

## Environmental Molecular Processes: Management of Simulation Data and Annotation

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The ‘Environment from the molecular level’ (eMinerals) project [1] is a NERC funded eScience pilot project focused on fundamental science problems associated with key environmental issues such as nuclear waste storage and pollution.

Aside from the scientific issues, this research is challenging both in terms of the computational power needed to tackle realistic system sizes with the required accuracy and the data management issues related to handling large amounts of data over a distributed virtual organisation. Hence the use of Grid computing together with associated data management technology provides enticing opportunities to facilitate and enhance this work.

The project involves the collaboration of environmental scientists, scientific code developers and computer scientists from Bath University, Cambridge University, CCLRC Daresbury Laboratory, Reading University, the Royal Institute and University College London.

From a data centric perspective, scientific research can be viewed by the sequence of events shown in Figure 1.

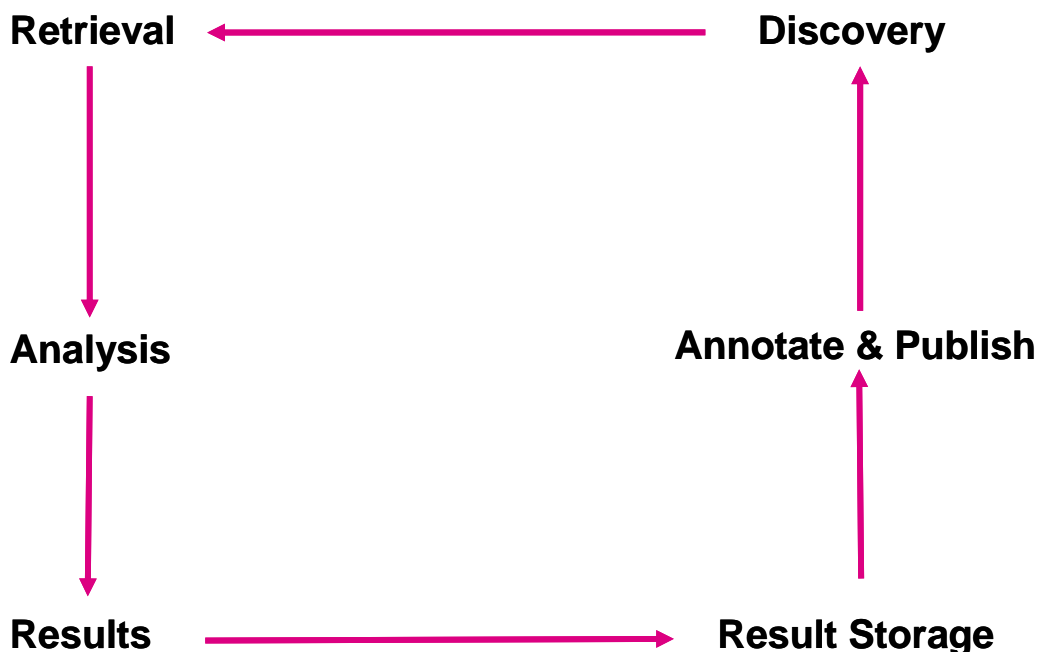


Figure 1: Data centric view of scientific workflow.

In general terms, research begins with some data, for example a crystal structure in a text file. Some analysis is performed on this data which in turn generates more data, i.e. results, usually in a number of text files. These results are then stored and annotated in some fashion after which a subset may be selected for publication or distribution to a wider community.

One of the principle challenges for the eMinerals project and the eScience programme in general is providing an effective and integrated infrastructure which facilitates each step of the data lifecycle for a distributed (both geographically and political) community. To this end a number of pieces of middleware have been developed and deployed for the project. This paper will elaborate on the data lifecycle shown in Figure 1, describing the pieces of middleware used, the issues motivating their need, and the benefits their use brings to the project.

## 1. DATA DISCOVERY

The majority of scientific data is typically stored in facility file storage, in journals or on personal machines or computation facilities. Much of the data is in arbitrary text files and few standard formats currently exist. This presents a major challenge in providing common tools to find the data in the first instance. It is currently necessary for a scientist to log onto each facility in turn and search for data they are interested in, that is, if the data is catalogued and available in the first place.

In many cases, as for the e-Mineral project scientists, their output files were originally scattered on a number of machines, uncatalogued and unavailable to anyone else. The immediate drawback is that of unnecessary repetition of computations elsewhere.

There are two main issues. First the results from within the project were stored by the individuals themselves thus not available to other members. Second that there are few access points for finding and downloading data from elsewhere in the community. To facilitate the management of individual's own data we have

deployed a version of the Storage Resource Broker [2] for distributed file storage and a relational database of metadata to describe the files and point to their location in SRB. More about these later in the paper. The important thing to note is that there is a significant amount of data held at scientific facilities or in databases, so our aim was to incorporate middleware that could integrate these heterogeneous data resources.

To that end CCLRC has developed a Data Portal [5] that provides parallel search capability via topics, of all the facilities it connects to. Search queries are specified by 'drilling down' within non-unique topic hierarchies. An example hierarchy could be:

Physics → Condensed Matter →  
Magnetism → Oxides → Manganites

By entering a topic users can browse *metadata* - description of file contents - displayed on the web pages. The user may then select files to download or transfer to a remote location for viewing, visualisation or analysis.

Currently the Data Portal technology is limited to downloading data in files and not in databases. However we are investigating the use of SRB's

integration with database records as a solution to this.

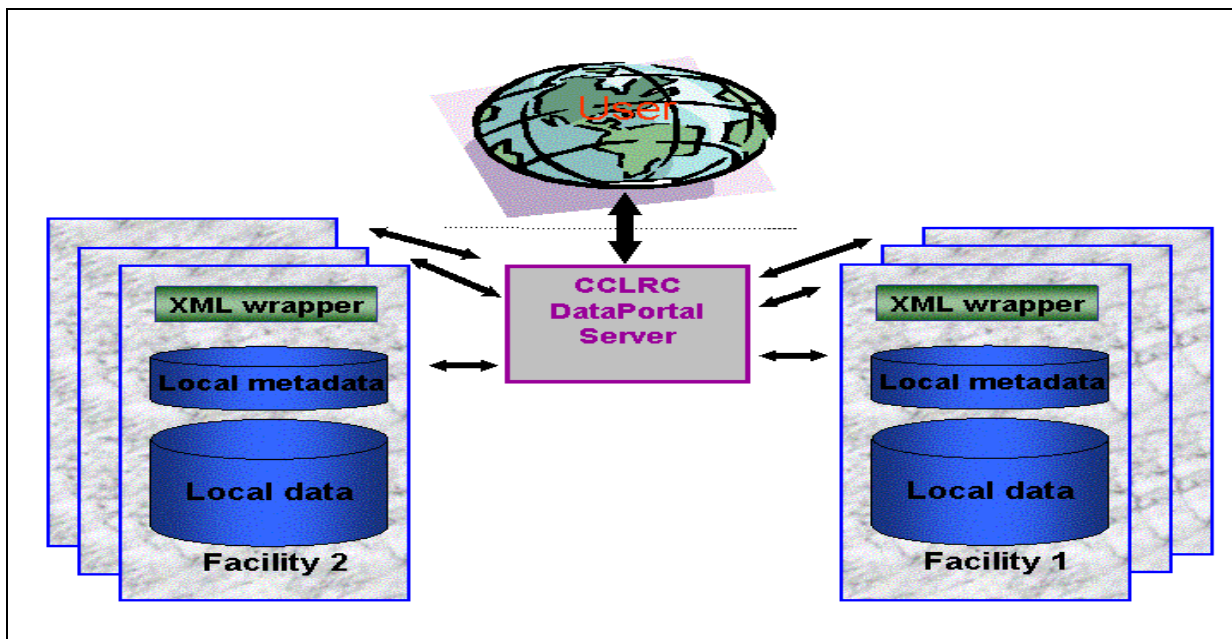


Figure 2: CCLRC Data Portal Architecture

A particular challenge is that each facility has a proprietary relational data model for describing their files. This has led to the development of an XML Wrapper for each facility to turn SQL results into a common XML format for transfer across the wire. This eases collation of the results and we simply use XSLT to display the results on the web pages in a variety of presentation formats.

This is just one of the ways that data can be sourced as input to analysis. Other methods include downloading data from a facility web site, amending a similar input file or copying from a journal.

An important issue to address is that often the data is retrieved in some proprietary format and must be converted to one suitable for a particular code. This is a common problem throughout the scientific community and often involves running conversion scripts or cutting and pasting information. We have made

some effort to address this in the use of Chemical Markup Language CML as a format for holding input data and as output from a number of scientific codes. Paper "The use of XML and CML in Computational Chemistry and Physics Programs" from these proceedings describes this in detail.

## 2. DATA RETRIEVAL

Prior to analysis it is necessary to have the input data transferred to the compute node. As described above the data may be transferred directly from the Data Portal via GridFTP [3] to the compute node. More likely however, some conversion is necessary or output files from previous calculations are amended for the new job, so the files could be sitting on the user's machine.

One of the key strengths of our infrastructure has been the ability to transfer files between the compute node or facility and the Storage Resource Broker (SRB) managed file storage. Input files can be transferred ready for

computation and results transferred back. This is made possible by the fact that the access to the SRB is provided on all compute facilities, including Condor [6], used by the project via the installation of SRB's command line utility called S-commands. On non-project facilities such as HPCx, users can either install S-commands in their home directory or preferably a shared version may be installed for general use.

First if the user has their files on their own machine they can use one of the many SRB client tools to upload them to SRB. After job submission to one of the machines on the eMinerals mini-grid, a pre-processing script uses S-commands - SRB's command line utility - to download the files directly from SRB to the execution directory.

### 3. DATA ANALYSIS

The next stage in the data lifecycle is Data Analysis which represents performing some manipulation on the data. In the context of the eMinerals project, this would typically involve running one or more scientific codes on the data and producing a set of output files. The computational requirements of the applications vary significantly. However they can be broadly classed as either High Throughput Computing (HTC) or High Performance Computing (HPC) applications.

The project makes use of a number of HPC facilities within the UK including the HPCx and the CSAR machines. In addition the project has a number of 16-node Beowulf clusters at Cambridge, UCL and Bath plus an IBM pSeries 24-node cluster at Reading.

For HTC applications, the project has set up a number of Condor Pools, the

most notable of which is the UCL pool which currently comprises around 960 machines.

See paper "Grid Tool Integration within the eMinerals Project" in these proceedings for more details on our grid infrastructure and middleware.

### 4. RESULTS STORAGE

Since all of the data is currently produced in flat files, the project has a number of file servers for their storage and these are at various locations in the UK. Storage Resource Broker was selected to provide a single point of access to these heterogeneous data resources. SRB is client-server based middleware initially developed in the mid-Nineties by San Diego Supercomputer Centre and is a means of allowing users to manage data storage and replication across the wide range of physical storage system types and locations available within UK e-Science, while still allowing having a single, stable access point to the data.

The SRB Client is an end user tool that provides a user interface to send requests to the SRB server. There are three main implementations of this: command line *S-commands*, MS Windows GUI *InQ* or Web based *MySRB*. A recent addition is the *MySRB* server component. This allows all access to storage via a thin client. The *MySRB* server is actually an application server middleware component that acts as a client to service multiple thin client sessions.

The S-commands unix-style tool has proven to be the most popular since it goes hand-in-hand with running computational analysis. As well as being able to transfer input files from SRB to the compute node(s), a post-

processing script also uploads the results to the user's chosen directory in SRB. On non-project facilities, users can simply use S-commands to upload their data once their job has completed.

## 5. DATA ANNOTATION AND PUBLISHING

The final stages of the data lifecycle are annotation and publishing. The data files themselves are uploaded to the SRB via the post-processing scripts or via the client tools. However the value of the data files would diminish rapidly if they were not annotated with relevant *metadata* describing the context and method of their generation. This step is essential if the data files are to be retrievable at a later date by others during the Data Discovery phase.

### 5.1 Metadata

Metadata is background information about data files and defines the who,

where, when, how of the data. We have created a relational database schema that can be used in multi-disciplinary scientific areas as shown in Figure 3: CCLRC Metadata Database Schema. A *DATASET* contains information and the physical location of a directory of files. Datasets are grouped into a *STUDY* with a name, start and end dates and originator. It also links to a list of people in the *PERSON* table who are the investigators along with their contact details. Each study has a list of associated categories in the *TOPIC* table. Users of the Data Portal use topics to find studies and datasets so it is important to capture as many relevant topics as possible.

We used this schema to create a catalogue of metadata for the project to annotate their files along with their physical location.

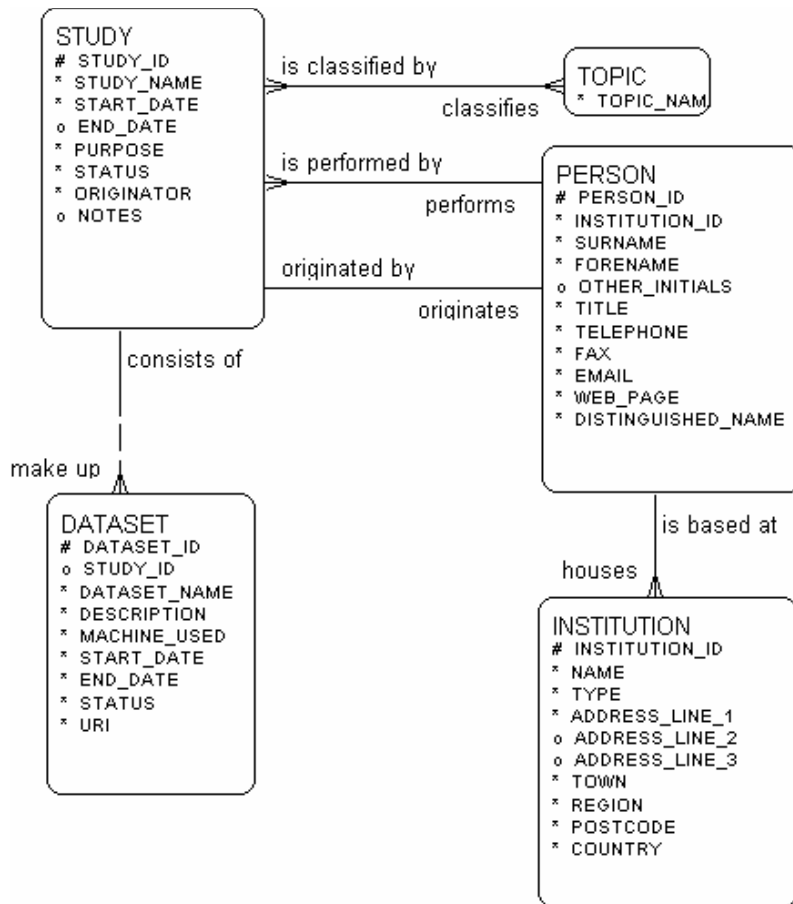


Figure 3: CCLRC Metadata Database Schema

Currently the metadata relating to scientific work is entered using forms-based web application known as the Metadata Editor. Within the metadata editor, individual computation simulations can be grouped into studies

and linked with topics that allow retrieval via the Data Portal at a later date.

This final step of publishing the metadata completes the data lifecycle loop shown in Figure 1.

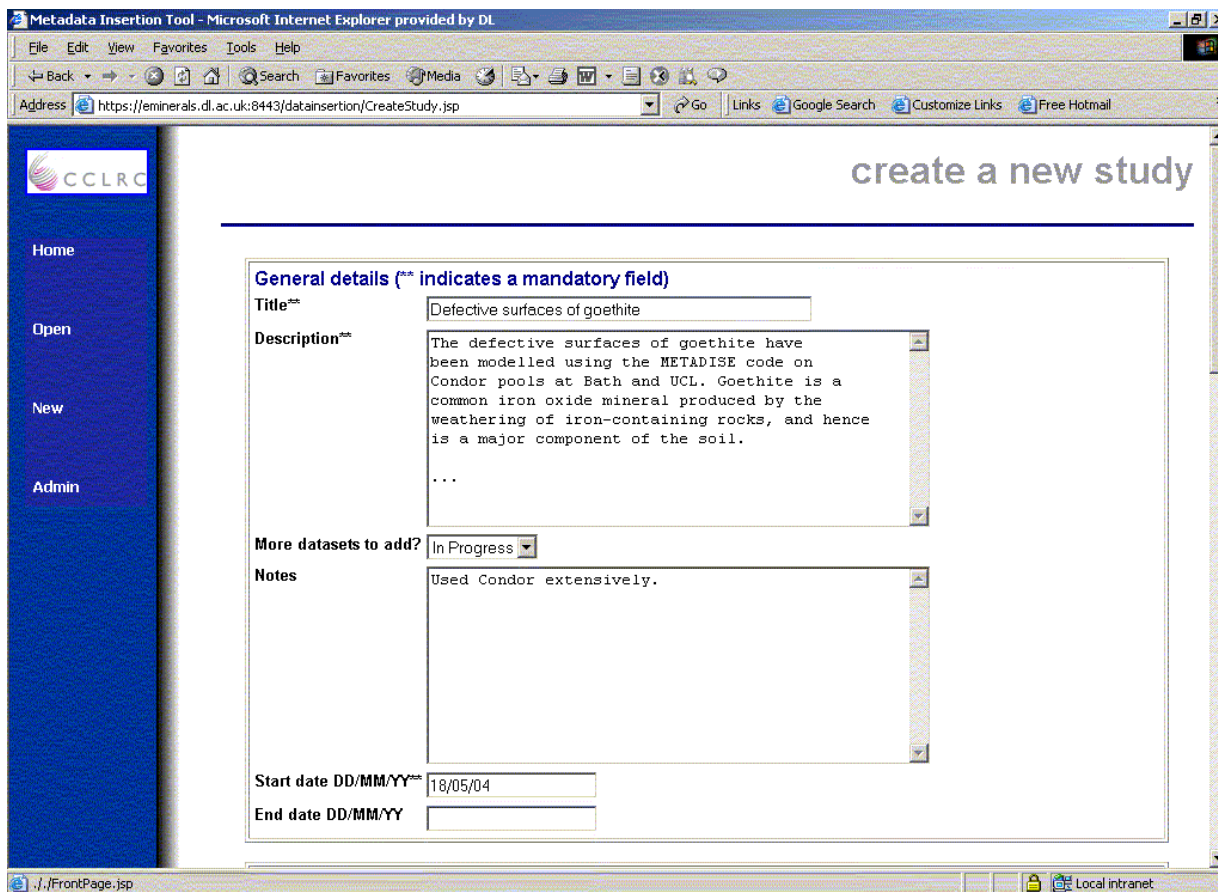


Figure 4: Create New Study Page in the Metadata Editor

## 6. ARCHITECTURE

Figure 5 shows the geographical distribution of the various software tools involved in the management of metadata and files. The central Storage Resource Broker software and database at CCLRC interacts with SRB software on each file server at Cambridge and

London. Users can upload or download their data files and arrange them in directories. If desirable they can then share their files by creating *studies* and *datasets* information via the Metadata Editor and linking the datasets to directories in SRB. Others can then browse the metadata and download them through the Data Portal.

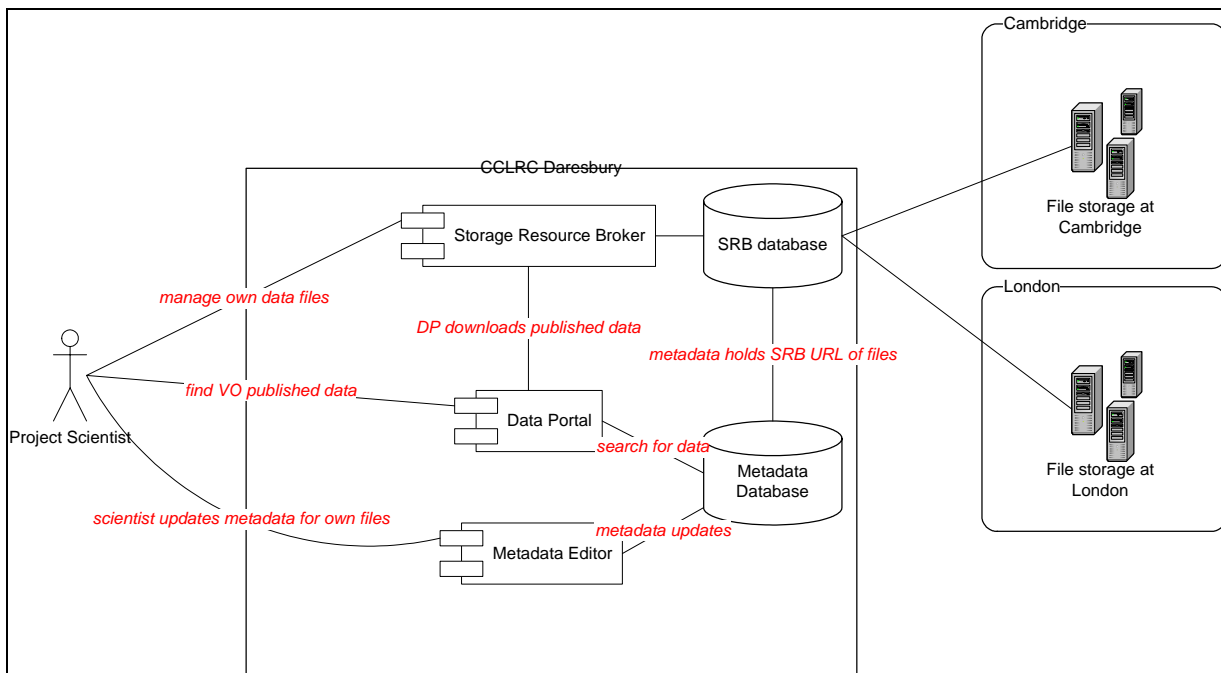


Figure 5: Data Management Architecture

## 7. SUMMARY

In this paper we have described a possible architecture for the whole data lifecycle. Its strength lies in the ability for users to access their data from home, work and compute nodes from a variety of different tools. Furthermore, we can now ensure that data is constantly available, is secure and is backed up, something that wasn't previously possible. Difficulties that we have encountered lie in the resistance to change within the community and in

encouraging users to annotate their data. Some progress has been made in encouraging the use of SRB in that many of the compute facilities within the project only allow data to be transferred in and out of SRB and not other machines directly. However SRB has been generally well received due to the choice of tools available on different platforms. Especially popular has been the S-command interface since Linux is the platform of choice amongst many users. More strategies are needed to encourage metadata creation.

## 8. REFERENCES

- [1] eMinerals web site <http://eminerals.org>
- [2] Storage Resource Broker <http://www.npaci.edu/DICE/SRB/>
- [3] GridFTP <http://www.globus.org/datagrid/gridftp.html>
- [4] CCLRC Metadata Editor [http://www.e-science.clrc.ac.uk/web/projects/scientific\\_metadatamngt](http://www.e-science.clrc.ac.uk/web/projects/scientific_metadatamngt)
- [5] CCLRC Data Portal <http://www.e-science.clrc.ac.uk/web/projects/dataportal>
- [6] Condor <http://www.cs.wisc.edu/condor/>