UT-BATTELLE

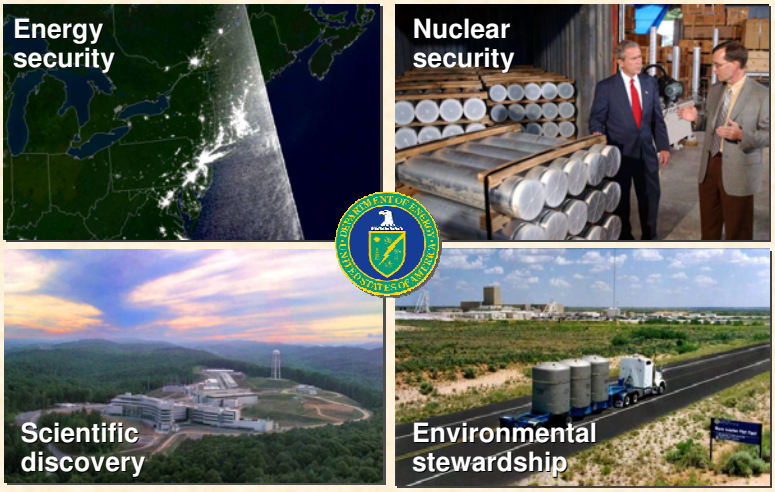
Advanced Scientific Computing: An Extraordinary Tool for Extraordinary Science

Presented at the
13th IEEE International Conference on High Performance Computing

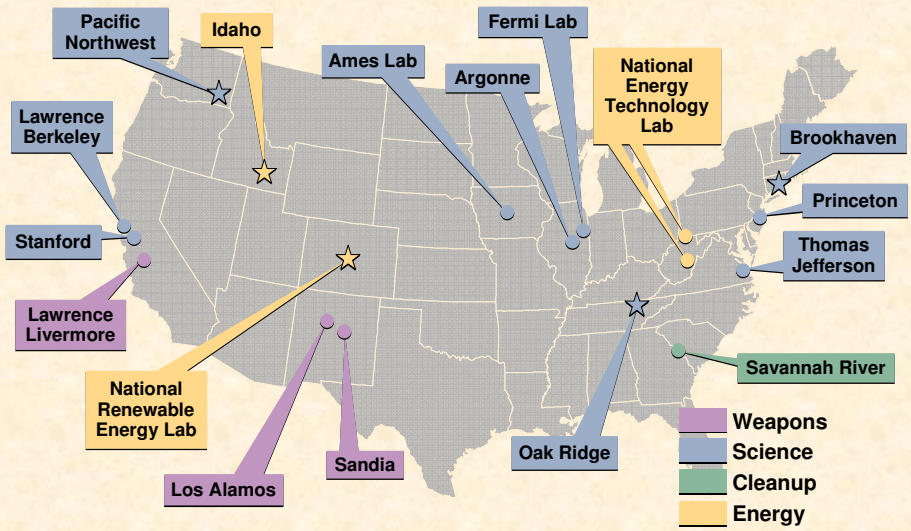
Jeffrey Wadsworth
Director, Oak Ridge National Laboratory

Bangalore, India
December 19, 2006

The U.S. Department of Energy: Innovation through science-driven development of new technologies



The U.S. national laboratories:
A comprehensive research system

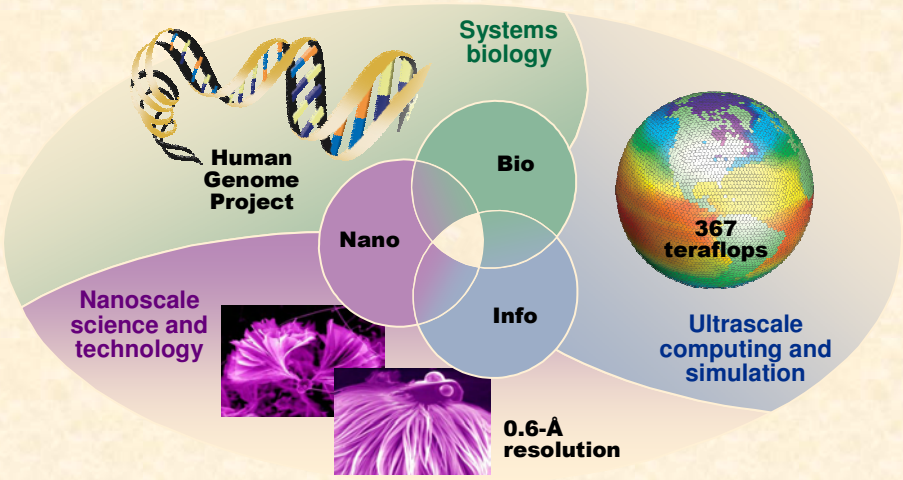


Oak Ridge National Laboratory
DOE's largest multiprogram science laboratory

- $1 billion budget
- 4,150 employees
- 3,000 research guests annually
- Managing the $1.1 billion U.S. ITER project
- Completing a $300 million modernization
- Nation's largest energy laboratory
- Nation's largest science facility: the $1.4 billion Spallation Neutron Source
- Nation's largest concentration of open source materials research
- Nation's largest unclassified scientific computing facility

Three closely linked global challenges call for a broad response

We are addressing the integrating scientific themes of the 21st century

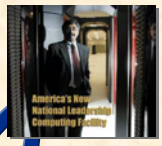


We are building on a tradition of excellence

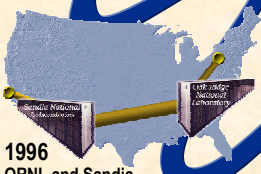
Computational milestones at ORNL

1991
ORNL Center for Computational Sciences established

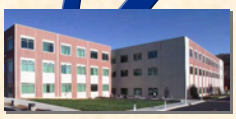
1998
First application to deliver sustained 1-TF performance



2004
ORNL selected to lead development of DOE's Leadership Computing Facility



1996
ORNL and Sandia National Laboratories create the first high-performance computational grid



2003
State-of-the-art Computational Sciences Building completed

2006
Cray XT3 upgraded to 54 TF

2005
20-TF Cray XT3 installed

Taking business risks: We made substantial investments in capability

- Computational Sciences Building
  - 40,000-ft^2 computer center
  - 12 MW of power
  - 4,800 tons of cooling water
- Joint Institute for Computational Sciences
- Positioned ORNL to win the competition for DOE's Leadership Computing Facility
- Other customers have expressed interest
- Infrastructure improvements are already under way

Today, ORNL is DOE's lead laboratory for open scientific computing

We are developing DOE's Leadership Computing Facility (LCF) to field a broad new capability for high-end science

- Provide leadership-class computing for science and engineering
- Procure and operate the largest-scale computer systems (beyond vendor design point) and develop high-end operating and application software
- Educate and train new computational scientists

We are engaging the political, scientific, and engineering communities to realize the breakthroughs promised by these extraordinary capabilities

Leadership Computing Facility

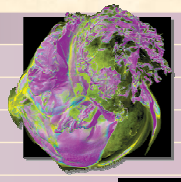
- Two primary systems
  - 18.5-TF Cray X1E Phoenix vector machine
  - 54-TF Cray XT3 Jaguar scalar machine (now being upgraded to 100 TF)
- Additional evaluation platforms and test systems
- High-Performance Storage System
- Visualization resources
  - 35-megapixel PowerWall
  - 64-node visualization cluster
  - Visualization Laboratory
- Multiple 10-Gb links to ESNet, Internet 2, National Lambda Rail, and TeraGrid

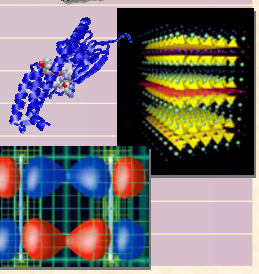
The LCF supports a broad spectrum of scientific domains and associated application codes

Scientific focus areas
Accelerator physics
Astrophysics
Chemistry
Climate change
Combustion
Computer science
Engineering
Fusion
High-energy physics
Life sciences
Materials sciences
Nuclear physics

Computational challenge

- Diverse capability requirements within each domain
- Bigger problems
  - Higher resolution
  - More grid points or particles
- Harder problems
  - More physics
  - More expensive grid points
  - More time steps
  - Tightly coupled





Research projects at the LCF

DOE's INCITE program: Innovative and Novel Computational Impact on Theory and Experiment

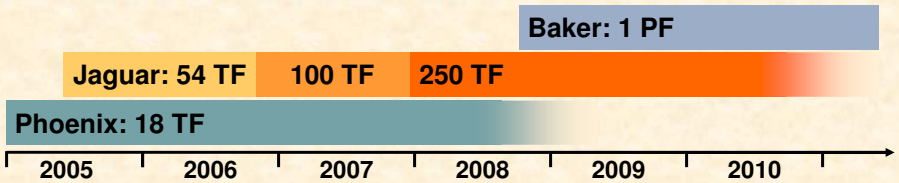
Boeing
Engineering physics:
Large-scale computational tools for flight vehicles

Harvard
Life sciences:
Molecular dynamics of molecular motors

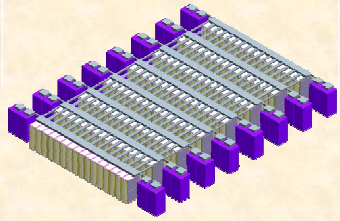
General Atomics
Fusion energy:
Plasma turbulence

Dreamworks Animation
Computer science:
Ray tracing

We are on a well-defined path to petaflops computing



54-TF Cray XT3 Jaguar



1-PF Cray "Baker"

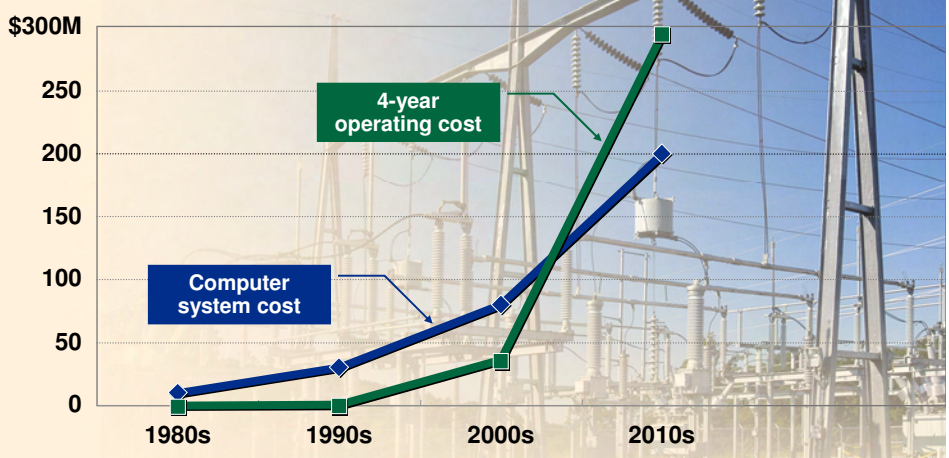
We expect to deploy the 1-PF Cray Baker system in 2008

System configuration

- 1 PF peak
- 23,936 multiple-core processors
- 136 cabinets
- $32 \times 34 \times 24$ topology
- 34 heat exchange units
- 7 MW of power

Our aggressive schedule recognizes how indispensable scientific computing has become to research

Operating a petascale computing system:
The infrastructure challenge



As computing power increases, so does the need for electric power

System	Peak performance	Number of cores	Power
Jaguar	25 TF	5,212	0.9 MW
Jaguar	50 TF	10,424	1.2 MW
Jaguar	100 TF	23,480	2.8 MW
Jaguar	250 TF	36,536	3.0 MW
Baker	1 PF	95,744	7.0 MW
Top500 (Nov 2006)	3.53 PF	1,020,901	~115 MW
Intel chips (1 year of production)	1600 PF	300,000,000	~50 GW

- We have partnered with our regional power provider, TVA, to deliver reliable, cost-effective power
- We are building a 70-MW substation (can be upgraded to 170 MW)
- We have upgraded our transmission capability (3 redundant feed circuits)

"Intel expects to sell 60 million dual-core chips this year, accounting for about a quarter of total processor sales"

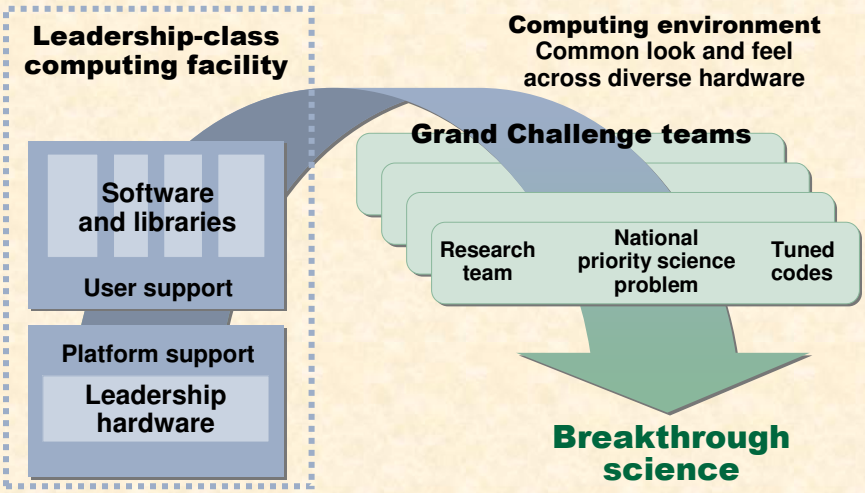
– Justin Rattner, Intel CTO (February 2006)

We are laying the foundation for science at the petascale

- Establishing a major new, fully integrated petascale computing environment
- Developing petascale software infrastructure to enable productive utilization and system management
- Empowering scientific and engineering progress and allied educational activities using petascale system
- Developing and educating the next-generation computational scientists who will use petascale systems to:
  - Increase our understanding of the world
  - Address global challenges in energy, environment, and national security

The goal is science

Facility plus hardware, software, and science teams all contribute to science breakthroughs



Science drivers

"Computational simulation offers to enhance, as well as leapfrog, theoretical and experimental progress in many areas of science and engineering…"

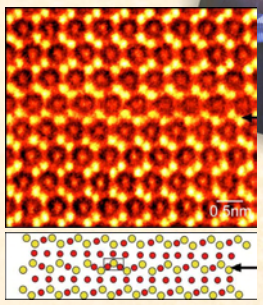
A Science-Based Case for Large-Scale Simulation (SCaLeS Report), Office of Science, U.S. DOE, July 2003

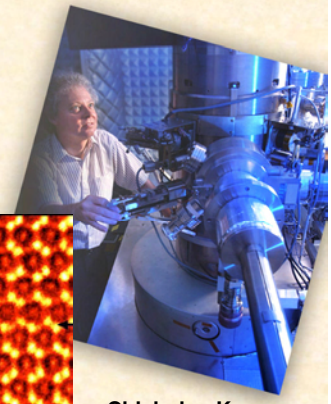
Advanced energy systems	Biotechnology	Environmental modeling	Nanotechnology
• Fuel cells • Magnetic fusion • Advanced fission reactors	• Genomics • Cellular dynamics • Bioenergy	• Climate prediction • Pollution remediation	• Sensors • Storage devices • Tailored materials

Intermetallic mystery solved through Z-contrast electron microscopy

Z-contrast reveals a complex dislocation that produces shear in two directions on adjacent planes

- Confirms a 1950 prediction by William Shockley
- Improves understanding of deformation and phase transformations in Laves phase materials (Cr_2Hf)
- Opens the door for new optimized intermetallics in high-performance applications
- Much understanding could be gained from atomistic simulations of the motion of this type of dislocation



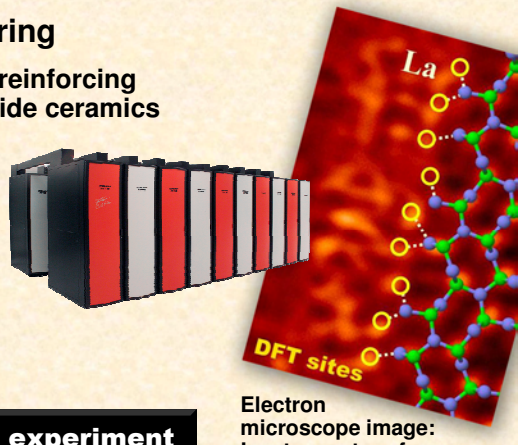


Chisholm, Kumar, and Hazzledine, *Science* 307, 701–703 (2005)

We can use modeling and simulation to drive materials development

Structural ceramic engineering

- Dopant additions can alter the reinforcing grains that toughen silicon nitride ceramics
- Using high-resolution electron microscopy and computer simulations, we have learned why these materials are so strong
- These findings provide a basis for the atomic-scale design of advanced ceramics



Electron microscope image: La atoms at surface of Si_3N_4 grain

Prediction precedes experiment

Realizing the promise of fusion requires petascale computing

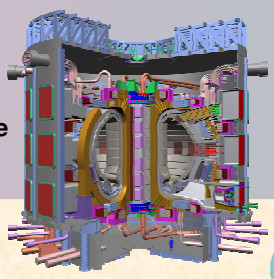
- Simulation plays a critical role in fusion research
  - Developing basic theory
  - Designing facilities
  - Planning and analyzing experiments
- ITER is the next step toward fusion power
  - Seven international parties are sharing the $12B cost
  - The cost to operate ITER could be ~$1M/day
  - Integrated simulation is essential
- Work is in progress to reduce the computing power needed to simulate ITER dynamics from ~10^{24} flops to 10^{15} flops (yottaflops to petaflops)
  - Better physics models
  - More efficient numerical algorithms

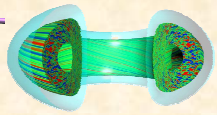
NEWSFOCUS

ITER's $12 Billion Gamble

Developing stable and efficient fusion devices:
Modeling and understanding plasma turbulence

Problem	Results
Model the interaction of turbulence on ion and electron spatial and temporal scales • Scales differ by orders of magnitude • Traditionally treated by separate simulations	New insights on how short-wavelength electron temperature gradient turbulence comes into play as long-wavelength (ion temperature gradient/ trapped electron mode) turbulence is suppressed in the pedestal (an edge transport barrier)

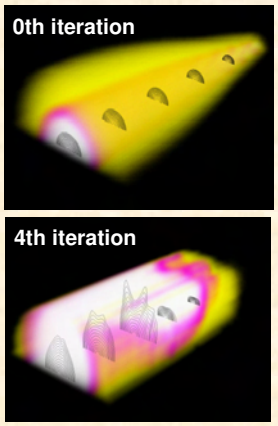




Ron Waltz, General Atomics

Developing stable and efficient fusion devices:
Ion cyclotron resonance heating of fusion plasmas

- Interaction of radio-frequency (RF) waves with fusion alpha particles must be understood and optimized for successful fusion power production
  - Increasing knowledge will help in planning and analysis of ITER experiments
- LCF computers have been used for self-consistent simulations of evolution of energetic ions in plasmas heated by RF waves in the ion cyclotron range of frequencies (ICRF)
- Using the AORSA code coupled to the CQL3D Fokker-Planck code, we can now simulate the evolution of ion distributions during ICRF heating



Bounce-averaged minority hydrogen distribution function in Alcator C-MOD

Don Batchelor, Oak Ridge National Laboratory

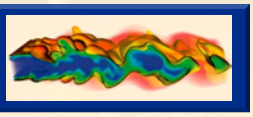
Improving energy security:
New insights into combustion

Problem
Understand the flamelet and thin-reaction zones where lean premixed combustion occurs

Key challenges
- Strong turbulence and chemistry interactions
- Combustion at lean flammability limit is difficult
  - Prone to extinction
  - Unburned hydrocarbon emission
  - Large-amplitude pressure oscillations
  - Emission of toxic CO

Simulation results
- Flame structure is penetrated by small-scale eddies
- Mean reaction rates still resemble a strained laminar flame
- Source terms that influence flame thickness are better understood

Increased efficiency and lower emissions in new land-based natural gas turbines

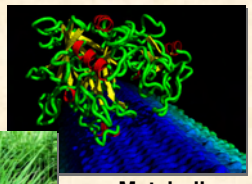


Jackie Chen, Sandia National Laboratories

Next-generation simulations in biology:
Creating efficient enzymes for cellulose degradation through protein engineering

Clostridium thermocellum growing on cellulose

- Ethanol production from cellulose can provide a pathway to renewable energy
- A detailed understanding of cellulase enzyme mechanisms has been gained from multiscale modeling
  - 1- to 100-ns trajectories for systems with >800,000 atoms
- Simulations with different substrates and mutant enzymes will lead to greater efficiency



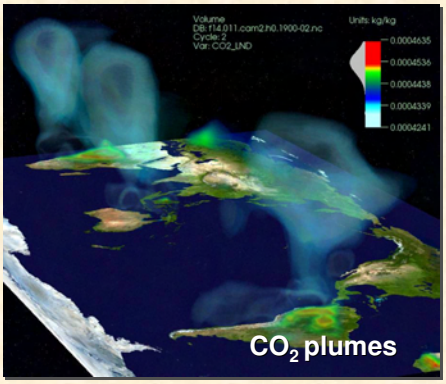
Metabolism of cellulose by exocellulase

Switchgrass

Pratul Agarwal, Oak Ridge National Laboratory

Advancing our ability to model and predict climate change

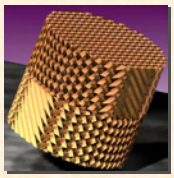
- New model algorithms and new scientific capabilities have been developed
  - New finite-volume method for simulating atmospheric dynamics
  - Alternative schemes for ocean models
  - New capabilities for simulating the carbon and sulfur cycles as part of the climate system
  - Assembly of a prototype carbon-climate-biogeochemistry model
- Improved regional detail requires high-end computational facilities



Warren Washington,
National Center for Atmospheric Research

Distillation columns consume 3% of the U.S. energy supply

- Complex corrugated packing geometry is empirically designed
- Current efforts allow two-phase computational fluid dynamics modeling of packing elements
- Whole-column modeling will require petascale computing



It should be possible to improve efficiency by 15%

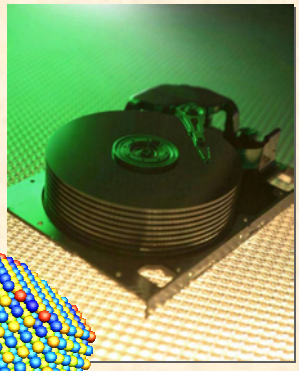
Insight into next-generation recording media:
Magnetic properties of FePt nanoparticles

Highly optimized calculations on LCF

- DFT calculations using codes optimized with Cray Center of Excellence
- Largest, most complex calculations of this type to date: ~50% of peak on 512 Jaguar processors (1 TF) for ~800 atoms
- Calculations with 2000 atoms planned

Results

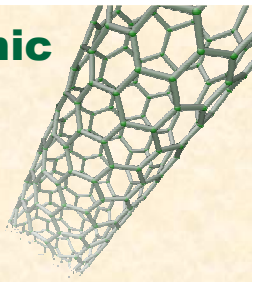
- Revealed, for first time, strong influence of nanoscale on magnetic structure of FePt nanoparticles
- Sensitivity of magnetic structure to small changes demonstrates importance of calculations for materials design and optimization



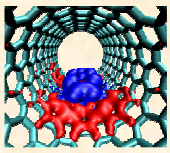
Industry candidate for next-generation magnetic recording (>1 Tb/in.^{2})

PI: Thomas Schulthess, Oak Ridge National Laboratory

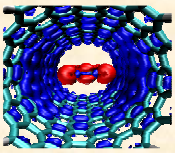
Large-scale quantum electronic structure calculations



- Self-assembled molecular electronics systems offer a promising path to future computers
- New theoretical and computational tools are enabling more rigorous, complete, and realistic modeling of molecular electronics devices
  - Electronic and structural properties of single-wall carbon nanotubes with encapsulated organic molecules
  - Quantum electron transport in molecular and nanoscale systems
- Stable and efficient doping of carbon nanotubes can be tailored using adequate doping molecules
- Combining experiment, theory, and simulation provides a solid basis for the optimal design of nanotube-based electronic devices



Charge transfer indicative of *n* doping



Charge transfer indicative of *p* doping

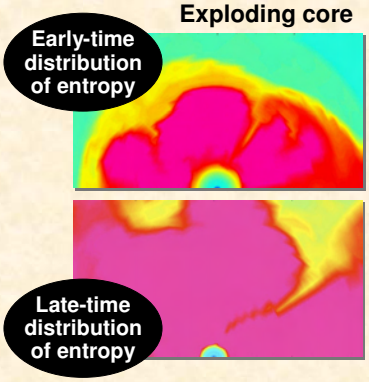
V. Munier and B. G. Sumpter, *J. Chem. Phys.* 123, 024705 (2005)

Evolution of supernovae

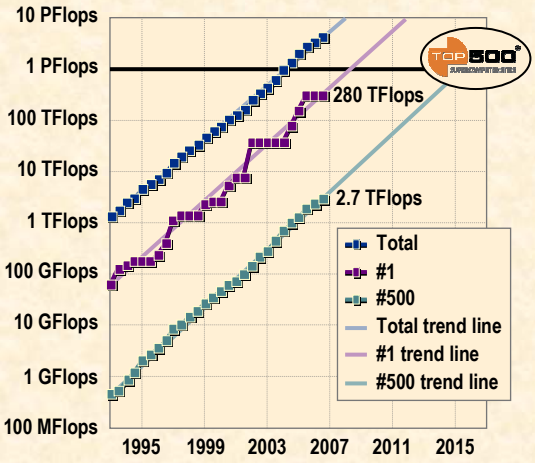
Challenge:
Incorporate all known physics into supernova models

- Explosions obtained for 11 and 15 solar-mass progenitors
- Explosions seem to be contingent on simulating **all** of the following:
  - Multidimensional hydro
  - Good transport (MGFLD)
  - Nuclear burning
  - Long physical times (equivalent to long run times)
- Researchers surprised that nuclear burning has an important dynamic effect
- New result builds on earlier supernova accretion shock instability (SASI) findings
  - Longer time scales required to observe explosion

Exploding core



Tony Mezzacappa,
Oak Ridge National Laboratory

We are on the threshold of a new era in scientific computing

- Studying scientific problems at an unprecedented level of detail
  - Accelerating scientific discovery
  - Delivering key insights
  - Solving global challenges
- Enabling the effective use of petascale computing for scientific research
  - Creating a comprehensive scientific computing software infrastructure for discovery at the petascale
  - Delivering a new generation of data management and knowledge discovery tools for data-intensive science