The Supercomputer Company

Update on Cray Earth Sciences Segment Activities and Roadmap

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12th ECMWF Workshop on Use of HPC in Meteorology

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Topics

- Cray Update
 - Highlights of the Past Year
- Earth Sciences Segment Activities
- Increasing System Scale
- Roadmap Update

The Supercomputer Company

Highlights of the Past Year

- Spain's National Institute of Meteorology (INM) Begins Production Weather Prediction on Cray X1E - June 23, 2005.
- Pittsburgh Unveils Big Ben the Supercomputer -July 20, 2005:
 - 10 Tflops XT3
 - Protein simulations, storm forecasting, global climate modeling, earthquake simulations.
- ERDC Supercomputer Most Powerful In DoD -Dec 8, 2005:
 - 24 Tflops XT3
 - Sea-ice and storm surge modeling









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- Cray Selected by UK'S AWE Jan 24, 2006:
 - 41 Tflops Cray XT3 selected by United Kingdom's Atomic Weapons Establishment.
 - Sustained performance 30 Times the existing Blue Oak System.
- Korea Meteorological Administration's New Cray X1E Supercomputer Is World's Fastest Weather Prediction System - Feb 06, 2006
 - 18.5 Tflops X1E.
- Cray X1E Supercomputer at India's NCMRWF
 Will Be the Most Powerful Weather Prediction
 System in the Region Mar 13, 2006.

राष्ट्रीय मध्यम अवधि मौसम पूर्वानुमान केन्द्र National Centre for Medium Range Weather Forecasting (NCMRWF) Department of Science & Technology

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Korea Meteorological Administration



- Swiss National Supercomputing Center Will Expand Cray XT3 System - May 17, 2006:
 - Upgrade Will Boost Computing Power to 8.6 Teraflops.
 - Climate and weather is 2nd largest user community: ECHAM5, CCSM, LM.



- Cray Signs \$200 Million Contract to Deliver
 World's Largest Supercomputer to Oak Ridge -June 15, 2006:
 - Multi-year contract with the U.S. Department of Energy's (DOE) Oak Ridge National Laboratory (ORNL) to provide the world's first petaflops-speed supercomputer.
 - DOE-NSF Climate-Science Computational End Station established at ORNL.



OAK RIDGE NATIONAL LABORATORY



- UK'S EPSRC Selects Cray Inc. to Negotiate Multi-Year Contract for HECToR Procurement - June 27, 2006:
 - EPSRC is the main funding agency in the UK for research in engineering and the physical sciences.
 - Next generation national high performance computing service for the UK academic community with an initial theoretical peak capability of over 50 Tflops.



Engineering and Physical Sciences Research Council

• Sandia Red Storm Moves to 120 Tflops.





- Cray Wins \$52M Contract with NERSC Aug 10, 2006:
 - Contract to install next-generation supercomputer at the DOE's National Energy Research Scientific Computing Center (NERSC).
 - The Hood system installed at NERSC will deliver sustained performance of at least 16 Tflops with a theoretical peak speed of 100 Tflops.
- Finland's CSC Supercomputer Center Selects Cray Hood System - Oct 9, 2006
 - CSC Finland, the Finnish IT center for science, will acquire a Cray Hood system delivering over 70 Tflops.





Finnish IT center for science



Significant Progress in the ES Market

- Key wins and upgrades: KMA, NCMRWF, INM, KMA, AWI, NMOO, CERFACS...
- CWO modeling represents significant usage of large scale wins: ORNL, PSC, CSCS, Sandia, ERDC, HECToR, CSC,...
- Establishment of the KMA-Cray Earth System Research Center.
- Leading weather and climate science on Cray systems:
 - IPCC assessments on ORNL X1E.
 - DOE/NSF Climate-Science Computational End Station at ORNL using X1E and XT3.
 - Partner in Germany-Korea cooperation "Earth System modelling and data analyses focusing on the East Asian region".
- Active participation in the community.
- Performance records on a number of leading weather and climate models.
 - Unprecedented scalability.









SEAM Scalability

- Spectral Element Atmospheric Model
- Spectral elements replace spherical harmonics in horizontal directions.
- Coupled to the Community Atmospheric Model (CAM)
- Run to 10km global resolution



Billion grid point simulation of a polar vortex that has trapped air at the pole.

Parallel Scalability



Performance of 4 fixed problem sizes, on up to 6K CPUs. The annotation gives the mean grid spacing at the equator (in km) and the number of vertical levels used for each problem.



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Increasing System Size

- Sandia National Laboratories Red Storm recently upgraded to 120 Tflops.
- NERSC 100 TFLOPS Hood in 2007.
- ORNL 50 TF, 100TF, 250TF, ...1 Pflop by end of 2008.
- Preferred bidder at EPSRC/HECToR
 - Initial peak capability of over 50 TFLOPs
- AWE: 41 Tflops XT3
- CSC: >70 Tflops Hood
- Inertia of experience...





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CSC



National Leadership Computing Facility

- Cray-ORNL Selected by DOE for National Leadership Computing Facility (NLCF).
- Goal: Deliver National Leadership Computing Facility for science:
 - Focused on grand challenge science and engineering applications
- Principal resource for SciDAC and other programs:
 - Specialized services to the scientific community: biology, climate, nanoscale science, fusion
- Today: 18 TF X1E and 50 TF XT3
- 250+ TF capability by 2007 and PF in late 2008.



OAK RIDGE NATIONAL LABORATORY

CCCS The Center for Computational Sciences DOE High Performance Computing Research Center





Combustion Plas

Plasma Behavior Simulation





Astrophysics

Jaguar <u>Since upgraded to 10,000+ processors</u> 5,294 processors and 11 TB of memory



Accepted in 2005 and routinely running applications requiring 4,000 to 5,000 processors

A "good" MPP will generate usage patterns like this: Lots of jobs using 1000s of processors

- 43% of time used by jobs using 40% of system or more
- 61% of time used by jobs requiring 1000+ processors



Machine Usage by Number of Processors



Oak Ridge National Laboratory

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Jaguar's Path to 250 TF

Jaguar 2006 upgrade

- Upgrade single-core to dualcore (2.6 GHz)
- Upgrade memory to maintain 2 GB per core
- Add 68 cabinets (total of 124)
- 11,508 dual-core compute sockets
- 119 TF peak
- 46 TB memory
- 900+ TB disk storage
- 55 GB/s disk bandwidth

Jaguar 2007 upgrade

- Upgrade 68 cabinets to multicore
- O(5000) dual-core compute sockets
- O(6000) multi-core compute sockets
- Double memory in upgraded nodes
- 250+ TF peak compute partition
- 50+ TF data analysis partition
- 70 TB memory



FOR COMPUTATIONAL SCIENCES

Petascale Ambitions

- Japan, Europe and US climate communities have all announced ambitions to reach Petaflop level by early in the next decade:
 - Japan Earth Simulator II (MEXT)
 - Europe ENES EVE:lab
 - US NSF Petascale Collaboratory
- US and Japanese government funding into R&D petascale computing:
 - MEXT Petaflop Project
 - DARPA HPCS
- Ongoing NSF "Track 1" solicitation for Petascale facility by 2011.
- First actual contract is between ORNL and Cray to deliver a Pflop by 2008.





Ministry of Education, Culture, Sports, Science and Technology





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Diverse Application Requirements

Table 2. Application computational, memory, data storage, and disk bandwidth requirements for various geoscience applications.



<u>Couple of</u> <u>comments:</u> - all apps will be "massively" parallel. - Definition of performance metrics vary

greatly.

Application Name/ Discipline	Problem	Max Required Sustained TFLOPS	System Memory (TBytes)	Mass Storage Archive Rate (PBytes/ year)	Disk Bandwidth for 5% overhead (GBytes/sec)
flow_solve/ oceanography	3-D turbulence	2.5	6.5	0.14	1.1
POP/ oceanography	10 km global mesoscale eddy	6	0.15	0.32-3.2	0.2-2.0
POP/ oceanography	5 km global mesoscale	120	1.5	3.2-32	2-20
MITgcm/ocean data assimilation	15 km global ocean	7.3	0.82	0.66	0.4
WRF/meteorology	10 m tornado simulation	150	20	2-24	25-300
	5 years of 3 km global nonhydro- static simulation	66	1.75	1.0	8
CAM/climate modeling	Five instances of T341L52	13	0.5	4.6	1.1
CRCP/climate modeling	2 km global sub-grid scale model	22	-	-	-
ABINIT/minerology	DFT calculation	1.6	-	-	-
inverse problem/regional seismology	100M point inverse problem	17	0.01	0.12	0.07
forward problem/global seismology	36.6 billion degrees of freedom	10.4	7.3	0.01	0.00002
LADHS/regional hydrology	100 m Columbia river basin	10	0.3	20.8	0.66

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Achieving Effective System Scalability

- Computation is increasingly cheap compared to data movement.
- Most hardware cost is in interconnect:
 - Packages, circuit boards, connectors, wires, routers, electrooptics, fibers, etc.
- Rate of increase in system scale is increasing:
 - Reliability, fault detection/containment/recovery requirements.
 - Network bandwidth becomes even more critical (cost and performance).
 - Need to get the system software right.
 - Scalability is primary determinant.
 - A holistic approach is mandatory: computing, system software, I/O, data management,....



Achieving Effective System Scalability

- Moore's Law has affected all systems:
 - Classic vector systems relied upon uniform connectivity to global shared memory (no memory hierarchy).
 - For vector systems to advance at Moore's Law rate, they have been forced to adopt hierarchical memory.
 - This is a system architecture issue; orthogonal to processor architecture.
- All systems are massively parallel...
- Only a question of how effectively they can scale and be utilized.
- Must invest in a wide range of technologies to achieve effective system scalability.



Cray MPP Experience and Lessons

- Began with MPP Advisory Group
 - Formed in 1991, a mechanism to engage user community to understand MPP issues.
- Cray XT3 is 3rd generation MPP product.
- 2 key areas:
- Lightweight Kernel:
 - Jitter free OS permits finest grain synchronization for MPP performance on broadest range of problems
 - No time sharing
 - No large SMPs
 - No paging
 - No spurious daemons
 - Minimal OS interrupts

Interconnect:

- Scalability in all aspects
- Interconnect architecture
- High bandwidth global I/O where files are equally accessible from any part of the system
- Administrative ease with single boot image and fast boot time
- Fast application launch
- Resiliency



Capability MPP Computing at Cray



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Summary

- Continued product innovation focused on high performance computing:
 - Leverage and integrate key technologies.
 - Invest in emerging technologies to meet future requirements.
 - Invest in customer relationships to further develop technologies.
- The successful realization of production petascale facilities will require both the earth system modeling and HPC vendor communities to maximize every level of parallelism available.
- Cray's MPP experience and technologies will play an important role in the realizing future needs of earth system modelers.

Thank you for your attention

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