Computer Science and Mathematics for Energy Problems of the 21st Century

DOE RAMS Program Review

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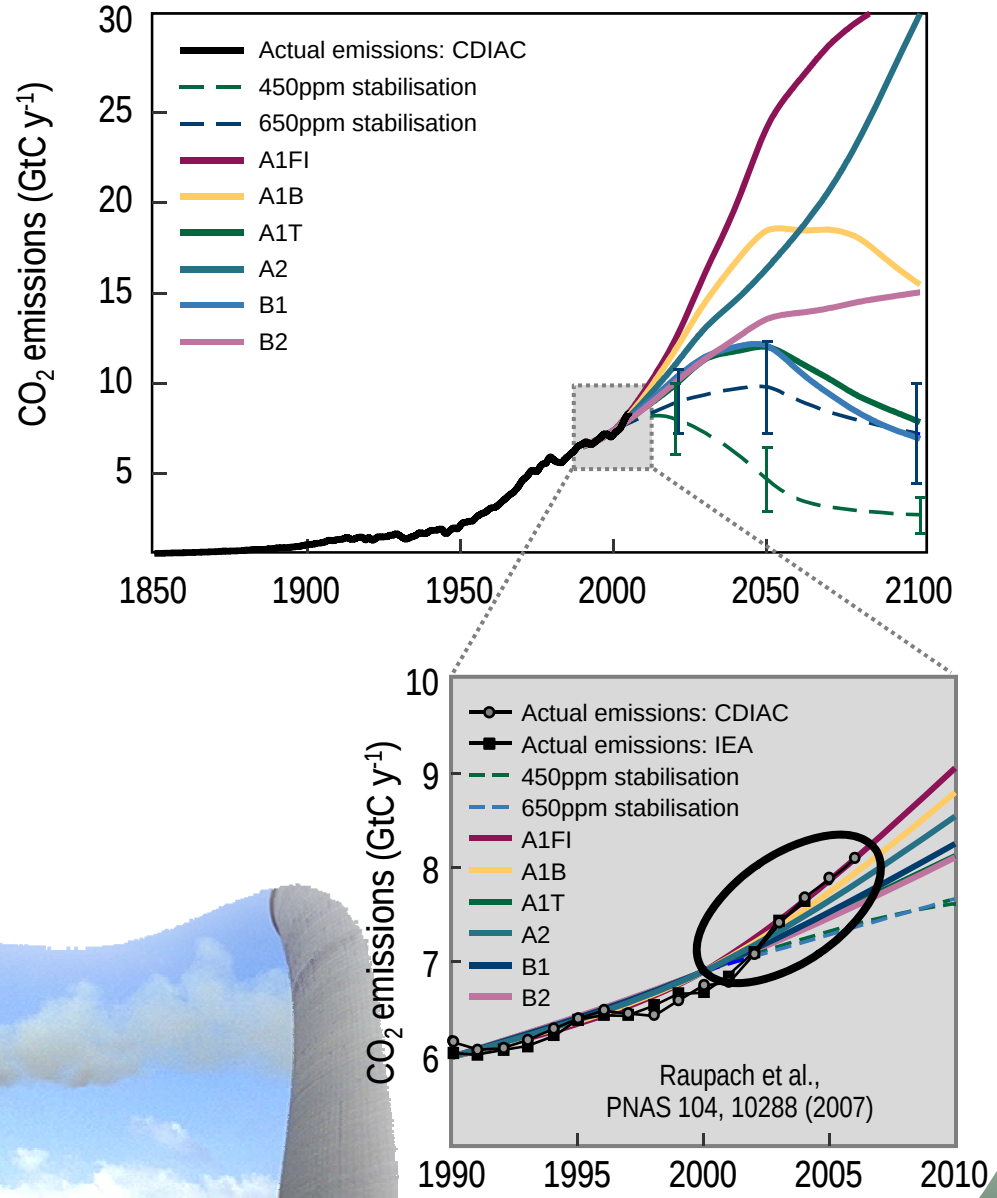
Computer Science
and Mathematics Division

ORNL
Dec. 3-4, 2008

Managed by UT-Battelle
for the Department of Energy

Human activity is affecting global climate

- Atmospheric CO_2 concentrations are increasing rapidly
  - 1990–1999: 1.5 ppm per year
  - 2000–2007: 2.0 ppm per year
  - 2007: 2.2 ppm per year
- Three processes are contributing to this increase:
  - Growth in world economy
  - Increase in carbon intensity
  - Decline in efficiency of CO_2 sinks on land and in oceans
- Climate forcing is both stronger than expected and sooner than expected



We are DOE's lead laboratory for open scientific computing

Compute performance
Today: 1.8 PF
December: 2.5PF

Why ORNL?

- World's most capable complex for computational science: Infrastructure, staff, multiagency programs
- Outcome: Sustained world leadership in transformational research and scientific discovery using advanced computing

Strategy

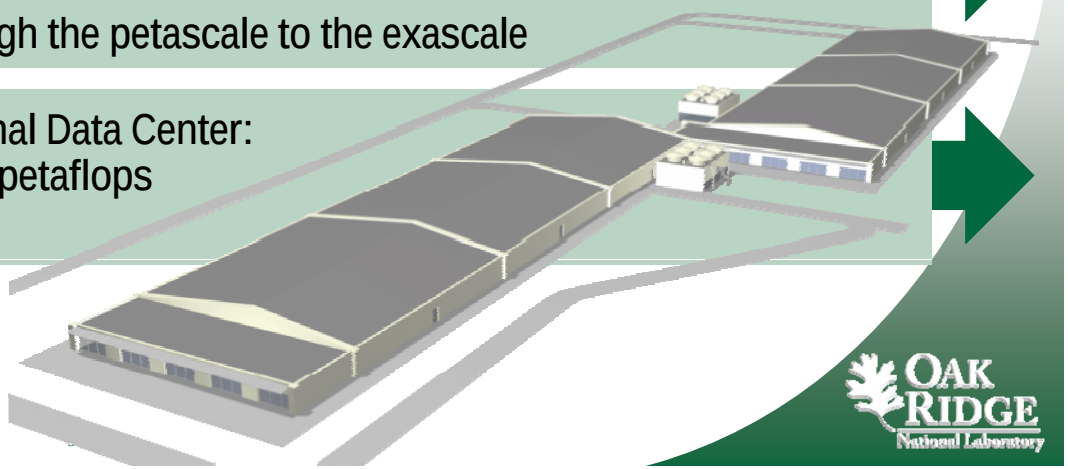
Provide the nation's most capable site for advancing through the petascale to the exascale and beyond	Execute multiagency programs for advanced architecture, extreme-scale software R&D, and transformational science	Attract top talent, deliver outstanding user program, educate and train next-generation researchers

Leadership areas

- Delivering leading-edge computational science for DOE missions
- Deploying and operating computational resources required to tackle national challenges in science, energy, and security
- Scaling applications through the petascale to the exascale

Infrastructure

- Multiprogram Computational Data Center: Infrastructure for 100–250 petaflops and 1 exaflops systems



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

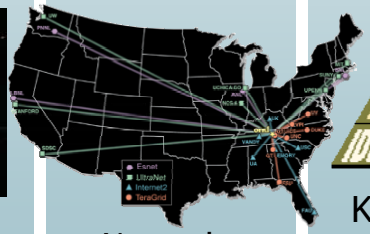
HPC experience and operations

Facilities and infrastructure

Data storage and file systems

Computer systems

Visualization



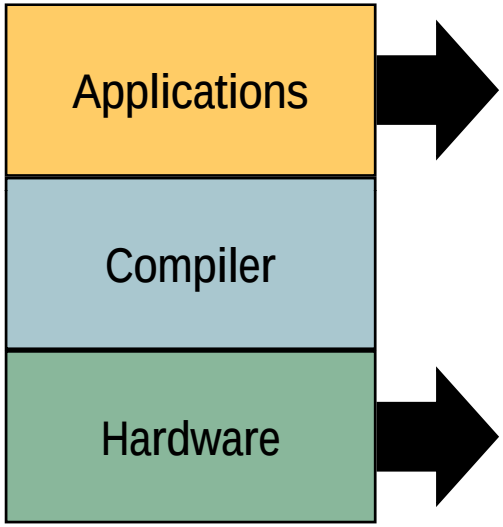
Networks

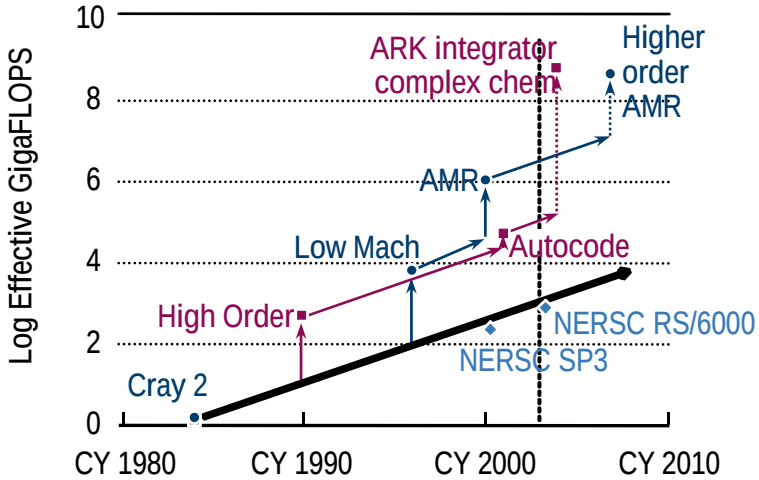
Knowledge discovery

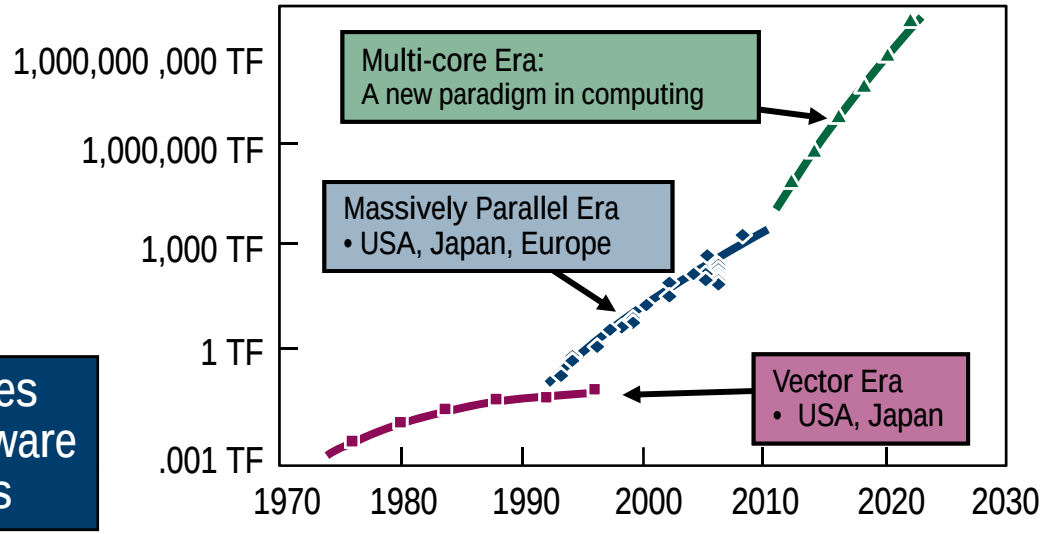
Recipe for leadership in open scientific computing

- **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**

Understanding the hardware and the applications are equally important

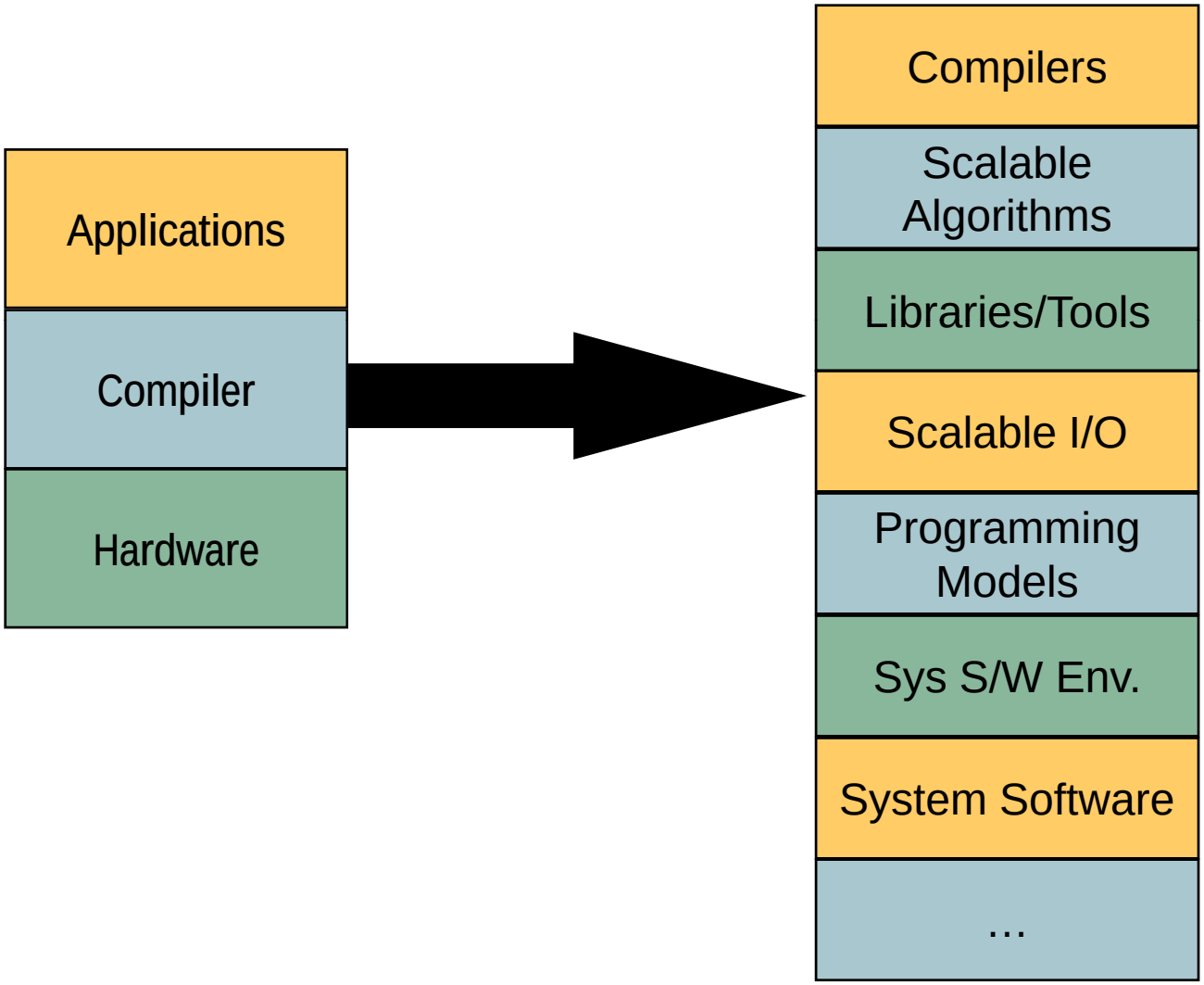






"Effective speed" increases came from both faster hardware and improved algorithms

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**

Extreme Scale Software Center (ESSC)

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

Multiresolution ADaptive NumErical Scientific Simulation (MADNESS)

Science Goals

Science Impact

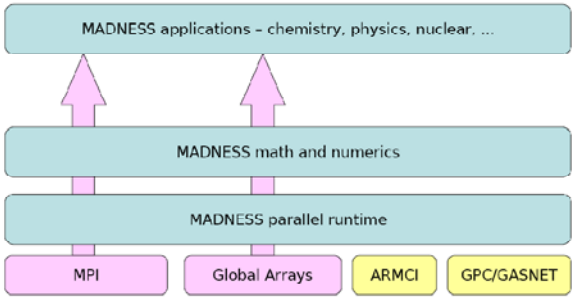
- Multi-resolution analysis in multi-wavelet bases
- Separated representations of functions and operators
- Partitioned singular value representations
- Bandwidth-limited bases for efficient sampling in space and evolution in time

Physical Models

- Fast algorithms with guaranteed precision
- Graphs

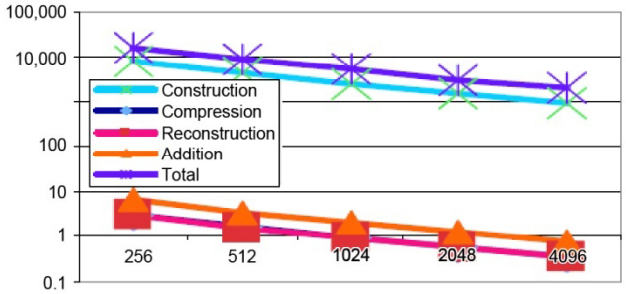
Algorithms

- 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



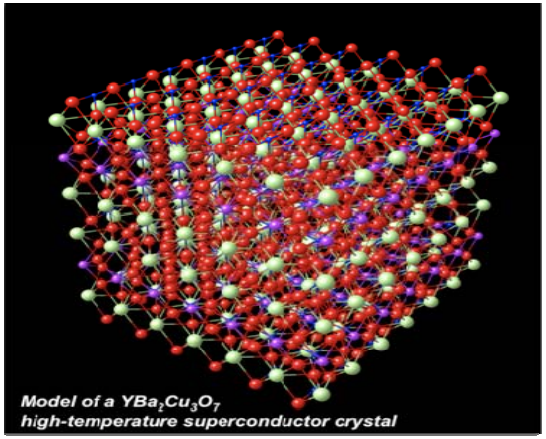
Scalability

Performance

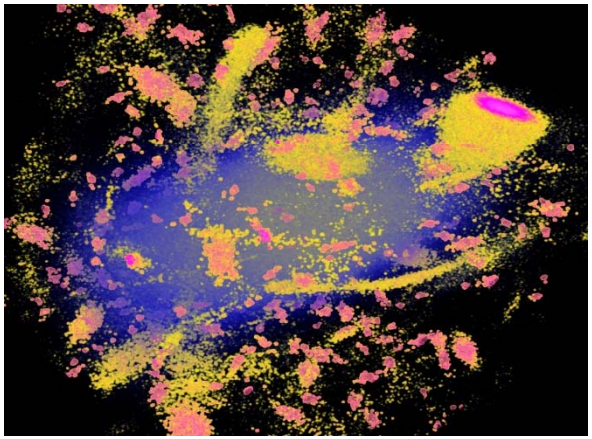


Advancing scientific discovery

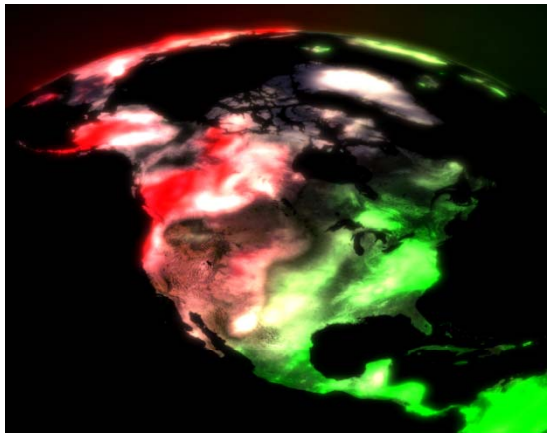
5 of top 10 ASCR science accomplishments in the past 18 months used LCF resources and staff



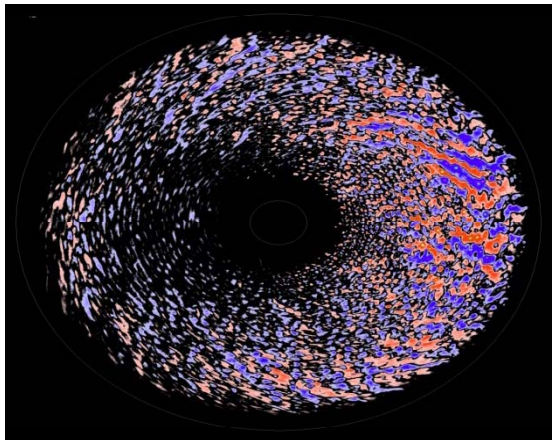
Electron pairing in HTSC cuprates
PRL (2007, 2008)



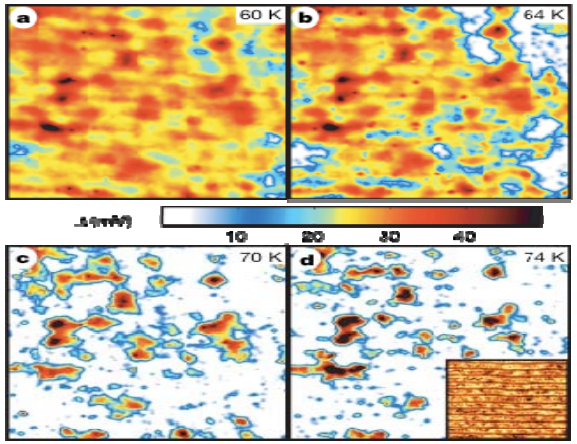
Shining a light on dark matter
Nature 454, 735 (2008)



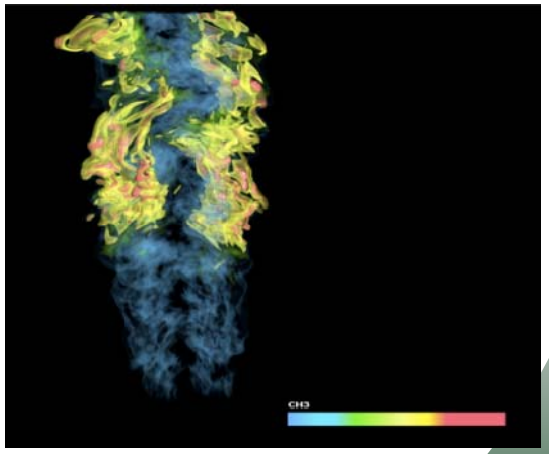
Modeling the full earth system



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

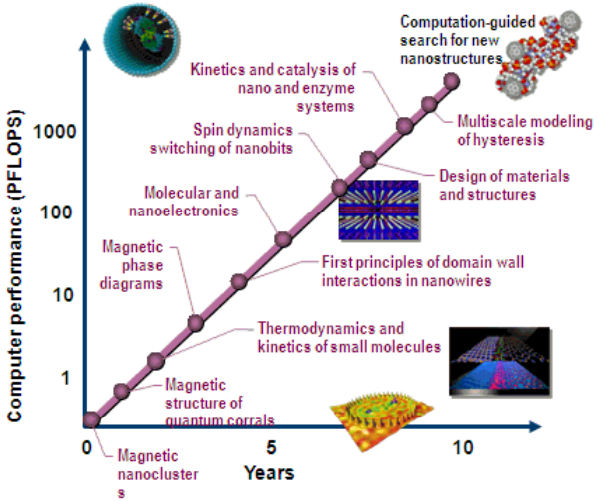


Nanoscale nonhomogeneities in high-temperature superconductors
Candidate for Gordon Bell prize



Stabilizing a lifted flame
Combust. Flame
(2008)

Science Roadmaps



Nanoscience

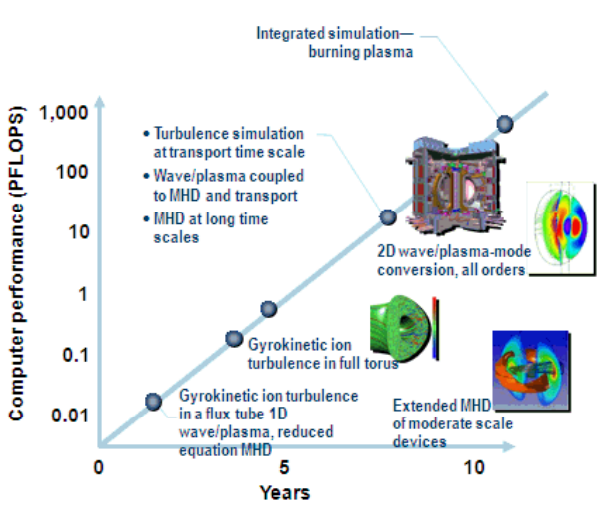
Expected outcomes

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

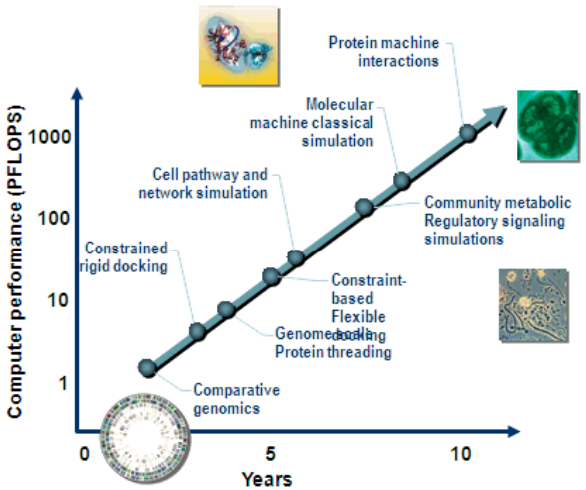
Expected outcomes

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

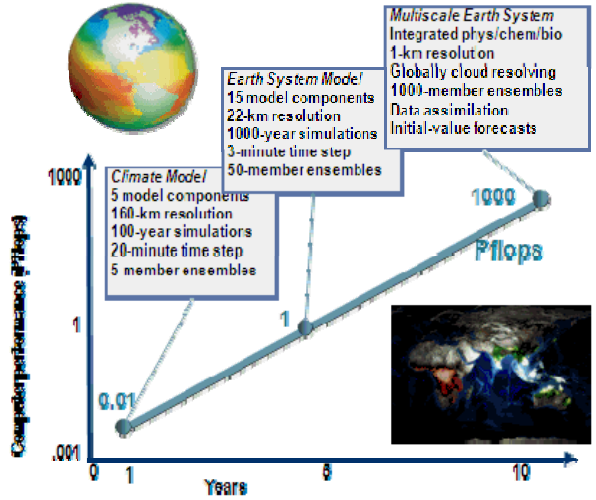
Expected outcomes

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

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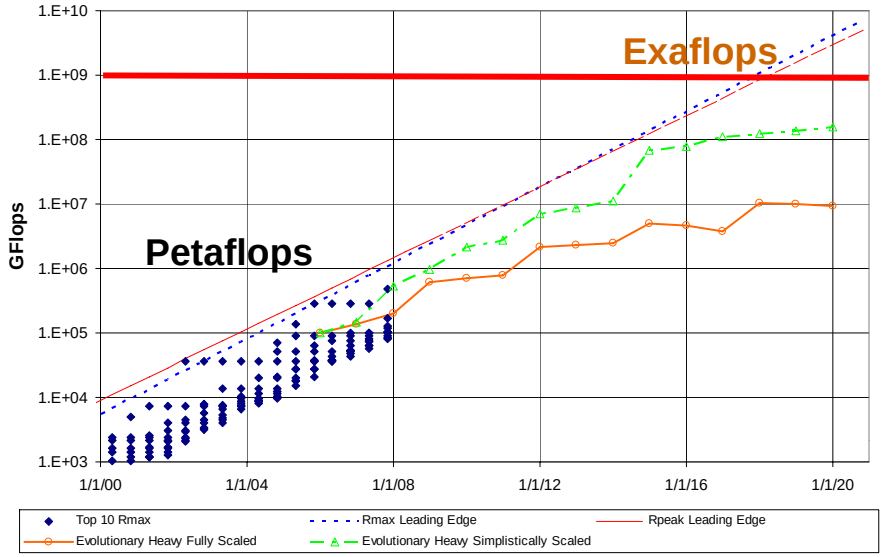
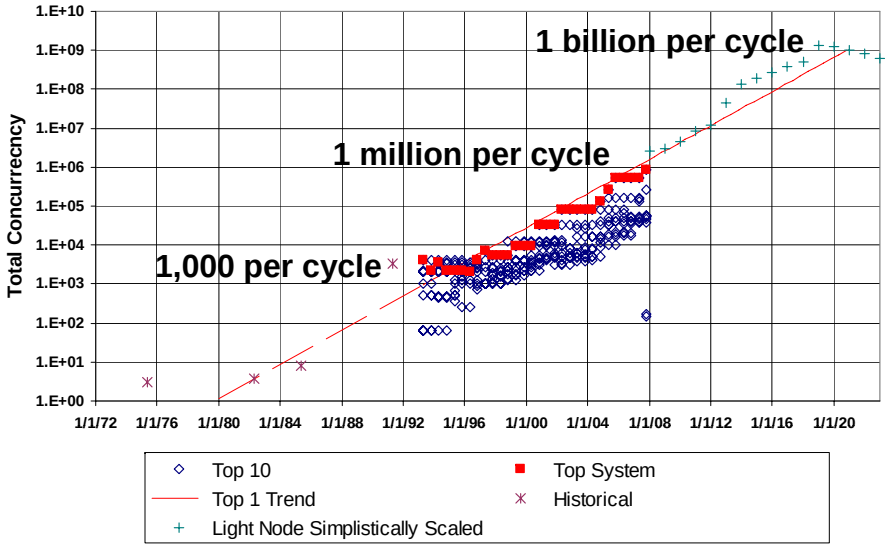
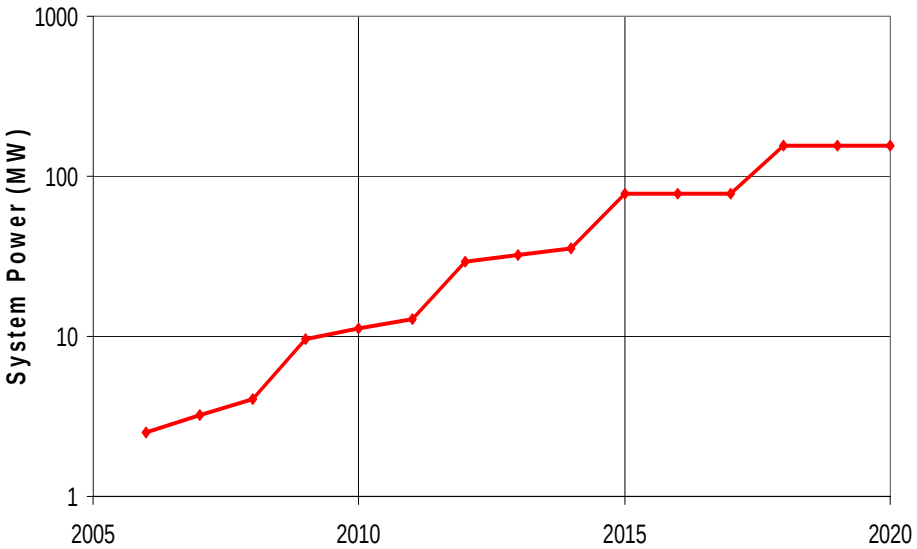
What do we have to look forward to?
Possible System/Power Models Beyond DARPA HPCS







- **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**

ADVISORY COMMITTEE
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Thomas Sterling, Warren Washington

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J. Cobb, Lead, TeraGrid

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Future Technologies

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Computational Mathematics

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D. D. Schmoyer
K. A. Stewart[6]
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Computational Earth Sciences

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C. Sonewald

M. L. Branstetter
D. J. Erickson
K. J. Evans
M. W. Ham
F. M. Hoffman
R. T. Mills
P. H. Worley

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Computational Astrophysics

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P. Boyd

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B. Messer[6a]

Complex Systems

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P. Boyd

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Computational Chemical Sciences

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D. Crawford[2]
T. Fridman[8]
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J. Huang[5]
A. Kalemos[5]
V. Meunier
W. Lu[2]
M. B. Nardelli[2]
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K. Saha[5]
W. A. Shelton
B. G. Sumpter

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Computational Materials Science

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L. C. Holbrook

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Y. Gao[2]
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I. Jouline[2]
P. R. Kent[8]
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P. K. Nukala
B. Radhakrishnan
G. B. Sarma
S. Simunovic
X. Tao[5]
X-G. Zhang
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J. Gergel

Facility 5600/5700
J. Gergel

ESH/Safety Officer
R. J. Toedte6

CSB Computing Center Manager
M. W. Dobbs[6]

[1]Co-op
[2]Joint Faculty/[2a]ORISE Faculty
[3]Wigner Fellow
[4]Householder Fellow
[5]Postdoc/[5a]Postmaster assign.
[6]Dual Assignment/[6a]Matrix/[6b] off-site
[7]Part-time
[8]JICS

1/28/2008

RAMS Projects by Group (CSR)

- **Computer Science Research**
  - **Cluster Account Management Program: C.A.M.P.**
  - **3-D Heat Conduction on a Linux Cluster using PVM**
  - **Achieving High Availability in Cluster Computing**
  - **Improving the Manageability of OSCAR**
  - **High Availability-Open Source Cluster Application Resources**
  - **Spallation Neutron Source Data and Analysis Portal**
  - **Message Passing Interface vs. Multi-threading: Which Parallelization Technique is More Efficient?**
  - **Virtualization in High-Performance Computing**
  - **Application of RT-RiboSyn to Measure Growth Rates of Shewanella oneidensis**
  - **A method to identify mass spectra of proteins containing post-translational modifications**
  - **Parallel Exact Stochastic Simulator**
  - **"Pathway Modeling of Shewanella denitrificans OS217"**
  - **Central Metabolism of Escherichia Coli in the Stationery State: Flux Balance Analysis and Gene Expression Data Comparison**
  - **Analysis Tools for the HPCC Benchmarking Suite**

RAMS Projects by Group (FT, CM and SDS)

- **Future Technologies**
  - **Analysis Tools for the HPCC Benchmarking Suite**
  - **Using OpenGL to Display Jumpshot Visualizations on the PowerWall**
- **Computational Mathematics**
  - **Statistical Methods for finding conserved patterns in DNA sequences**
  - **Research in the Effectiveness of Singular Value Decomposition of Pixel Data to Decrease the Amount of Essential Data to be Processed**
  - **Visualization of Oxidation Reduction Simulations**
  - **A method to identify mass spectra of proteins containing post-translational modifications**
  - **Parallel Exact Stochastic Simulator**
  - **"Pathway Modeling of Shewanella denitrificans OS217"**
  - **Central Metabolism of Escherichia Coli in the Stationery State: Flux Balance Analysis and Gene Expression Data Comparison**
- **Statistics and Data Science**
  - **RobustMap: A Fast and Robust Algorithm for Dimension Reduction and Clustering**
  - **A Laboratory Information Management System For Protein Complex Research**
  - **A Multiscale Algorithm for Dimension Reduction and Clustering**

RAMS Projects by Group (CMS)

- **Computational Materials Sciences**
  - **The Basic Linear Algebra Subroutine (BLAS) & C++: Creating a Simple and Generic Interface Between the Two**
  - **Scientific Visualization of Superconducting Materials**
  - **Three-Dimensional Grain Growth Model Using the Phase Field Approach**
  - **Fiber Bundle Modeling for Nacre Fracture Simulation**
  - **Development of the Plone Website for Computational Materials Science Group**
  - **Large Scale Simulations of Thin Film Grain Growth**
  - **A method to identify mass spectra of proteins containing post-translational modifications**
  - **Parallel Exact Stochastic Simulator**
  - **"Pathway Modeling of Shewanella denitrificans OS217"**
  - **Central Metabolism of Escherichia Coli in the Stationery State: Flux Balance Analysis and Gene Expression Data Comparison**

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RAMS Projects by Group (CSys, CCS and CES)

- **Complex Systems**
  - **Comparison Algorithm for Descent Speeds in Local Minimization Processes for TRUST**
  - **Porting the CESAR Source Localization of Underwater Targets Code to the Intel Visual Fortran Compiler**
  - **Source Localization in a Moving Sensor Field**
  - **Algorithms for The Computed Tomography Imaging Spectrometer**
  - **Streaming Singular Value Decomposition (SVD)**
  - **Advances in Algorithms for Processing, CTIS Flash Hyperspectral Imagery**
- **Computational Chemical Sciences**
  - **Computational Modeling of Scanning Microscopy**
  - **Molecular Dynamics Simulations of Methanol in Single-Walled Carbon Nanotubes (SWNTs)**
- **Computational Earth Sciences**
  - **A Practical Map-Analysis Tool for Detecting Dispersal Corridors**

Vehicles of cooperation with ORNL

Undergraduate	Graduate	Postdoctoral	Faculty
• Co-op program • DHS HS-STEM Internship • HERE@ORNL • Laboratory Technology Program • Nuclear Engineering Science Laboratory Synthesis Internship • Research Alliance in Math and Science • Science Undergraduate Laboratory Internship	• Advanced Short-Term Research Opportunity • HERE@ORNL • Nuclear Engineering Science Laboratory Synthesis Internship • Research Alliance in Math and Science • Post-Master's Research Participation	• Advanced Short-Term Research Opportunity • Eugene Wigner Fellows* • Clifford Shull Fellows: Neutron science • Alston Householder Fellows: Scientific computing* • Instrument Development Fellows • Postdoctoral research associates*	• DHS Summer Research Team • Visiting / summer faculty* • HERE@ORNL* • NRC Faculty Research Participation • Sabbaticals and summer research*

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***Mentoring for RAMS students**

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