

Grid Enabled Workflows: An Example From Computational Chemistry

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The field of computational chemistry is ideally suited to the utilization of a grid enabled workflow. We discuss a case study where existing tools and services are employed to integrate the task of remote job execution with the desktop tasks of building, manipulating, and visualizing chemical structures. The discussion will focus on how the GDIS[1] program was enhanced with new features and capabilities for enabling the submission, monitoring, and retrieval of results from the ARCS[2] compute infrastructure. In particular, issues relating to the discovery of desired programs, efficient re-use of previously uploaded data sets, and the archiving of output results will be shown.

The GDIS program is primarily used to visualize chemical systems such as unit cells, surfaces, polymers, and isolated molecules. It also contains other useful features such as dislocation building, nanotube construction, and iso-surface visualization. However, its key features rest in the ability to read and write numerous input file formats for computational chemistry packages such as GAMESS[3], GULP[4], and SIESTA[5] and, in addition, process the output files of these programs to provide some simple job analysis.

The ARCS compute infrastructure provides convenient and standards based methods for secure authentication, resource discovery, job submission and monitoring, and data storage. These services were accessed primarily through the web-based interface provided by the GRISU[6] framework.

In this discussion, we will demonstrate how the existing software package GDIS, aimed at computational chemistry users, was adapted and enhanced to provide the convenience of a grid based workflow by consuming services provided by the ARCS compute infrastructure.

References

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