LLNL-UCSD Scientific Data Management Status Report
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Reagan W. Moore
Mike Norman
Tim Barnett
Robert Harkness
David Pierce
Leesa Brieger
Arun Jagatheesan

The LLNL UCSD collaboration has the goal of demonstrating the use of advanced data management mechanisms in support of two important scientific applications: Global Climate Change impact on water resources, and Cosmology studies of the structure of the early universe. The scientific applications drive the requirements for scientific data management by generating large simulation output files at LLNL, moving the data to storage systems at SDSC, and publishing derived data products in digital library technology for use by the broader research community.

The specific activities for the last two months have been hindered by delays in establishment of user accounts. A second issue is the installation of disk cache at LLNL, on which data grid technology can be deployed. A third issue is the establishment of a higher-speed network between LLNL and UCSD for moving larger amounts of data for remote analysis.

On the other hand, substantial progress has been made in readying the application codes for large-scale analyses.

Global Climate Change simulation:

Research on Global Climate Change was recognized as the 8th most important research effort in 2005 in a Science article,

> Science 23 December 2005:
> Vol. 310. no. 5756, pp. 1880 – 1885

The article references research conducted by Tim Barnett:

> T. P. Barnett et al., "Penetration of Human-Induced Warming into the World's Oceans," Science 309, 284 (2005)

The following simulations have been run at LLNL:
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The following data sets have been moved to SIO for analysis.
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The system stages the data through SDSC to workstations at SIO. A digital library for managing the data has been established using the Storage Resource Broker data grid. This is available at:
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The SRB collection name is
/LLNL/home/climate.scripps

ENZO Cosmology Simulation

The ENZO cosmology code has been parallelized and validated for a massive 1024^3 simulation of the early structure of the universe.

An effort has started to organize all previous ENZO simulations into a digital library for access by the cosmology community.

LSST Preservation Effort

SDSC has modeled a preservation environment based on experiences working with the 2-Micron All Sky Survey. This collection consists of 5 million images and 10-Terabytes of data. Thus it represents approximately the amount of data that will be generated in a single day by the LSST. A preservation environment provides three essential capabilities:

- Authenticity. This is the set of descriptive metadata that defines all information needed to correctly interpret each image. The metadata includes the information present in the FITS header, and also information about the observation process, seeing conditions, and calibration. Authenticity information is typically static, and can be acquired at the time the data is put into a preservation environment.
- Integrity. This is the set of information needed to assert that the data are being correctly managed, with appropriate mechanisms for access controls, mitigation of the risk of data loss, and validation of checksums.
- Infrastructure independence. This is the set of mechanisms that enable the migration of the preserved records onto new technology, including new storage systems, new databases, new access mechanisms, and new information encoding formats.

The Storage Resource Broker data grid provides the mechanisms needed for authenticity, integrity, and infrastructure independence. Authenticity information is managed as metadata associated with each image. The metadata is packaged with each image, and is also extracted into a metadata catalog to support queries. A notable requirement is support for schema extension, needed to allow future metadata attributes to be easily added to new images.

Integrity metadata is managed as state information associated with each image. The state information must be updated consistently after each operation. Since large collections are inherently distributed (multiple copies, multiple sources, multiple users), it is not possible to keep all state information consistently updated. An example is the act of modifying one image in a replicated data set. The update of the replicas does not occur immediately. Instead a flag is set that asserts that at some point in the future the replicas need to be synchronized.

The generalization of this approach is to implement three types of operations:

- Access constraints that are checked on each operation using static metadata.
- Local procedural operations that are self-contained and modify the associated metadata consistently.
- Global procedural operations that require execution of subsequent operations to build a consistent set of state information. These are turned into local procedural operations with additional status information that denotes what needs to be done to create globally consistent state information. A future operation can then be done to bring the state information back to a consistent state.

The experience with the SRB is that it is possible to build shared collections that are managed with deferred state consistency. An NSF funded project at SDSC on "dynamic consistency constraints" is developing a new rule-oriented data system that will enable deferred state consistency when the rules themselves are dynamically changed. The goal is to be able to build a preservation environment in which the governing policies can change over time as technology improves, without having to re-write code.

For the 2MASS collection, the types of operations that were needed for integrity included:

- Checksum validation. No storage system is reliable. Current bit error rates are on the order of 10^(-13) to 10^(-14). When petabytes of data are stored, you are guaranteed that multiple errors are present. The current TCP/IP data transfer mechanisms also have a bit error rate on the order of 10^(-13). This implies that moving 10 TBs of data will introduce an error. To overcome an imperfect world, the SRB supports md5 checksum generation at the source, validation of the checksum after movement, and validation of checksums at future dates. A synchronization command enables validation of the integrity of a collection, replacement of corrupted data by a good replica, and even synchronization with data collections that reside outside of the SRB data grid environment.
- Consistency checking of images and information mined from images. The NVO has released two FITS image header validation tools. The locations of the stars in the image are used to correct errors in the specification of the pointing information.
- Generation of standard data products. For the LSST, the comparison of images between different surveys implies a standard plate for each area of the sky. SDSC is using the mosaic technology from the NVO and IPAC to create standard plates for 2MASS. The plates are published in the hyperAtlas digital library proposed by Roy Williams of Caltech. Current technology requires 200,000 CPU-hours to do the projection. For this to be done in a single day, a cluster with 8,000 nodes is required.

- Creation of LSST catalog. The information that is mined from the standard plates can be compared with information mined from the original raw data. SDSC is starting a project to compare star locations and magnitudes mined from the mosaics with the information mined in the original 2MASS survey. The goal is to quantify the impact on the accuracy of the mined information by the use of standard plates.

An NSF sponsored workshop was held at SDSC on December 8-9, 2005 to assess the use of the Storage Resource Broker data grid technology in preservation environments. The workshop identified governance as a major concern. The institution that builds the preservation environment may not persist, and support for a collection may be lost. The workshop report identifies mechanisms to federate multiple independent institutions with different governance policies to ensure that no single governance policy will put the data at risk.

References:

1. Science 23 December 2005: Vol. 310. no. 5756, pp. 1880 – 1885
2. T. P. Barnett et al., "Penetration of Human-Induced Warming into the World's Oceans," Science 309, 284 (2005)
3. R. Moore, “SRB Preservation Assessment Workshop”, December 2005, SDSC Technical Report TR-2006-01.