A Composable Scientific Data Management Architecture

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Scientific Data Management

• Applications becoming dominated by moving, finding, archiving large data

• Users are concerned with longevity
  — Robustness and longevity two primary concerns in recent cyberinfrastructure analysis at IU
  — Rightfully or not, they believe open source provides it

• Need more automation of data management and metadata creation
Scientific Data Libraries

- Data model defines structures that I/O libraries can directly understand/manipulate
- Scientific data libraries manage complex data structures directly and record metadata such as type, size, shape, numerical format, etc.

<table>
<thead>
<tr>
<th>I/O system</th>
<th>Data models</th>
</tr>
</thead>
<tbody>
<tr>
<td>UNIX</td>
<td>Sequence of bytes</td>
</tr>
<tr>
<td>netCDF (network Common Data Form)</td>
<td>Annotated multi-dimensional arrays of typed elements</td>
</tr>
<tr>
<td>HDF5 (Hierarchical Data Format)</td>
<td>Annotated multi-dimensional arrays of multi-element records Hierarchical groups of objects.</td>
</tr>
</tbody>
</table>
High Level Data Models

• Pros
  — Data structures closely match what scientific applications use;
  — Self-contained data files with metadata stored in addition to the basic datasets.

• Cons
  — May be too specific to a class of applications, thus not useful in other application areas;
  — Translations between high-level abstraction and low-level storage system model are required, some may be inefficient, and increase the data transfer cost.
Metadata Management Systems

- Metadata makes other data useful
- **Separating metadata** from described datasets has proven utility
- The earliest and still most commonly used technology: **file naming conventions**.
- Existing general-purpose metadata management systems include **SRB/MCAT, OGSA-DAI, MCS, SAM, Chimera**, etc.
Data Grids

- **Grid**: a set of services for configuring, launching, monitoring, controlling work

- A data grid provides an architecture of managing and analyzing large-scale, shared, and widely distributed datasets.

- Data grids focus on:
  - Secure and efficient data transfer
  - Metadata services

- Data grid efforts include: SDSS, ESG, European DataGrid, FusionGrid, GriPhyN, PPDG, etc.
SRB/MCAT

• **SRB** is a client-server middleware that provides distributed clients with an uniform interface to access heterogeneous data storage resources.

• **MCAT** is a metadata repository for SRB resource discovery.

• **MCAT system-level** metadata categories include Data Object, Resource, Collection, User, Method
SRB/MCAT

MCAT has introduced several concepts of metadata categorization for apps. However:
- a universal metadata schema is more useful at abstract level than at practical level;
- MCAT has rather limited support for application-level metadata;
- as with any integrated software system, MCAT has implementation limitations;
- SRB/MCAT is not an open source software.
OGSA-DAI

- Provides uniform service interfaces to access data from distributed sources via the Grid
- Promotes standards for grid database services, initially focusing on consistent access to existing autonomously managed databases
- Does not create new data storage/management systems, but makes them more readily usable within a Grid framework
- Can be considered as a grid transport layer of relational and XML database queries, mainly concerned with large scale integration/federation
Obsidian Goals

• Unattended data collection
• Multiple storage levels and hierarchies
• Large size data objects
• Composable modules
  — Each part does one thing, but does it well
• Ability to define user-specified metadata schemas, instead of one size fits all approach
• Open source components with proven robustness
• Support for Unix and Windows platforms
Modules Implied by Requirements

- Annotation Manager
- MDB Handler
- Logical Collection Manager
- Data Object Accessor
- Unique ID Generator
- Physical Location Tracker
Architecture Overview

Scientific Application

- Annotation Manager
- Physical Location Tracker
- Logical Collection Manager
- Unique ID Generator
- Data Object Accessor
- MDB Handler

MySQL, Access, Scp

HSI, WinZip
Obsidian

- Supports each needed module with at least one implementation
- Has been used for collaborations in
  - bioinformatics
  - x-ray crystallography
  - astronomy
  - clinical radiation therapy
Application 1: Platcom

• Platcom is an integrated **comparative genome analysis system** developed at IUB School of Informatics.

• Building and updating a pairwise comparison database require over **48,000 jobs** initially, and a few hundred more monthly afterwards.

• Data management needs:
  – interface with batch queuing system PBS;
  – automatic and secure transfer of large amount of computation input/output files;
  – archive history and performance metadata;
  – failed job discovery and re-submission.
Application 1: Platcom

Platcom

Annotation Manager
Physical Location Tracker
Logical Collection Manager
Unique ID Generator
Data Object Accessor
MDB Handler

MySQL
Access
Scp

HSI
WinZip
Application 2: X-Ray Crystallography

• IU Molecular Structure Center remotely manages X-ray crystallography data collections of large molecule samples

• To date over 2 terabytes of data; extending to include earlier data from past decade involves multiple petabytes

• **Data management needs:**
  – track physical locations of different kinds of data objects, including CCD frames and lab camera images;
  – archive metadata about environment under which the datasets are collected;
  – archive metadata about sample providers and instrument operators;
  – move data objects and metadata among front end collectors, staging computers, tape systems like HPSS
Application 2: X-Ray Crystallography

X-Ray Crystallography

- Annotation Manager
- Physical Location Tracker
- Logical Collection Manager
- Unique ID Generator
- Data Object Accessor
- MDB Handler

- Humidity
- Temp
- CCD
- NOx
- Sample Info
- Collections

- MySQL
- Access
- Scp

- HSI
- WinZip
Application 3: Radiation Therapy

• In radiation therapy of cancers, large amount of data are produced from patient pretreatment imaging scans

• Collaboration with one of the clinical practices at Radiation Oncology Department, University of Maryland School of Medicine

• **Data management needs:**
  – Automatically locate a patient’s treatment files, whether on hard disk or tape, through a few variations of queries;
  – Automatically build a MS Access database of specified treatment parameter combinations and populate it with existing patient data to facilitate clinical trial designs.
Application 3: Radiation Therapy

Radiation Therapy

- Annotation Manager
- Physical Location Tracker
- Logical Collection Manager
- Unique ID Generator
- Data Object Accessor
- MDB Handler

MySQL, Access, Scp, HSI, WinZip
Application 4: Automated Photometry

- Facilitate managing astronomical data collected from Morgan-Monroe Station of the Goethe Link Observatory telescopes.

- Data are produced from a wide range of instruments including:
  - CCD images in FITS format
  - Thermometer readings and precipitation records
  - Weighing scale readings for liquid NOx
  - Telescope and dome control parameters

- **Data management needs:**
  - Data direct from A2D cards on instruments
  - Transfer across low-bandwidth connections
  - Support scientific queries involving large amounts of complex computation
Application 4: Automated Photometry

MMSF RoboScope

Annotation Manager
Physical Location Tracker
Logical Collection Manager
Unique ID Generator
Data Object Accessor
MDB Handler

MySQL
Access
Scp

HSI
WinZip
Summary

• Obsidian’s modular approach to creating data management systems allows using only what is needed for particular application

• End-user defined schema are superior to putting user metadata into DB text fields

• Does not replace need for application communities to define ontologies, agree upon terms, definitions, and interfaces