eIUS Use Case - Earth Sciences

1. Tony is a Physics Research Fellow at a large UK university. One of his main research areas is the unusual behaviour of materials under particular conditions of temperature and pressure. Today on his way home Tony thinks of a paper he has read in the latest issue of 'Physics and Chemistry of Minerals'. Rose, a physicist at a prestigious Scottish university has published the preliminary results of her study on the unusual behaviour of Silver 3 Cyanocobaltate Ag3[Co(CN)6], a material that shrinks instead of expanding at high temperatures. This is a very exciting piece of research news for Tony, as in the past few years he himself was involved with researching the atypical behaviour of materials. In particular he has tried to understand why silica glass, unlike other glasses, becomes easier to compress at particular high pressure levels.

2. In her research Rose has used hight throughput computing to run parallel simulation codes via the eMinerals toolkit, a set of grid-based tools for simulation scientists that are designed to cover the whole job life cycle, from submitting jobs to a grid environment, through to extracting the core information for analysis, and sharing with collaborators. This approach provided Rose with high-definition graphs that mapped the temperature-volume dependency much more accurately than any results Tony could get by running successive simulation sessions on his computer. He feels very excited with the prospect of being able to analyse 200-point simulation graphs displaying the performance of silica glass in high pressure conditions.

3. Tony is keen to find out more about the grid computing tools Rose mentioned in her paper. After dinner, instead of watching TV as usual, he decides to check the eMinerals website on his laptop. Following the comprehensive online instructions, he easily manages to run some simple simulation tests, and within a few hours he is able to access the first set of high resolution graphs the system has automatically generated for him.

4. During the following weeks Tony becomes familiar with the eMinerals tools as he uses them to run more complex simulation codes. After about a month of extensive parameter sampling Tony comes up with a rather unexpected result. The greater level of detail available with the high resolution graphs has revealed a previously unnoticeable effect that may be able to provide an explanation for the unusual behaviour of silica glass at high pressures. Tony decides to email some of the graphs to Hilary, a close collaborator at a research university in the South of England.

5. One morning a couple of days later Hilary enters her office, and before starting her usual work routine she accesses and adds a new entry to her online calendar. She has been extremely intrigued lately by the graphs Tony had emailed her. Although she had not planed to attend the JISC Conference this year, she has eventually decided to go, as she is keen to watch an eMinerals demonstration scheduled to take place on their stand. Hilary uses the online facility provided on the conference website to book a slot on the specially designed WiFi networking space for a meeting with Tony and Rose who plan to attend too.

6. On the conference day the three meet as planned, and Rose shows Tony and Hilary on her WiFi enabled laptop some customization tools she uses for running her simulation codes. Then they move down to the demonstration area. On the eMinerals stand, Jeremy, one of Rose's PhD students who uses

eMinerals extensively in his research, demonstrate the newest addition to the eMinerals Toolkit. The Multicast Application Sharing Tool (MAST) turns out to be an application specially designed to enhance collaboration within an Access Grid session by allowing real time visualisation and annotation of simulations across geographically distributed teams. Jeremy demonstrates how to run a set of simulation codes and share the automatically generated graphs with remote collaborators who can remotely annotate the graphs in real time.

7. Impressed with the MAST demonstration, Tony and Hilary decide to explore the online collaboration and data sharing facilities provided by the tool. Rose offers to help by remotely annotating their shared simulation graphs. A few days after the conference Tony contacts Jeremy, who helps him and Hilary set up and customise MAST for their computers. Over the following weeks Tony and Hilary test the tool's functionality, and encourage a few colleagues from the Special Interest Group in Mineralogy to try it out. The possibility to visualize and comment upon shared simulation graphs in real time without needing to be physically present looks extremely appealing to their colleagues. One of them suggests that a section of next year's Annual Meeting of the Mineralogy SIG be held online using MAST, in order to allow a larger participation of researchers from both the UK and abroad.

8. Six month from Tony's initial email, Hillary feels reasonably confident with using the eMinerals tools. As she checks the photos on her digital camera one evening, she comes across a photo of Jeremy talking on the eMinerals stand at the JISC conference. She remembers him telling her after the demonstration how beneficial he thought MAST was for his PhD research, as it provided a unique opportunity for him to witness geographically distributed researchers addressing practical issues related to analysing and annotating simulation graphs online. Computer simulation scientists should consider using MAST as an informal way of teaching research skills to their students, Hillary recalls Jeremy suggesting in the end of their chat.

9. A few days later, prompted by Jeremy's remarks, Hilary decides to introduce Barbara, one of her PhD students, to the eMinerals toolkit. They have agreed to write a paper together for the Journal of Applied Crystallography. As Barbara becomes acquainted with the eMinerals tools she discovers its file management capabilities. The simulations she is supposed to run involve a large number of input and output files, which are managed via a distributed file system based on Storage Resource Broker [SRB]. The system automatically integrates with the Data Grid and provides a complete and secure archive of all input and output files. Barbara is pleased that she doesn't need to send any output files to Hilary, and indeed to any other collaborators. All she needs to do is upload them in the web-based SRB tool, and all authorized users can access them, or click a button and see their automatic transformation in web reports.

10. Three months into researching and writing the paper with Barbara Hilary is very pleased with this new way of research collaboration. By keeping track of both data and information about data, the eMinerals toolkit has so far helped her avoid a typical case of bad data sharing, in which the PhD student who runs the simulations finishes, leaving the supervisor helplessly attempting to find results through the paper. Six weeks later Hilary receives an email confirming that their paper has been admitted for publication.

Tools identified in the experience report research cycle

Literature review
* Physics and Chemistry of Minerals

Data collection
* Storage Resource Broker [SRB]
* National Grid Service

Data analysis
* Chemical Markup Language
* XML data formats

Discus/compare results
* Multicast Application Sharing Tool [MAST]
* Access Grid

Publish
* Journal of Applied Crystallography