Grid-Enabling an Existing Instrument-Based National Service

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Abstract

Recent work by the 'CombeChem' project together with the UK National Crystallography Service (NCS) has integrated the NCS into an e-Science environment. The existing high-throughput crystallography facility is enhanced by on-line feedback with the ability to monitor and steer diffraction experiments remotely. Security mechanisms are used to determine authorisation attributes and hence to allow user interaction at appropriate stages, together with access of a database recording the status of the submitted samples. The user can monitor the position of their samples, be alerted to all stages from submission to experiment and then analysis, visualise raw data as it is generated, be involved in the key decision-making during the parameterisation and initialization of the experiment and then track the data collection to ensure its successful completion. Results data are staged to a secure area and made available for download (either the raw diffraction data or a refined structure generated by NCS staff).

1. Introduction

This paper reports on our experiences when designing and implementing the Grid infrastructure to support access to the UK EPSRC National Crystallography Service (NCS) high-performance small-molecule (e.g. non-protein) crystallography diffractometer instrumentation facility [1]. The geographically-dispersed clients of this facility comprise several hundred academic users located throughout the UK who currently submit over 1000 samples a year in addition to 1000 originating within the department. This throughput is approximately an order of magnitude higher than a typical crystallography laboratory. The paper reviews the real problems that we encountered in practice.

As part of the UK National *e*-Science programme [2], the CombeChem project [3, 4, 5] and the NCS initially developed a proof-of-concept demonstration outlining how the Grid could enable an *e*-Science enhancement for structural chemistry. This initial work confirmed the feasibility of the proposed NCS Grid-enabled service, designed to increase and enhance user interaction with experiments and also provide efficient management of the resulting data. Our objective was to adopt an *e*-Science approach to enable crystal structure results to be rapidly and efficiently generated, disseminated and reused [6]

The Grid can potentially provide many applications to Service Crystallography. The primary benefits would be where the physical location of the user is distant from the service (which is inevitable whenever a national service is provided in any discipline). The implementation of such an infrastructure has a number of advantages over a conventional laboratory that would be of considerable worth to the service crystallographer [7]. A massively increased interaction between local experts and users would allow both chemists unskilled in the art of crystallography and "trained" crystallographers alike to participate in, or conduct their own, experiments remotely. Enabling remote control for the expert user will assist in "dark" laboratory instrument automation, allowing service operators to concentrate on other matters. Furthermore,