

eScience for materials research with intensive computational, data and collaborative requirements

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This talk will focus on the application of eScience technologies to support small-scale collaborations of researchers. In particular, many tasks in science, whether simulation or data analysis, require the running of many instances of a similar computational processes. Such combinatorial or ensemble studies are ideal for grid computing. But just running large-scale studies over grid computing resources is only part of the picture; we also need to consider how to set-up and manage many compute jobs. Moreover, data management is a significant part of the picture, involving collaborative sharing of data, management of metadata, and retrieval/sharing of the information content of data. In this talk we describe work the UK *e*Minerals project has been carrying out to develop a collaborative/community grid infrastructure and associated job, data management and collaboration tools for simulation scientists. One key aspect in this work is the use of XML for data representation. Increasingly experimentalists are requiring significant computing resources for data analysis and modelling — one example is the use of Reverse Monte Carlo modelling of total scattering data in neutron and X-ray diffraction — so that the approaches and tools described in this talk will be of direct relevance to data/analysis-intensive experimental work. Some of the tools described in this talk are being adapted for routine use on the UK Diamond and ISIS facilities. For more information, please see <http://www.eminerals.org/>.