A Progress Report on the Cray X1 Evaluation by CCS at ORNL

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Oak Ridge National Laboratory

Presented to

CUG

18 May 2004

Knoxville, TN, USA

Presentation Highlights

- ORNL CCS is an Advanced Computing Research Testbed Facility for DOE
- Cray X1 arrived at ORNL in March 2003
- Early evaluation started immediately
  - Microbenchmarks, Kernels
  - Important DOE applications
  - System scaled up over past year
  - Workshops
  - System opened to many users
- Current X1 evaluation has produced impressive results on important DOE applications
  - Presented at Cray X1 external review in February
- Close collaboration with Cray
  - Resolved issues, such as a scaling bug
  - Identified opportunities for improvements in future designs
- National Leadership Class Facility funded last week

Center for Computational Sciences at ORNL

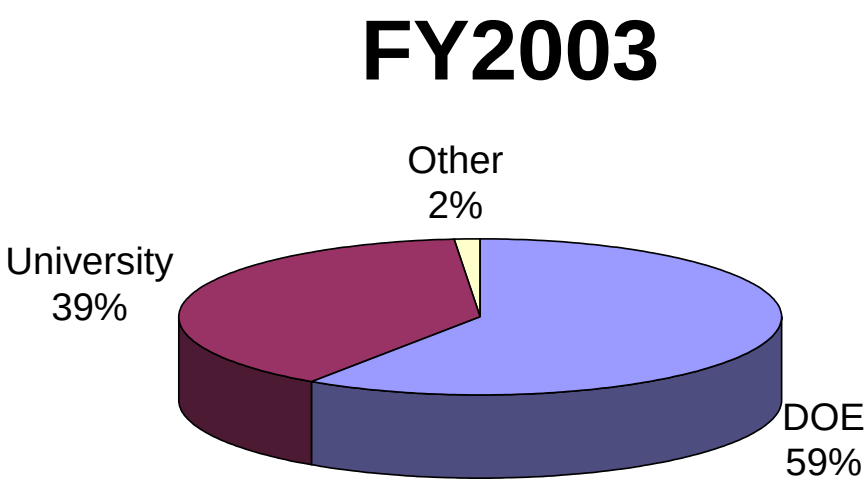
- is a DOE Advanced Computing Research Testbed
  - Computational science partnerships
    - Provide tailored HEC resources to specific, focused scientific communities to support their exploration of new research capabilities
  - Technology assessment
    - Assess the potential of new computing technologies
- Requires interdisciplinary teams
  - Applications, mathematics, computer science
- Requires close collaboration with vendors

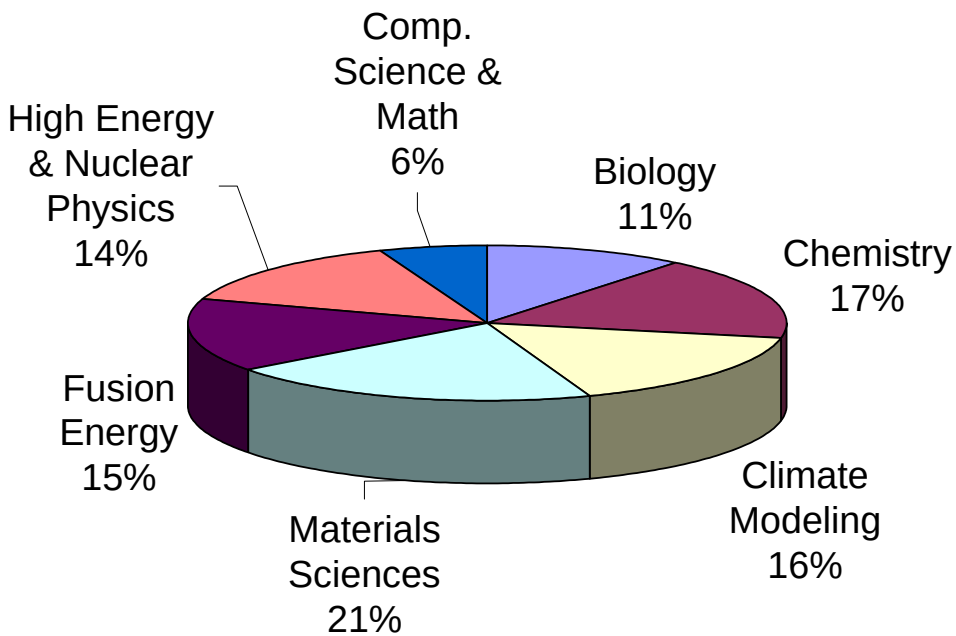
CCS (cont)

- Procure the largest scale systems (beyond vendors design point)
  - Develop software to manage systems on this scale
  - Enable application science
- Deliver leadership-class computing for DOE science
  - By 2005: 50x performance on major scientific simulations
  - By 2008: ***1000x*** performance

CCS is a national resource for academic and DOE communities

- Works very closely with, and are part of, the scientific user communities to anticipate their needs



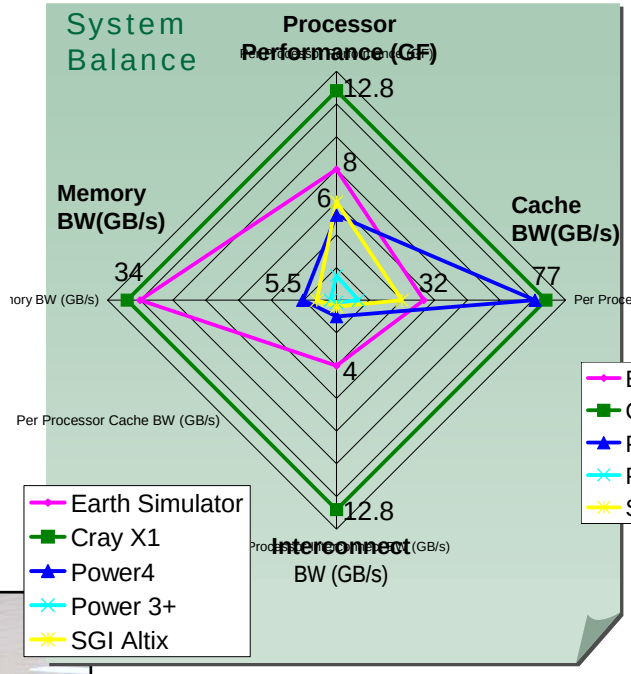


Technical Assessment Activities at CCS

- Evaluations underway
  - Cray X1
  - SGI Altix
  - IBM p690 w/ Federation
- Investigating component technologies
  - Elan 3, 4
  - Infiniband
  - Reconfigurable computing
  - Programming models
  - *Operating systems*
  - *File systems*

Motivation for Cray X1 Evaluation

- X1 offered system balance not available in other systems
- DOE/CCS began discussions w/ Cray in 2002
- In August 2002, DOE funded ORNL proposal to 256 MSP system



Deployment History

Date	Cabinets	Processors (MSP)	Memory (GB)	I/O (TB)
March 03	1	32	128	8
June 03	2	64	256	16
July 03	4	128	512	16
November 03	8	256	1024	32

CCS Early Evaluation Tasks

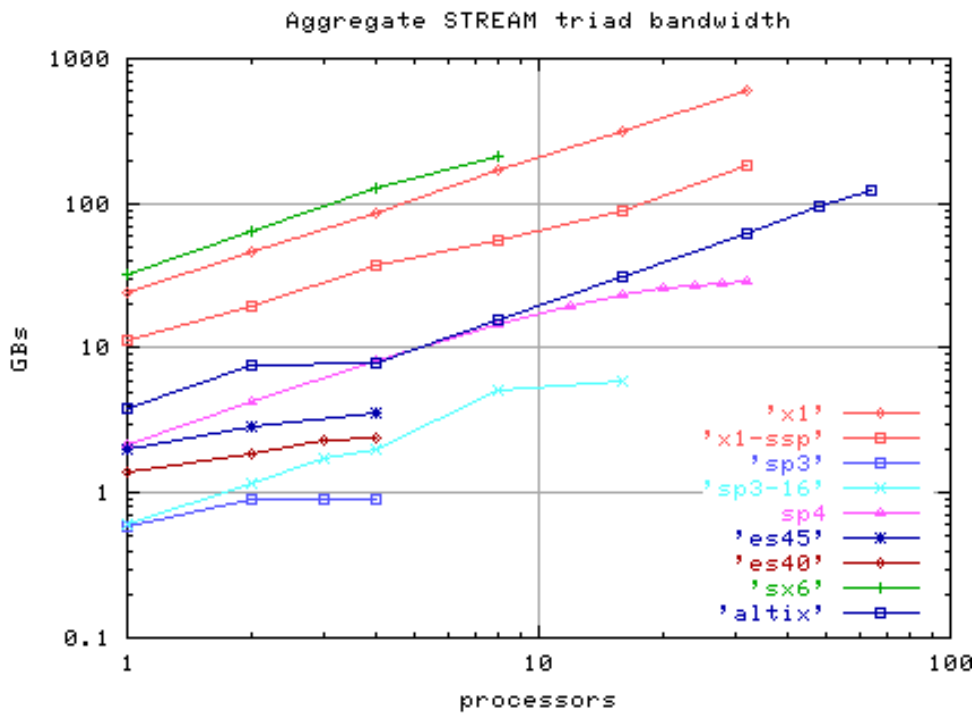
- Evaluate benchmark and application performance to compare with other systems
- Determine the most effective approaches for using the Cray X1
- Evaluate system and system administration software reliability and performance
- Predict scalability, both in terms of problem size and number of processors
- Collaborate with Cray to incorporate this information and experience into their next generation designs

Early Evaluation Methodology

- Hierarchical
  - Microbenchmarks → Kernels → Benchmarks → Applications
- Staged
  - Subsystems reevaluated following each expansion or upgrade
- Open
  - Fully disclose the test codes and results
  - Share results with vendors, colleagues, applications teams
  - http://www.csm.ornl.gov/evaluation

Microbenchmarks

- Euroben, STREAMS, and MAPS microbenchmarks characterized the underlying architectural components



See complete, current details at **www.csm.ornl.gov/~dunigan/cray/**

HPC Challenge

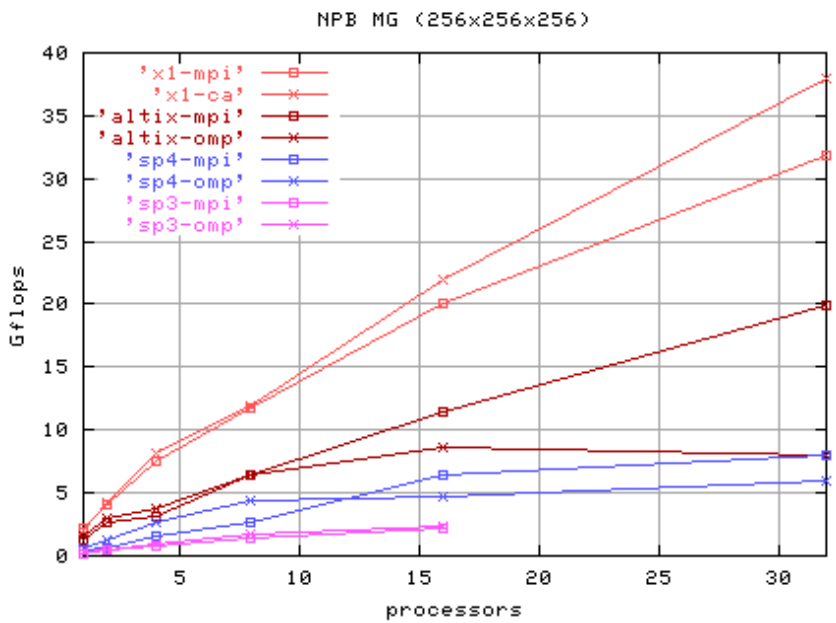
- New set of performance evaluation tests measuring wide array of system characteristics
- Need benchmarks in alternate languages (UPC, CAF)

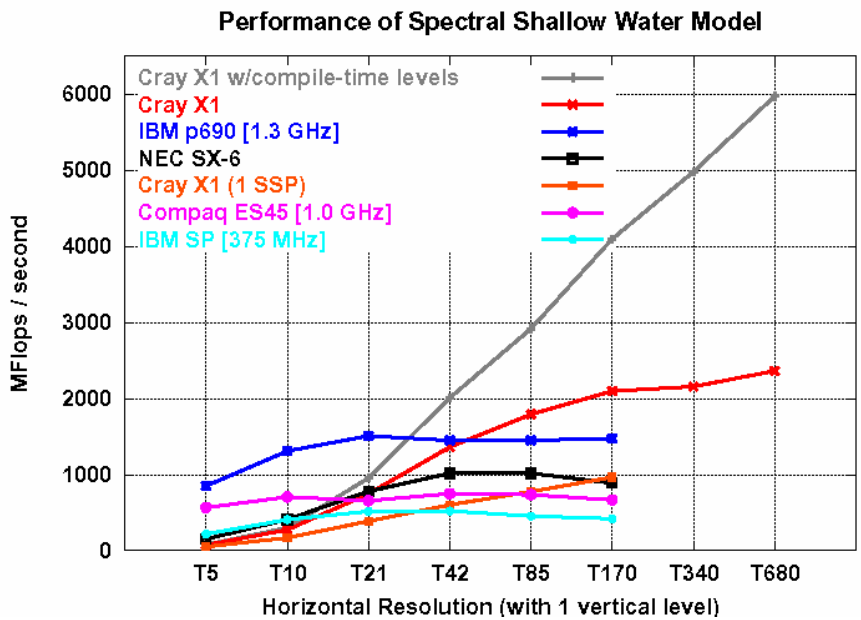
Computer	Run	Processors	HPL (system performance)	PTRANS (system performance)	*STREAM Triad (per CPU)	Random Access MPI (per CPU)	Random Ring Latency (per CPU)	Random Ring Bandwidth (per CPU)
System	Type	#	TFlop/s	GB/s	GB/s	Gup/s	usec	GB/s
Cray X1	base	64	0.522	3.229	14.99	0.00521	20.34	0.9407
HP AlphaServer SC45	base	128	0.19	1.507	0.803	0.00133	37.31	0.0278
HP Integrity zx6000	base	128	0.331	4.607	1.956	0.00145	32.44	0.0435
IBM p690	base	64	0.181	0.477	1.148	0.00057	101.96	0.0149
IBM p690	base	256	0.654	0.833	1.19	0.00031	373.99	0.0046
SGI Altix	base	32	0.131	0.7	0.896	0.00152	7.71	0.0258
SGI Altix	base	128	0.52	0.727	0.746	0.00089	24.34	0.0193

See HPCC talks tomorrow…

Kernels

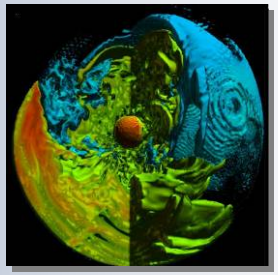
- Kernels from NAS, ParkBench, Euroben, and kernels from important DOE applications
- Experiment w/ vendor libs, alternate languages

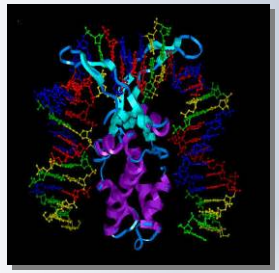




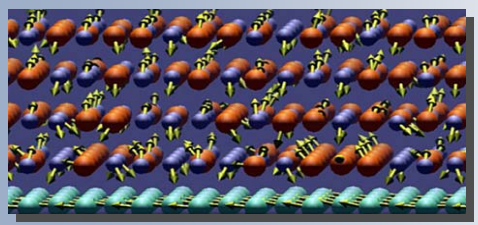
Focused on critical scientific challenges

SciDAC Astrophysics

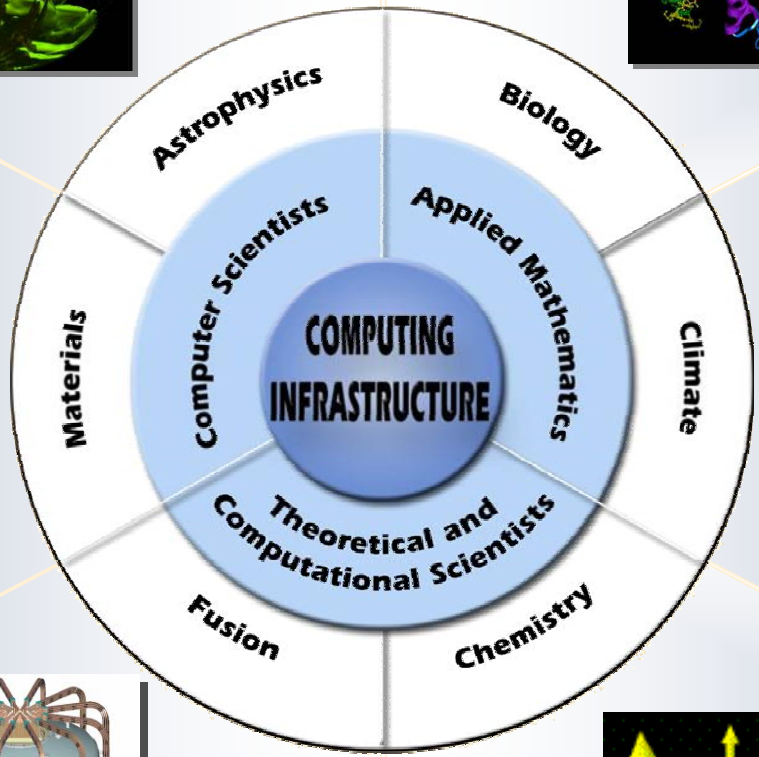


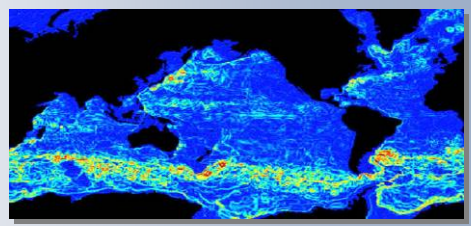


Genomes to Life



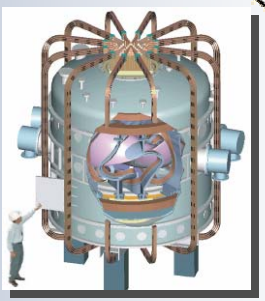
Nanophase Materials

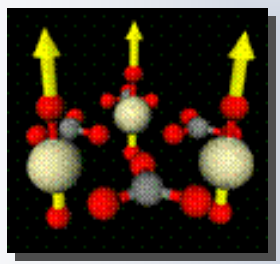




SciDAC Climate

SciDAC Fusion

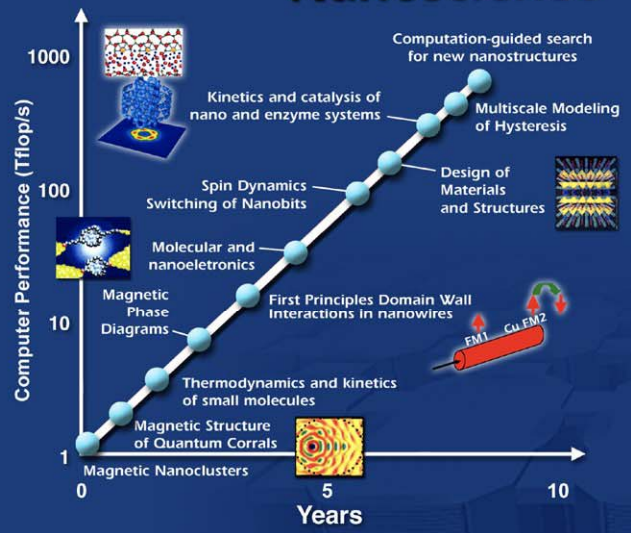




SciDAC Chemistry

Delivering Science and Leadership in High-end Computing

Nanoscience



Expected Outcomes

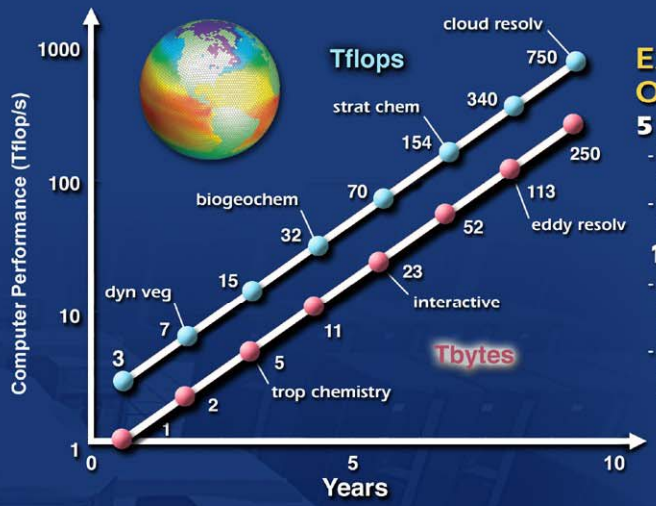
5 years

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

10 years

- Multi-scale modeling of molecular electronic devices
- Computation-guided search for new materials/nanostructures

Climate



Expected Outcomes

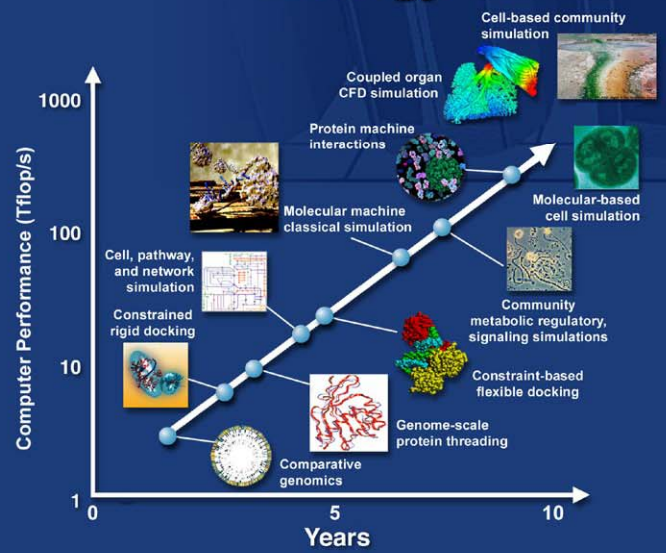
5 years

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

10 years

- Cloud-resolving 30-km spatial resolution atmosphere climate simulation
- Fully coupled, physics, chemistry, biology Earth system model

Biology



Expected Outcomes

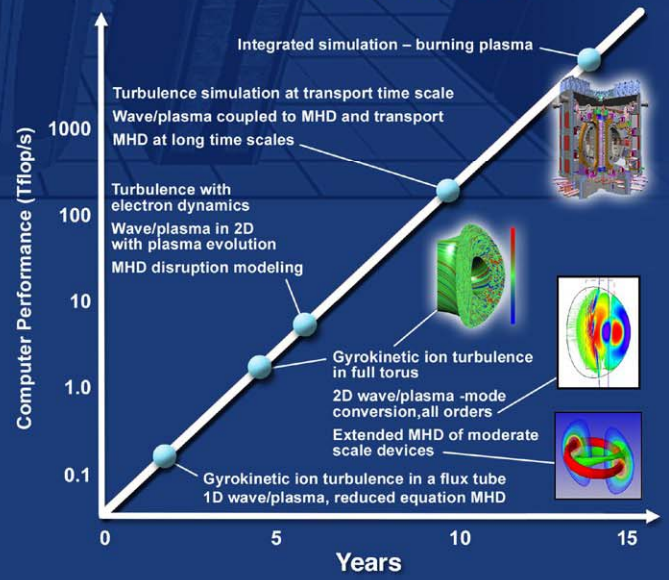
5 years

- Metabolic flux modeling for Hydrogen and Carbon fixation pathways
- Constrained flexible docking simulations of interacting proteins

10 years

- Multi-scale stochastic simulations of combined microbial metabolic, regulatory and protein interaction networks
- Dynamics simulations of complex molecular machines

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 - multi-physics predictions for ITER

Center for Computational Sciences
Oak Ridge National Laboratory

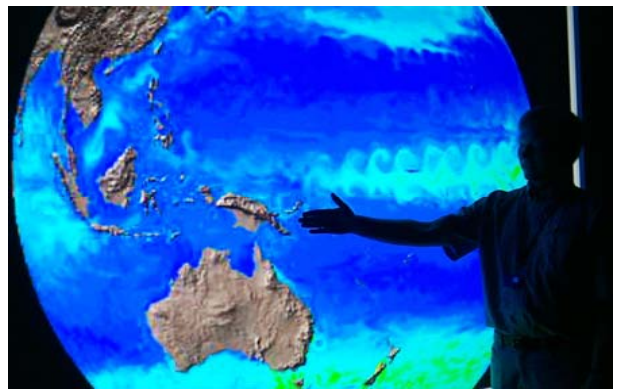
Office of Science
U.S. Department of Energy
ORNL 2003-03017A/jcs

Application Highlights from Cray X1 Evaluation

- Large-scale simulations of high-temperature superconductors
  - 25 times faster than on an IBM Power4 cluster using the same number of processors
- Parallel ocean program (POP v1.4.3) is
  - 50 percent higher than on Japan's Earth Simulator
  - 5 times higher than on an IBM Power4 cluster
- Fusion application, global GYRO transport,
  - 16 times faster on the X1 than on an IBM Power3.
  - Increased performance allowed simulations to fully resolve questions raised by a prior study
- Transport kernel in the AGILE-BOLTZTRAN astrophysics code
  - 15 times faster than on an IBM Power4 cluster using the same number of processors
- Molecular dynamics simulations related to the phenomenon of photon echo
  - 8 times faster than previously achieved

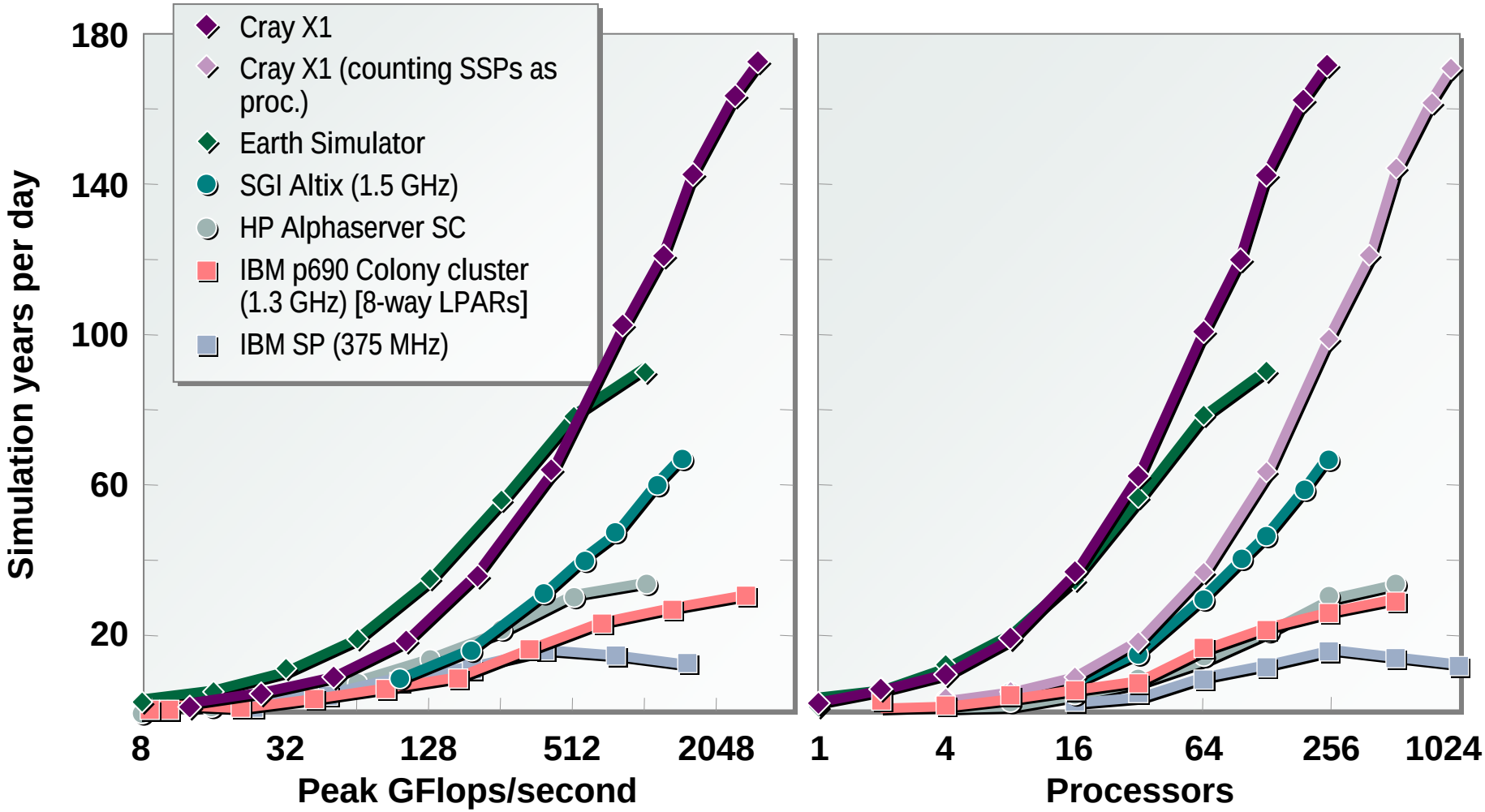
Climate Modeling

- Community Climate System Model (CCSM) is the primary model for global climate simulation in the USA
  - Community Atmosphere Model (CAM)
  - Community Land Model (CLM)
  - Parallel Ocean Program (POP)
  - Los Alamos Sea Ice Model (CICE)
  - Coupler (CPL)



- Recently, preparing for and running Intergovernmental Panel on Climate Change (IPCC) experiments

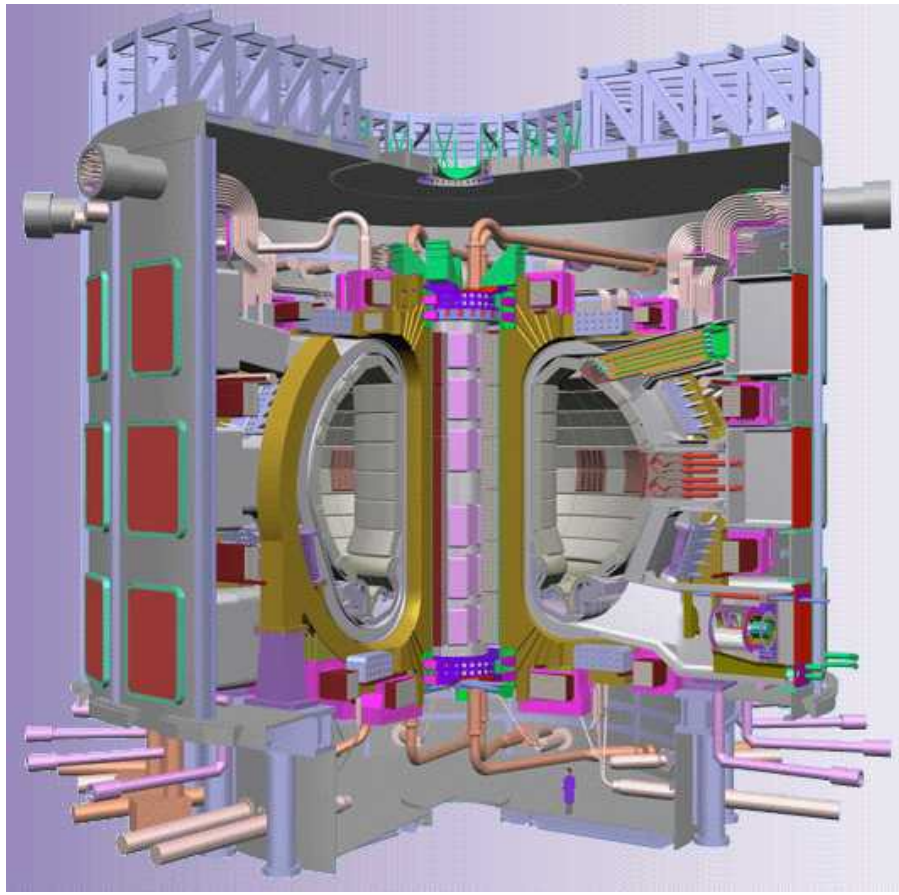
Parallel Ocean Program benchmark

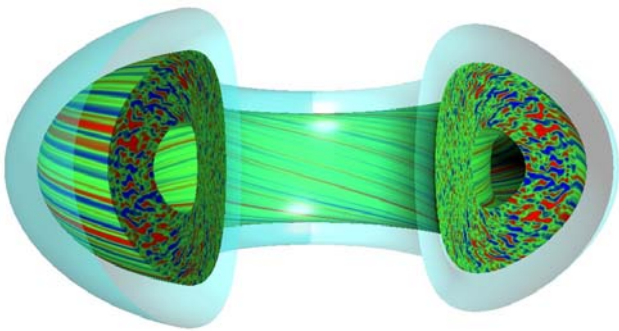


See POP, CLM, CCSM talks today and Thursday.

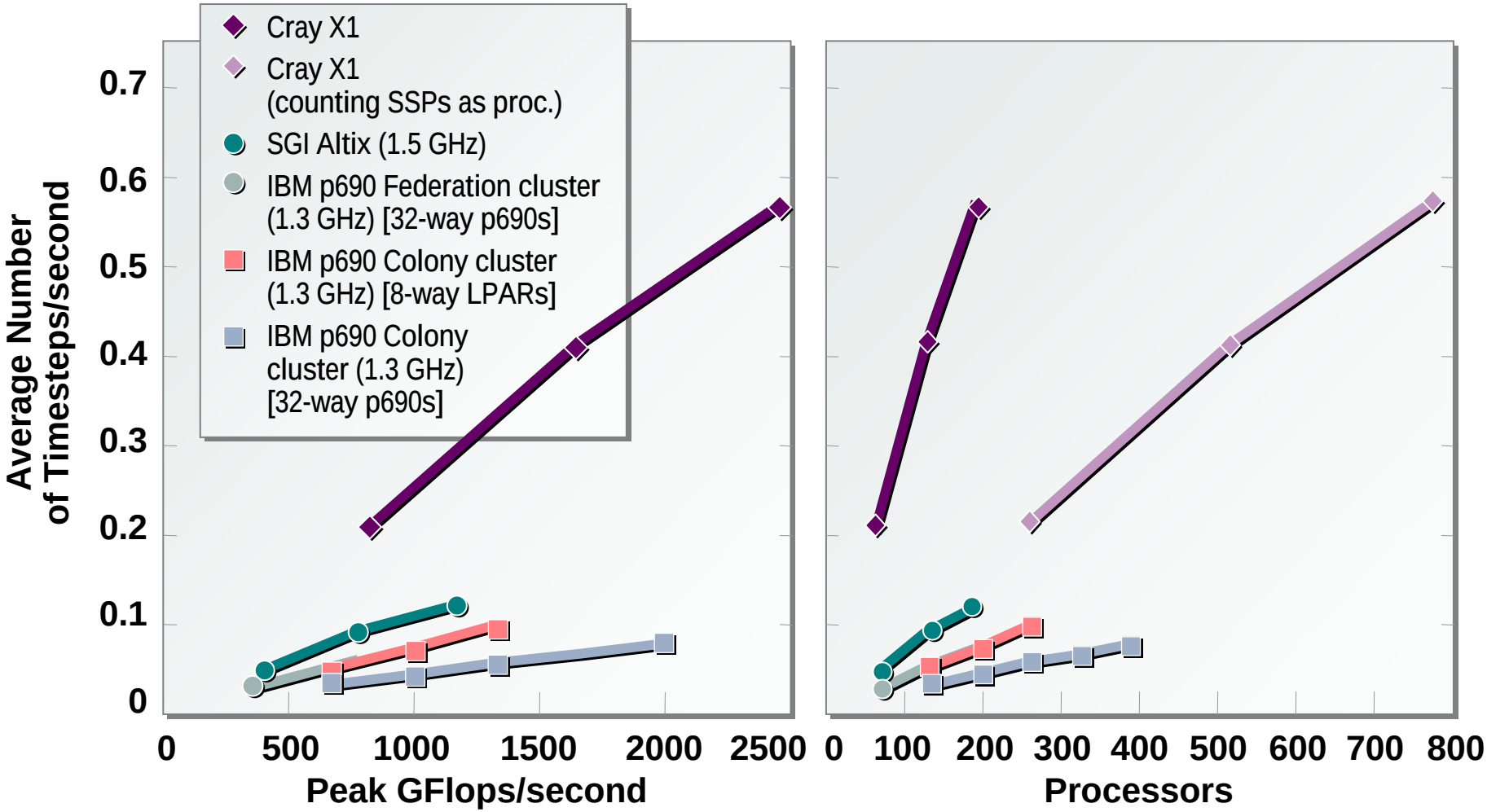
Fusion

- Advances in understanding tokamak plasma behavior are necessary for the design of large scale reactor devices (like ITER)
- Multiple applications used to simulate various phenomena w/ different algorithms
  - GYRO
  - NIMROD
  - AORSA3D
  - GTC





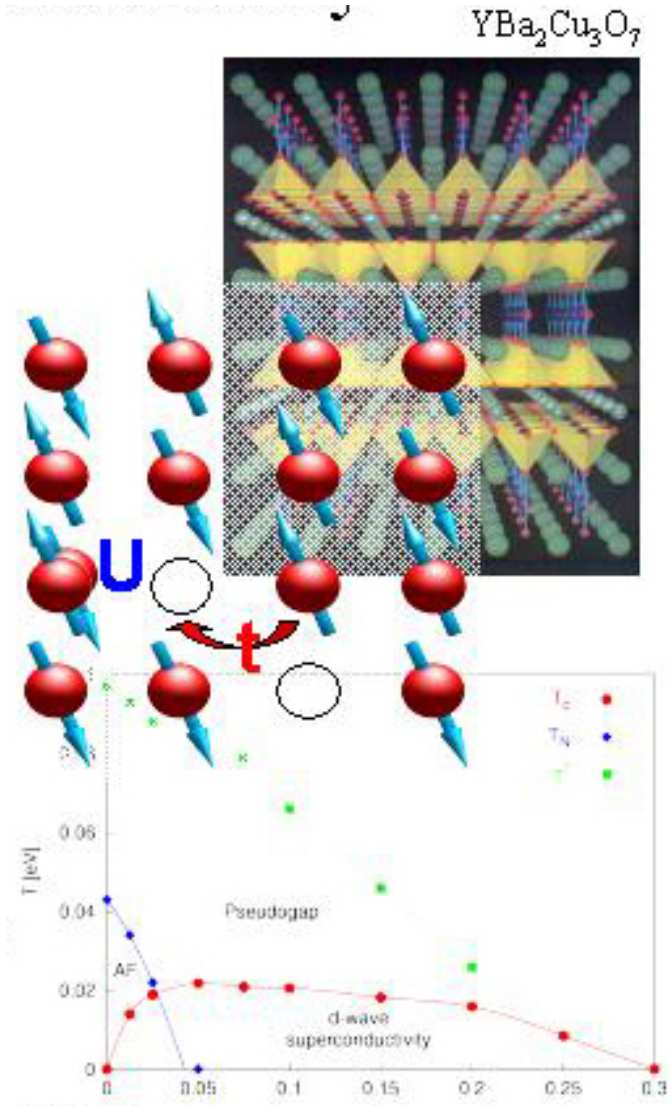
Fusion – GYRO GTC 64-mode benchmark



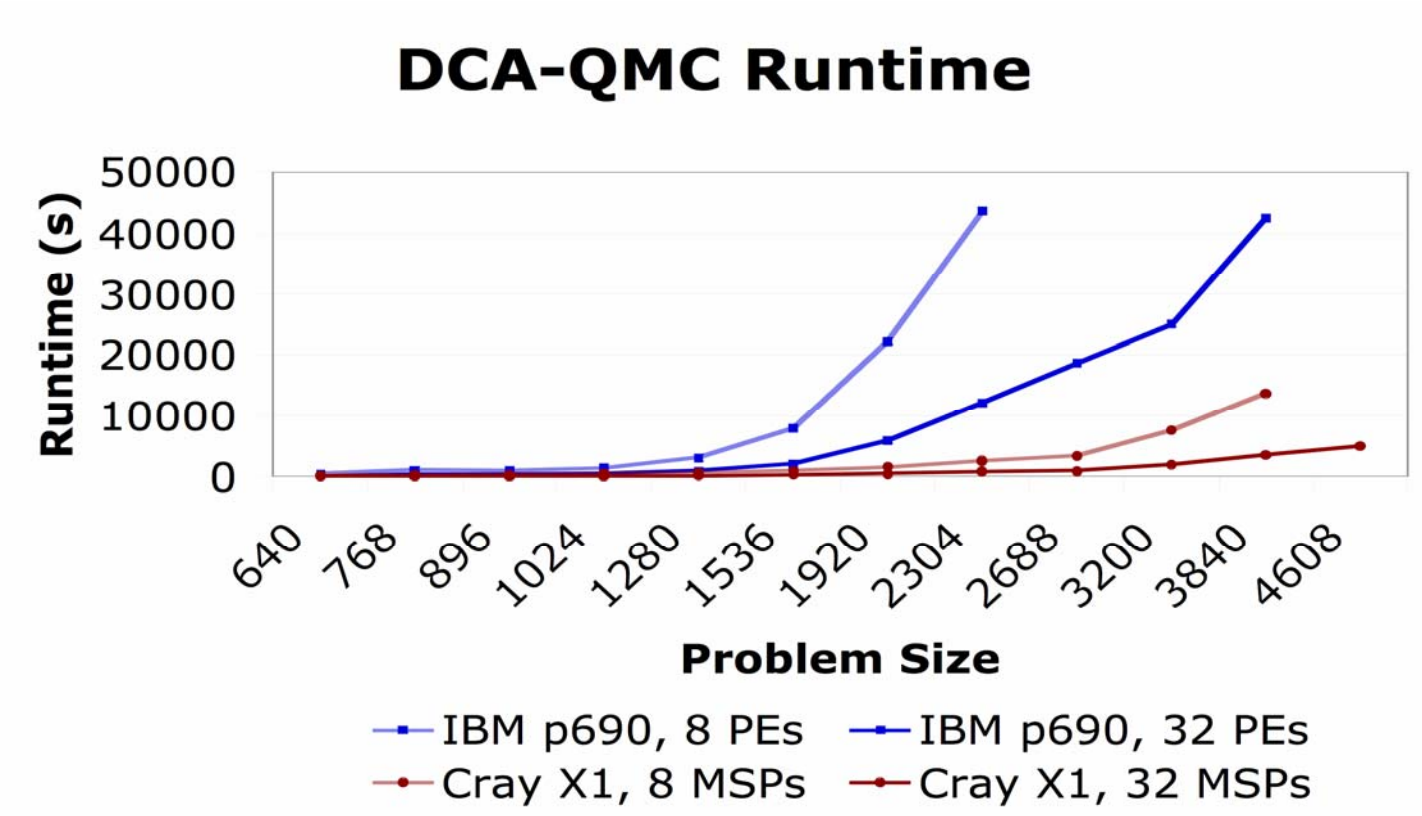
See GTC and GYRO talks Thursday.

Materials

- Simulation of materials science promotes
  - understanding of new phenomena like high-temperature superconductors
  - design of materials with specific properties, such as magnetism for a disk drive
- Applications include
  - DCA-QMC
    - Dynamic cluster approximation-quantum Monte-Carlo
  - LSMS
    - Locally-Self-Consistent Multiple-Scattering



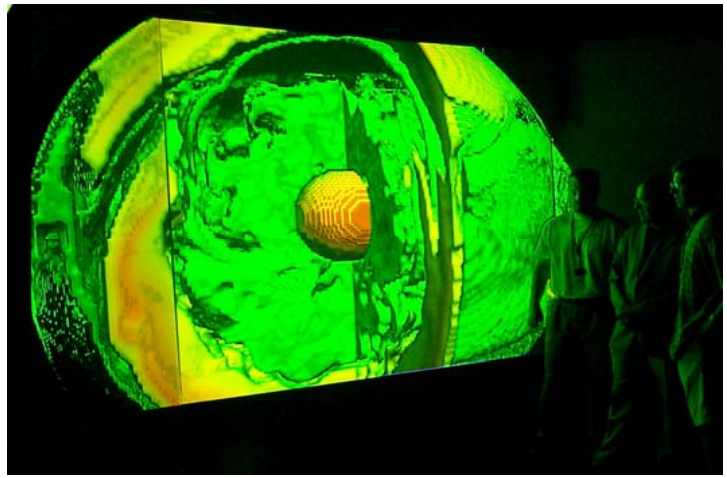
Materials Scaling



See Superconductors talk Thursday.

Astrophysics

- AGILE-BOLTZTRAN is a primary application for the SciDAC Terascale Supernova Initiative
  - Adaptive mesh hydrodynamics
  - Radiation transport, sparse



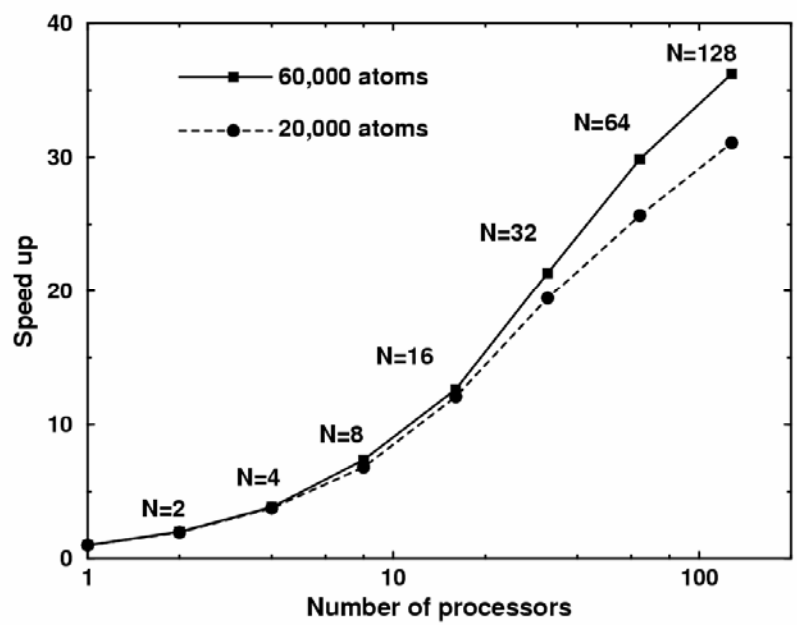
Transport step is at heart of AGILE-BOLTZTRAN overall solution step and of every radiation transport/hydrodynamics simulation

Problem Size = Number Mass Shells X Number Angular Quadratures X Number Frequencies

Problem Size8	No. Proc.	Power4 (Sec)	Cray X1 (Sec)	Speedup
100 X 6 X 12	1	19.1	3.8	5
100 X 16 X 16	100	100 (5 Nodes)	6.5 (25 Nodes)	15

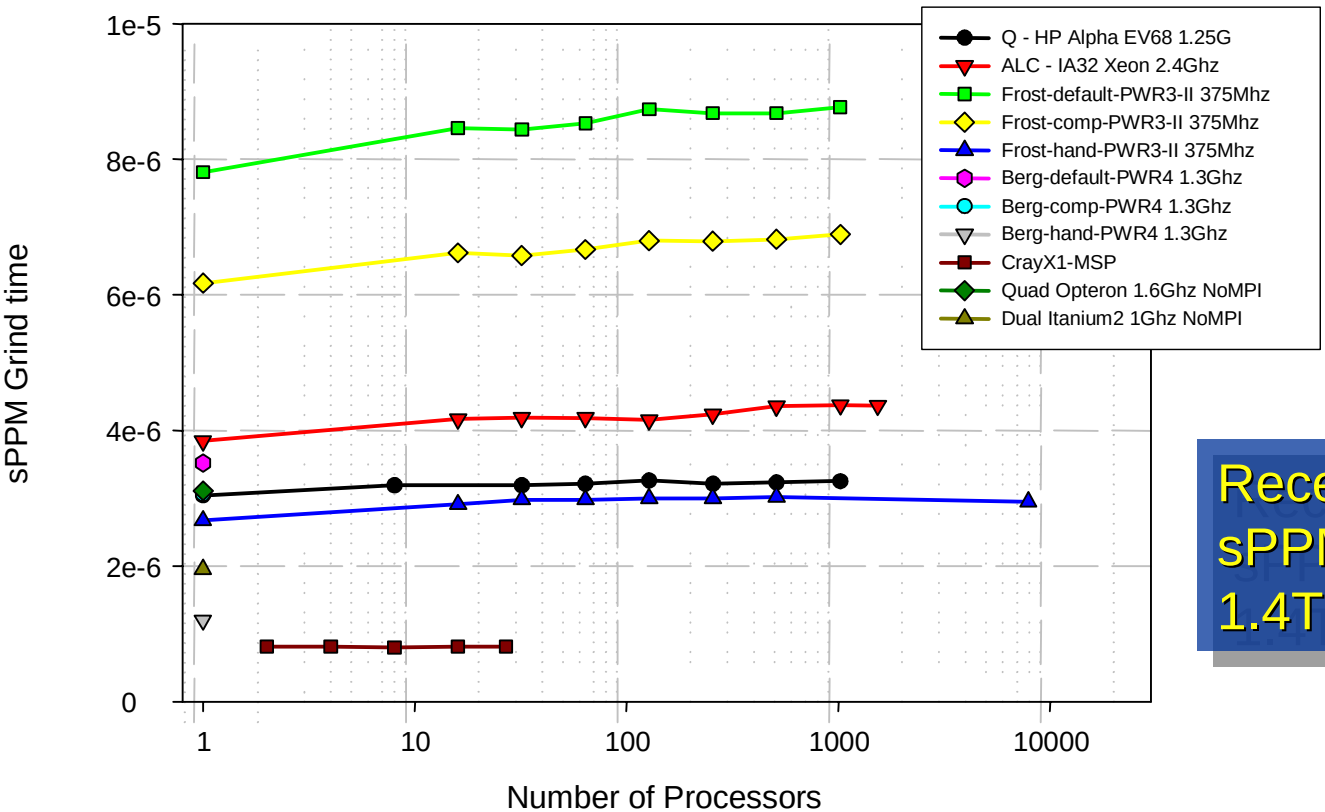
Biology

- AMBER is a popular application used for atomistic modeling of biological systems using molecular dynamics simulation
  - Current techniques fall short of simulating biologically relevant time scales by several orders of magnitude



sPPM

- Solves a 3-D gas dynamics problem on a uniform Cartesian mesh, using a simplified version of the Piecewise Parabolic Method



Recent efforts to optimize sPPM resulted in 1.4TF/s on 252 processors

Additional Examples in Report

- Atomic and molecular physics
- Chemistry
  - NWCHEM using ARMCI, Global Array Toolkit
- Cosmology
- System software and machine administration
- *Programming models*

See Atomic/molecular physics talk Thursday.
See Global Arrays talk Thursday

Outreach activities included workshops w/ user community
(http://www.csm.ornl.gov/meetings/)

- Applications Workshops, November 5-6, 2002
  - Climate, Materials, Biology, Fusion, Chemistry, Astrophysics
  - Cray, ORNL, LANL, PNNL, NCI
- Cray X1 Tutorial, November 7, 2002
  - >100 attendees from 20+ sites
- Cray-Fusion Workshop, February 3-4, 2003
  - Cray, ORNL, PPPL, U. Wisconsin, U. Iowa, General Atomics
- SciDAC CCSM Workshop: Porting CCSM to the Cray X1
  - NCAR, February 6, 2003 (followed CCSM Software Engineering Working Group meeting)
  - Cray, NEC, ORNL, NCAR, LANL
- Computational Materials Science: Early Evaluation of the Cray X1
  - Austin, March 2, 2003 (in conjunction with APS Meeting)
  - Invitees from 15 sites
- Cray Biology Workshop, March 18, 2003
- Others…

Announcement of National Leadership Computing Facility: A Partnership in Computational Sciences

- Last week's announcement
- Evaluations will continue on new platforms at larger scale … stay tuned

See tomorrow's keynote…

Related Presentations at CUG

Monday	1A	1:00	Cray X1 Optimization	John Levesque and Jim Schwarzmeier, Cray Inc., and Patrick Worley (ORNL)
Monday	2A	3:15	Cray X1 Optimization (continued)	John Levesque and Jim Schwarzmeier, Cray Inc., and Patrick Worley (ORNL)
Tuesday	5A	2:00	The Performance Evolution of the Parallel Ocean Program on the Cray X1	Patrick Worley (ORNL) and John Levesque, Cray Inc.
Tuesday	5A	2:30	Exploiting Architectural Support for Shared Memory Communication on the Cray X1 to Optimize Bandwidth Intensive Computations	Jarek Nieplocha and Manojkumar Krishnan, PNNL
Wednesday	8	8:30	Keynote Address	Thomas Zacharia (ORNL)
Wednesday	9	11:30	CSA (Cray Standard Accounting) Is No More - Panel Discussion	Jim Glidewell (BCS), Liam Forbes (ARSC), Arthur Bland (ORNL), and Michael Pettipher (MCC)
Thursday	13A	8:30	Performance Study of the 3D Particle-in-Cell Code GTC on the Cray X1	Stephane Ethier (ORNL)
Thursday	13B	8:30	Experience with the Full CCSM	John Drake and Pat Worley (ORNL) and Matthew Cordery and Ilene Carpenter, Cray Inc.
Thursday	14A	12:00	Optimizing Performance of Global Arrays Toolkit on the Cray X1	Jarek Nieplocha, PNNL
Thursday	14B	11:00	Towards Full Simulation of High-Temperature Superconductors	Thomas Maier, James B. White III (Trey), and Thomas Schulthess (ORNL)
Thursday	14B	11:30	GYRO—Analyzing New Physics in Record Time on the Cray X1	Mark Fahey (ORNL) and Jeff Candy, General Atomics
Thursday	14B	12:00	Computational Atomic and Molecular Physics	Michael Pindzola, F.J. Robicheaux, S.D. Loch, and U. Kleiman, Auburn University; D.R. Schultz, T. Minami, and T-G. Lee, (ORNL) D.C. Griffin and C.P. Ballance, Rollins College; J.P. Colgan and C.J. Fontes, (LANL); N.R. Badnell, A.D. Whiteford, M.G. O'Mullane, and H.P. Summers, University of Strathclyde; K. Berrington, Sheffield Hallam University
Thursday	15A	2:30	Dangerously Clever X1 Application Tricks	James B. White III (Trey) (ORNL)
Thursday	15B	3:00	Porting and Performance of PCM on the Cray X1	Vince Wayland (ORNL)
Thursday	16C	4:00	Adventures in Vectorizing the Community Land Model	James B. White III (Trey) and Forrest Hoffman (ORNL); Mariana Vertenstein, NCAR

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- Early evaluation started immediately
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  - Important DOE applications
  - Workshops
  - System opened to many users
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- Current X1 evaluation has produced impressive results on important DOE applications
- Close collaboration with Cray
  - Resolved issues, such as a scaling bug
  - Identified opportunities for improvements in future designs
- National Leadership Class Facility funded last week

More Info and Acknowledgements

Email: vetterjs@ornl.gov, vetter@computer.org

URLs: www.csm.ornl.gov

perc.nersc.gov

www.csm.ornl.gov/evaluation

www.ccs.ornl.gov

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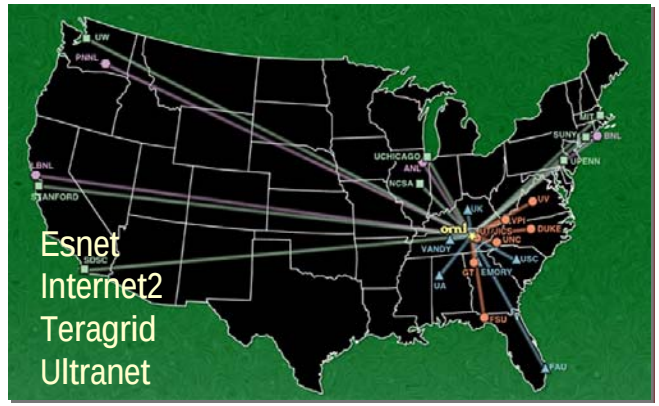
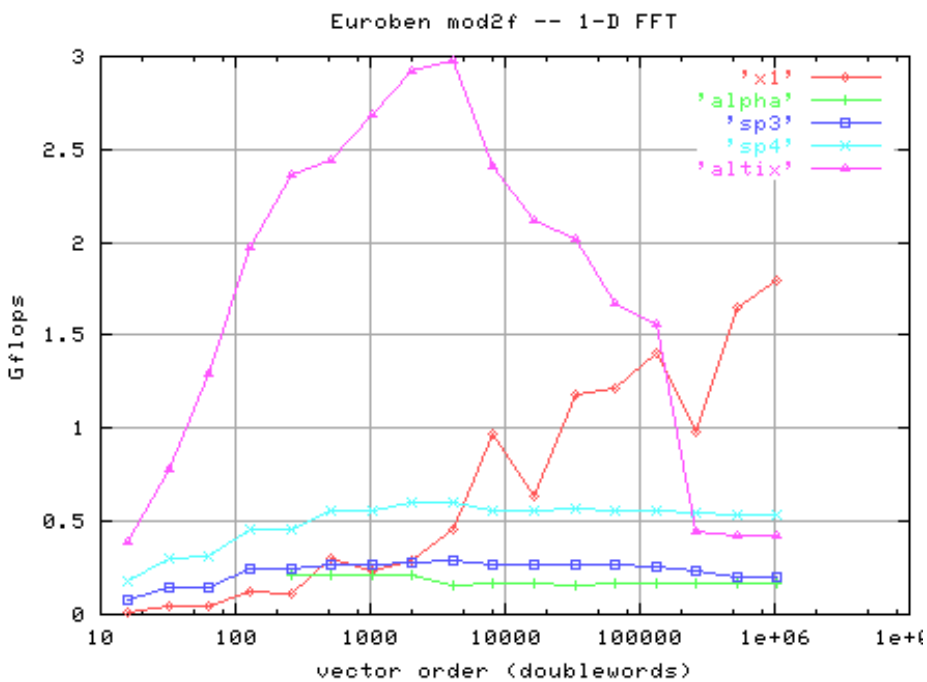
Bonus Slides

New world-class facility for leadership class computers

- 170,000 sq.ft. building
  - office space for 350 staff members
  - 40,000 ft2 computer center with 36-in. raised floor
  - 8 MW of power (expandable) @ 5c/kWhr
- Visualization lab w/ Cave, Powerwall, Access Grid, etc.



- State-of-the-Art network connectivity
- 5PB of HPSS storage


Euroben mod2f -- 1-D FFT
Gflops
vector order (doublewords)
'x1'
'alpha'
'sp3'
'sp4'
'altix'
0
0.5
1
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