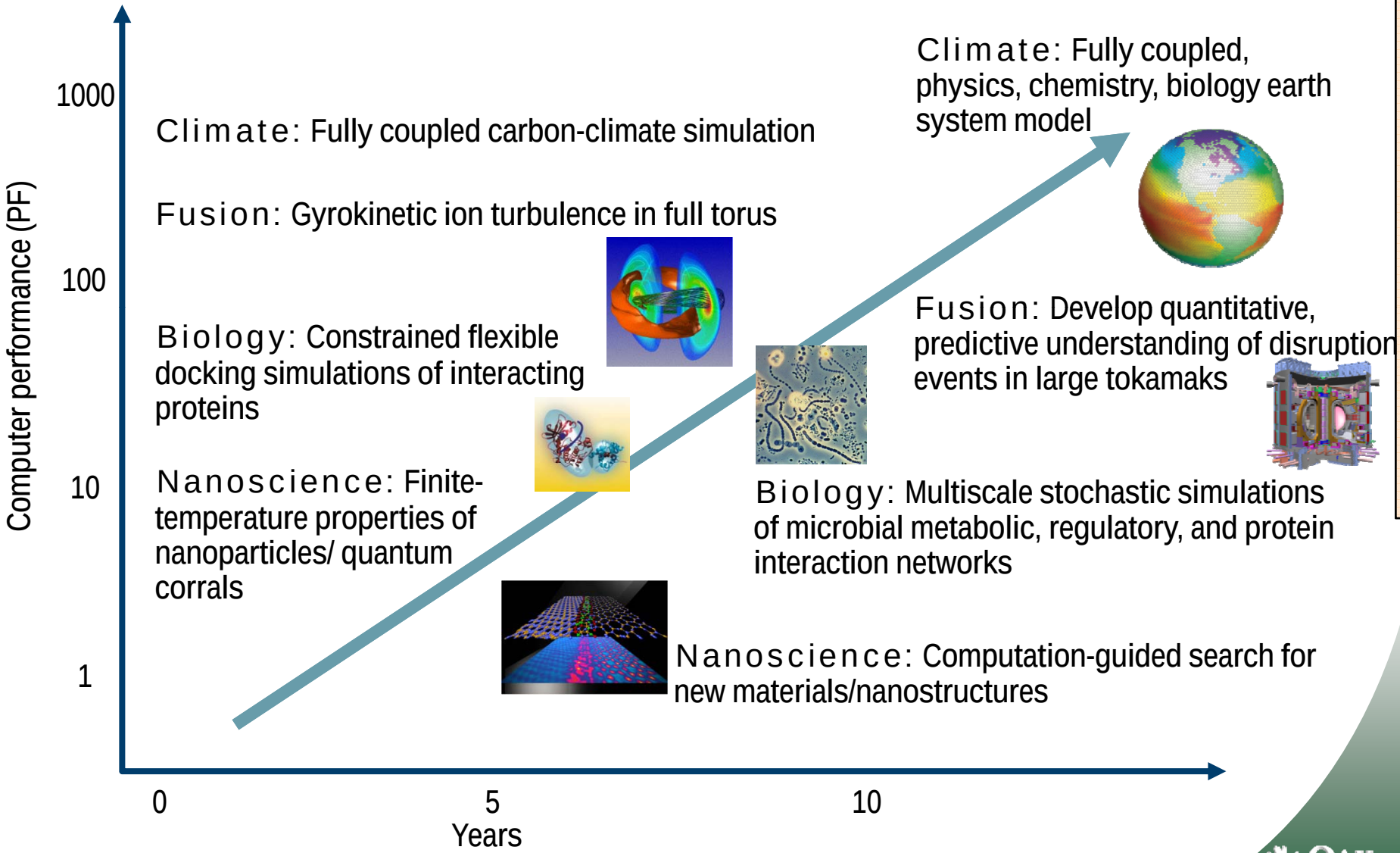
Science advances for the next decade require leadership computing



Scalable Applications

Chemistry Example: Multiresolution ADaptive NumErical Scientific Simulation (MADNESS)

Scalable Applications

Science Goals

Science Impact

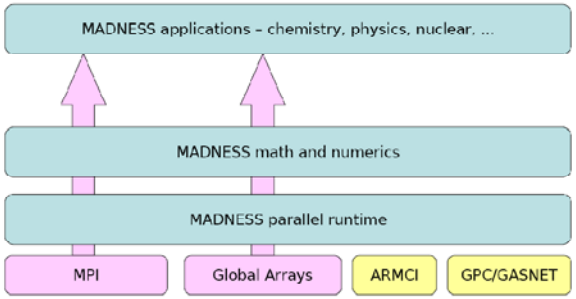
- Multi-resolution analysis in multi-wavelet bases
- Separated representations of functions and operators
- Partitioned singular value representations
- Bandwidth-limited bases for efficient sampling in space and evolution in time

Physical Models

Algorithms

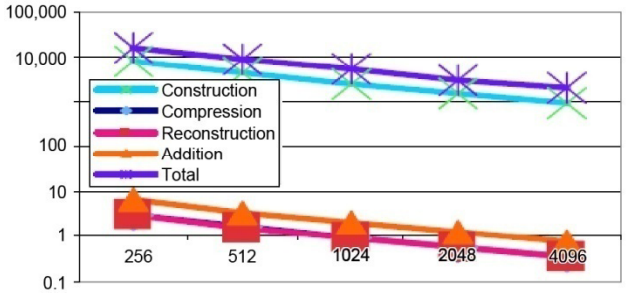
- Fast algorithms with guaranteed precision
- Graphs

- Runtime responsible for
  - scheduling and placement,
  - managing data dependencies,
  - hiding latency, and
  - Medium to coarse grain concurrency
- Compatible with existing models
  - MPI, Global Arrays
- Borrow successful concepts from Cilk, Charm++, Python



Scalability

Performance



New cross-cutting initiative: Climate Change Impacts

Opportunity:

- Launch and lead a national effort to provide the scientific basis for evaluation of climate change consequences in the context of sustainable production and use of interrelated resources
- The transition from climate change science to climate change impacts
- Collaborative support (ASCR and BER) of AR5 by allocation of a billion hours of computer time to the climate end station accessible via the earth systems grid and people resources to support the collaboration

ORNL resources:

- Computational climate science and Earth system model (ESM) integration
- Carbon cycle and ecosystem science
- Expertise in assessment of climate change impacts and response
- LCF and NSF track 2 system
- Climate data analytics, management, and distribution (CDIAC, ARM)
- NSF National Ecological Observatory Network site
- Longstanding partnerships with NSF/NCAR, NASA, and NOAA

Strategy:

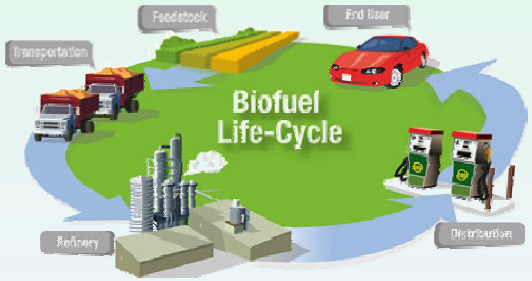
- Develop and deploy a multiagency strategy to build a climate center of excellence to tackle problems at energy-carbon-water interface
- Leverage ultrascale computing and broad environmental R&D base to build reliable climate prediction and assessment capabilities
- Develop and deploy observational field platforms that address multifactor forcings and inform ESMs
- Build stronger relationship with PCMDI
- Provide NOAA/NSF computing resources at ORNL

Outcome: A cross-cutting national program for understanding climate change impacts

New cross-cutting initiative: Emerging S&T for Bioenergy

Opportunity:

- Design and develop a national decision support framework for addressing the overall sustainability and security of bioenergy infrastructure
- Position ORNL as a world leader in geospatial science and technology to impact other scientific and technological missions such as climate and national security



ORNL resources:

- Capability integration across
  - Biomass assessment
  - Infrastructure modeling and simulation
  - Supply chain analysis
- Program leaderships in
  - Sustainability and ecosystem science
  - GIScience and technology
  - Transportation science and technology
  - Climate change science
- Knowledge Discovery via dynamic data analytics, management, and distribution
- High-performance computing and visualization (EVEREST)

Strategy:

- Develop and deploy a multiagency strategy to support a bioenergy sustainability center at ORNL
- Develop and deploy a multiagency strategy to build a GIST center of excellence to address cross-disciplinary problems

Outcome: Cross-cutting national programs in bioenergy infrastructure modeling and geospatial science and technology

OAK RIDGE National Laboratory

Expand Partnership in Energy Research:

Opportunity:

- Modeling and Simulation drives the agenda for energy storage systems, non-petroleum transportation systems, and nuclear energy
- Leadership in energy efficiency and security by simulation and modeling of the electric grid
- Simulation and modeling of the relationships between clean energy technologies and population
- Use HPC to assess bridging strategies for reducing dependencies on foreign oil
- Continued leadership role in development of enrichment models

ORNL resources:

- LCF
- NICS
- EVEREST
- USEC Cluster
- OIC
- IAA/ESSC
- First generation scalable codes
- Staff expertise in chemistry, materials, and scientific computing

Strategy:

- Build out computational Engineering and Energy Sciences group to deliver scalable code to support clean energy challenges
- Achieve transformational technology innovations in energy security by building tools and visualization capabilities for million-core exascale systems
- Investments in modeling and simulation supporting nuclear energy and battery storage
- Leadership role in NEAMS program development
- Leadership role in FSP program development

Outcome: An integrated simulation system for addressing energy problems of national importance

Expand Partnerships in National Security

Opportunity:

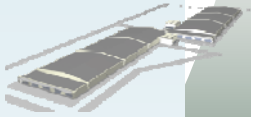
- Leadership in Knowledge Discovery from dynamic disparate data
- DOE classified computing
- Advance the use of modeling and simulation in the classified community
- Infrastructure modeling and vulnerability analysis
- Leadership role in advancing cybersecurity
- Center of excellence in Quantum Information Sciences (QIS)
- Advance extreme scale high-performance computing in national security
- Push the frontier in data center energy efficiency

ORNL resources:

- Existing, extensive, wide spectrum of funded work and relationships across a number of agencies
- MRF facility
- Classified computing and networks
- Extreme Scale Software Center (ESSC)

Strategy:

- Personnel exchanges
  - IPA's
  - Assignments (customers working here)
- Continue to build on existing customer relationships
  - DHS
  - DoD
  - Intelligence Comm.
  - IN/NNSA
- Expand the ESSC
- MCDC



Outcome: Leadership in computing and computational sciences role in national security

Expand university partnerships:

Opportunity:

- Leadership role in NSF computing strategy from Track-1 to Track-3 (campus)
- Leadership in data management, storage, and analytics
- Leadership in development of scalable software in multiple domains
- Expanded presence in: climate change and environment, and computational systems biology/medicine

ORNL resources:

- JICS/NICS
- Master agreement with core universities
- ORAU Fellowships
- JFU/JFO & GC
- OIC & Eugene

Strategy:

- FY09 proposals from ORNL/University partners against multiple OCI calls (Track-2d, XD, DataNet)
- FY09 NSF PetaApps proposals (round 2)
- Deliver on endstation activities in chemistry (Harrison), biology (Kale), and materials (Ceperley)
- Build out JICS focus areas with UT-CEE, UT-HSC, St. Jude, Georgetown, Howard, …

Outcome: A cross-cutting national program

We have an extraordinary opportunity in computing for sustained leadership and scientific impact

Discussion