

Early Operations Experience with the Cray X1 at the Oak Ridge National Laboratory Center for Computational Sciences

**Arthur Bland, Richard Alexander, Steven M. Carter,
Kenneth D. Matney, Sr., Oak Ridge National Laboratory**

ABSTRACT: Oak Ridge National Laboratory (ORNL) has a history of acquiring, evaluating, and hardening early high-performance computing systems. In March 2003, ORNL acquired one of the first production Cray X1 systems. We describe our experiences with installing, integrating, and maintaining this system, along with plans for expansion and further system development.

1. Introduction

The Center for Computational Sciences (CCS) at the Oak Ridge National Laboratory (ORNL) is an advanced computing research test bed sponsored by the U.S. Department of Energy's (DOE) Office of Advanced Scientific Computing Research. Its primary mission is to evaluate and bring to production readiness new computer architectures and to apply those resources to solving important scientific problems for the DOE. In 2002 the CCS proposed evaluating the Cray X1 for use as a scientific computing system by the DOE Office of Science. The first phase of this five-phase plan was funded and the first of eight cabinets was installed in March 2003. In collaboration with other national laboratories and universities, the CCS is currently evaluating the system to determine its strengths and weaknesses. The ultimate goal of the project is to provide data for the DOE in its selection of the architecture of a leadership class computer system for open scientific research. The CCS has outlined a path to this goal that grows the Cray X1 and then upgrades to the follow-on system, code-named "Black Widow."

2. Overview of the CCS

The CCS was founded in 1991 by the DOE as part of the High Performance Computing and Communications program and was one of two high-performance computing research centers created in DOE national laboratories. At the time massively parallel computer systems were just starting to make their commercial debut into a marketplace for scientific computing that had been dominated by parallel vector systems from Cray Research. ORNL was well suited to this task having had a Cray X-MP system as well as six years experience converting vector applications to run on experimental parallel systems such as the Intel i/PSC series of systems.

From the beginning, the CCS had three primary missions:

- Evaluate experimental new architectures to see how they work for DOE Office of Science applications;
- Work with the manufacturers of these systems to bring the systems to production readiness;
- Use these new systems on a few applications that are both important to the nation, and cannot be addressed with the conventional computer systems of the day.

Over the last decade, the applications of interest at the CCS have centered around six major areas:

- Materials Science – Many of ORNL's major programs center on materials science. ORNL is the site of the ongoing construction of the nation's largest unclassified science project, the Spallation Neutron Source. This \$1.4 billion project will provide neutron streams for exploring the structure of both hard and soft materials.
- Global Climate Change – The DOE has a major program in global climate modelling to understand the energy needs of the world and the impact of energy production and usage on our environment. The CCS has a major program in Climate and Carbon Research.
- Computational Biology – The fields of genomics and proteomics require massive computational power to understand the basis of all life. DOE's biology program began with the Manhattan Project to understand the effects of radiation on cellular biology. That program has grown into a major effort in genomics.
- Fusion – Fusion reactors hold the promise of providing virtually unlimited power from abundant fuel. Modelling these reactors has proven to be a daunting task that requires the most powerful computers available.
- Computational Chemistry – Modelling of complex chemical processes help understand everything from combustion to drug design.

- Astrophysics – Basic research into the origins of the universe provides an understanding of the nature of matter and energy. Modelling a supernova explosion is among the most computationally complex phenomena being attempted today.

Today the CCS provides a capability computing center with over 6 TFLOP/s of peak capacity for DOE researchers and our university partners. The DOE Scientific Discovery through Advanced Computing (SciDAC) program is a \$50 million program to develop a new generation of scientific application programs and is a major initiative within the DOE. The CCS was selected to provide the majority of the compute infrastructure for SciDAC.

ORNL and the CCS have a long history of evaluating new, experimental computer architectures. In all, over 30 different computer systems have been evaluated over the last 15 years, with many more under active or planned evaluation. Some of the major systems where ORNL has evaluated a prototype, beta, or serial number one system include: KSR-1, Intel i/PSC-1, i/PSC-2, i/PSC-860, Intel Touchstone Sigma and Paragon MP, IBM Winterhawk-1, Winterhawk-2, Nighthawk-1, Nighthawk-2, S80, Regatta H, Compaq AlphaServer SC40 and SC45, and the Cray X1. In the near future, the CCS is planning evaluations of the SGI Altix with Madison processors, the Red Storm system jointly designed by Sandia National Laboratories and Cray, Inc., the IBM Blue Gene/D system, and the Cray Black Widow machine.

3. Facilities and Infrastructure

The CCS provides the facilities, computing, networking, visualization, and archival storage resources needed by the DOE Office of Science's computational scientists.

3.1 Computational Science Building

ORNL has long recognized that computational science is an equal "third-leg" of the scientific discovery triangle with experiment and theory. However, the facilities needed to support leadership class computers have not been funded by the DOE for unclassified scientific research. To bridge the gap, in 2002 ORNL broke ground on a new computational sciences building (CSB) as well as another new building to house the Joint Institute for Computational Sciences (JICS). The CSB provides 170,000 square feet of space to house the laboratory's computing infrastructure. The center piece is a 40,000 square foot computer room with up to eight megawatts of power and up to 4,800 tons of air conditioning. When completed in June 2003, this will be the nation's largest computer center for scientific research. The CSB also houses the fibre-optic communications hub for the laboratory, providing direct access to high-speed, wide-area networks linking ORNL to

other major research laboratories and universities. Adjacent to the computer room is a new 1,700 square foot visualization theater to help the researchers glean understanding and knowledge from the terabytes of data generated by their simulations. Finally, the building has office space for 450 staff members of the Computing and Computational Sciences Directorate of ORNL. An additional 52,000 square foot building to house JICS is under construction across the street from the CSB. JICS is the university outreach arm of the CCS and this building will provide laboratory, office, classroom, and conference space for faculty and students collaborating with ORNL researchers.

3.2 Computer Systems

The major production computer system of the CCS is a 4.5 TFLOP/s IBM Power4 Regatta H system. The machine is composed of 27 nodes, each with 32 processors and from 32 GB to 128 GB of memory. The system is linked with two planes of IBM's Switch2 or "Colony" interconnect providing high-speed communications among the nodes of the machine. In 2003, the CCS will be partnering with IBM to test the next-generation interconnect technology, code-named "Federation". This will provide an order of magnitude increase in the bandwidth between nodes while cutting the latency in half.

The second major system is the new Cray X1 system. Today, this machine has 32 MSPs and 128 GB of memory for a total of 400 GFLOP/s of peak performance. By the end of September 2003, the system will be expanded to 256 MSPs and 1 TB of memory, providing a peak performance of 3.2 TFLOP/s.

Additional systems include a 1 TFLOP/s IBM Power3 system and a 427 GFLOP/s Compaq SC40. This summer, we will also add a 1.5 TFLOP/s SGI Altix system with 256 Madison processors and 2 TB of globally addressable memory.

3.3 Networking

Gone are the days of hungry graduate students and researchers making the pilgrimage to the computer center to worship at the alter of the giant brain. Today, the majority of the researchers using high-performance computers around the world will never get near or see the computer system. Fully two-thirds of the users of the CCS are located outside of Oak Ridge. Thus our challenge is to provide the networking infrastructure and tools to make accessing the computers and their data just as fast, convenient, and secure as if the resources were local to the user. The CCS has two primary connections to our users. For DOE users, the CCS is connected to the DOE's Energy Sciences network-ESnet-which is a private research network. ESnet provides an OC12 connection (622 mega-bits per second) linking to an OC48 (2 Gbps) backbone. To link to our university partners, ORNL has contracted with Qwest to provide an OC192 (10 Gbps) link from ORNL to Atlanta where it

connects to the Internet2 backbone and links to major research universities around the country. But providing the wires is only the first piece of a complex stack of software to make the computers truly accessible to our distant users. The CCS is an active participant in the DOE Science Grid project. This project will provide seamless connectivity and high bandwidth between sites through the addition of grid middleware and tools to our computers.

3.4 Visualization, Data Analysis, and Archival Storage

In a world where a single climate calculation can easily generate tens of terabytes of data, a supernova simulation might generate 100s of terabytes, and experimental results from experimental devices can take petabytes, a leadership class computing center must have tools to manage the explosion of data. The CCS is building a new visualization theater based on the Sandia National Laboratories Views Corridor research. This 20+ megapixel display system will provide state-of-the-art resolution for seeing the complex structures of turbulence in a supernova explosion, or the sub-atomic structure of a new material. The new SGI Altix system will have 2 TB of globally addressable memory to ease the task of finding information from these massive datasets. In collaboration with four other national laboratories and IBM, the CCS is a developer of the High Performance Storage System (HPSS). This system provides scalable bandwidth, metadata management, and archive size for the most demanding data centers. Together, these systems provide an environment that simplifies the task of converting data into knowledge.

4. Early Operational Experiences

By and large, the Cray X1 installation and early operational experiences have been as expected. The hardware has been very stable. At delivery there was one node board that had to be reseated and one disk drive failed. Both of these occurred in the first two days of operation of the machine. Since that time, we have had one additional hardware problem, a failed power supply on a node board, and a case of the L0 diagnostic controller hanging and requiring a reboot. I give the hardware an “Exceeds Expectations” for reliability.

The software is a different story. It was known that UNICOS/mp was a new operating system and as such, would have some rough edges. Overall, the system is “Meeting Expectations” but it has a long way to go before it is a stable production system. On the other hand, the system is more stable than we had feared it might be. According to Cray’s internal “Cruise” system, the CCS machine is showing a MTTI of 86 hours on software. But this doesn’t tell the entire story. This only includes actual panics or crashes of the operating system. There have been numerous occasions when PSCHED quits dispatching jobs or everything in the system will hang. But even these problems have not been a major problem for us in early software development and testing.

The system arrived on Tuesday, March 18, 2003. It is a 32 MSP, liquid cooled chassis with a single IOC attached. Power was turned on Wednesday, March 19th. By the end of the day Wednesday, the diagnostic programs were running. On Thursday, March 20th, the operating system was first started. The operating system had been preinstalled at the factory by our on-site analyst team of Jeff Becklehimer and Sherri Ball along with the CCS system administrators Ken Matney, Steven Carter, and Richard Alexander. On Friday, March 21st, the initial acceptance test for this cabinet was run and passed without any problems.

The following week began the work to integrate the Cray X1 into the CCS operational environment. The CCS uses DCE for the authentication and authorization mechanism on all of our other computers and our archival storage system. However, DCE is not available for UNICOS/mp and is losing support on other platforms. So the CCS is in the process of converting to an LDAP based system for authorization and using Kerberos 5 for authentication. Since neither of these is supported on UNICOS/mp, we began with porting Kerberos 5 to the system. There were several compiler problems that seemed to prevent building Kerberos 5, so Cray provided a version that the Army High Performance Computing Center was able to get working. In parallel, we developed scripts to export a password file out of the DCE registry to the Cray and that is run several times per day to keep accounts and passwords up to date. Users log on to the Cray and then use KINIT to authenticate to DCE and obtain tickets which are then passed to our DFS file system gateway. Once authenticated in this manner, the user can access his home directory without further use of passwords.

There were a number of minor configuration challenges to work through. Sendmail would not deliver mail to external machines. There were debugging problems with the NFS gateway to DFS when using TCP protocol. The compiler performance on the CPES was poor. And configuring fiber channel disk services for optimal I/O performance turned out to be a challenge.

There are three rather major problems that ORNL sees with the Cray X1. The first is the link between the X1 and network through the Cray Network Subsystem (CNS). While a great improvement over the ION used with the early production machines, it is still a slow and expensive solution for connecting the X1 to the network. Driving the network takes a significant fraction of an MSP; the performance is poor for small packets, and only marginally better for large packets. To get around some of this problem, we are using UDP for NFS traffic, but that has additional problems in that the TCP_ASSIST feature of the CNS cannot be used to consolidate many small packets into larger packets to limit the overhead of the X1. However,

the X1 MSP is not a good CPU for doing IP protocol processing. At a minimum, we need to be able to aggregate services over multiple CNS systems with single streams sharing several parallel paths. We also believe there is a need to open up the protocol so that the fiber channel link between the X1 and the CNS can be routed to other devices, such as NFS or HPSS servers as a way of minimizing the overhead and latency between the boxes.

A second problem is the need for a user selectable authentication and authorization systems such as PAM from Linux. The current requirement for password files as the only authentication method is inadequate. With more and more need for computer security and every site and agency selecting differing methods for implementing security, Cray needs to adopt a standard method of implementing site specific security policies. However, implementing such a change is not as easy as it may seem. Since most of the work of authentication and manipulation of the password file is done in LIBC, changes to this library will require the implementation of dynamic libraries in UNICOS/mp. Otherwise, every change to the authentication method will require that all codes be relinked.

A third area for improvement is the programming environment. Compile time started as very slow and has improved markedly. However, compiling codes still takes much longer on the X1 than on other systems. Cray has promised a cross compile environment will be available, soon. This may solve part of the problem, but the underlying network slowness, slow NFS mounts, and slow compiler all make program development a more painful process than on other supercomputer systems. It is important for Cray, working with their early deployment sites, to solve these problems quickly.

While there are challenges yet to be resolved, the CCS has found the Cray X1 to have excellent hardware reliability and better than expected software stability. As with any new system, there are some areas that need work, but we have received excellent support from both our local Cray team and from the software development organization.

5. Future Plans

Oak Ridge National Laboratory and the CCS have had over 18 years experience using parallel cluster computers from every major vendor and using Beowulf style clusters of commodity systems. All of our major applications have been ported to run on distributed memory systems. In this process, we have found a number of applications that run very well on cluster systems. For example, the LSMS electronic structure code was developed on our 3000+ processor Intel Paragon system and provides near linear scaling to at least thousands of processors and achieves over 70% of the peak performance of most major

microprocessors. However, we find that many applications need a more robust memory architecture, higher bandwidth communications, and lower latency synchronization mechanisms than commodity systems provide. For example, the Coupled Climate System Model (CCSM) code accesses essentially all of memory on every time step. It also requires tight synchronization between the constituent parts of the model. This type of code does not get a high percentage of the peak performance of cluster style systems. On the CCS IBM Power4 cluster, CCSM achieves less than 5% of the peak performance of the system. While the vectorization is not yet complete, we expect CCSM to achieve a substantially higher percentage of the peak performance on the X1, similar to climate codes that ran on vector machines in the past.

The DOE is already pursuing leadership class systems in the 100+ TFLOP/s range through the Accelerated Strategic Computing Initiative (ASCI) at Lawrence Livermore, Los Alamos, and Sandia National Laboratories. The CCS applauds these efforts and expects that for certain applications, these will be the highest performing, most cost effective types of systems. To complement this work, the CCS believes that it is imperative that we also explore the limits of scalability and system performance using processors and system architectures that are specifically designed for scientific processing, such as the Cray X1, Red Storm, and Black Widow systems. The CCS has laid out a road map for this project and taken the first steps. The plan is to start with a 256 MSP X1 system to start porting and testing applications. This will be installed at the CCS by the end of September 2003. In 2004, we propose to increase the size of the system to 640 or more MSPs. The desire is to begin to test the limits of the scalability of the hardware and software and to provide a machine that is a substantial computational resource to the DOE. Also in 2004, the CCS will work closely with Sandia National Laboratory and Cray to evaluate the first Red Storm system at Sandia, and later a second system that we plan to install at Oak Ridge. This will give the DOE a head-to-head comparison of the best of the MPP clusters and the best scalable vector system. From there, the plan calls for scaling the X1 up to 40+ TFLOP/s in 2005 and expanding that to a 100+ TFLOP/s Black Widow system in 2006.

6. Summary

The CCS has entered into a strategic partnership with Cray to test, evaluate, and deploy a leadership class computer system for the unclassified scientific research community in the United States. Such a system is vital to our national interests. Our early experiences with the Cray X1 demonstrate excellent performance on our applications, but as with many early systems, it has a few rough edges. Cray has been exceptionally responsive to solving the problems and meeting the needs of the early X1 customers.

7. About the Authors

Arthur Bland is Director of Operations of the Center for Computational Sciences at the Oak Ridge National Laboratory. Richard Alexander is the Group leader of the Computer Systems group in the CCS. Kenneth Matney and Steven Carter are the primary system administrators of the Cray X1. All can be reached at P.O. Box 2008, Oak Ridge, TN, 37831-6203.

Email addresses are: BlandAS@ornl.gov, Alexar@ccs.ornl.gov, matneykdsr@ornl.gov, and cartersm@ornl.gov.

Research sponsored by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research; U.S. Department of Energy, under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.