A Grid Computing Prototype for Integrated Solvent and Process Design

Athanasios I. Papadopoulos(a) and Patrick Linke(b)

(a) Chemical Process Engineering Research Institute, Greece
(b) University of Surrey, U.K.

Grid technologies have received a lot of attention by the scientific community recently; however, developments are at their infancy and very few engineering applications have been reported to date. The Process Engineering domain makes an interesting application area for Grid technologies as the problem solving and decision-making generally involves multiple software and data resources and heavy computations. There are also numerous highly computationally demanding computer aided chemical engineering applications that can benefit from distributed Grid computing such as molecular simulations and large-scale optimisations. In theory, Grid technologies would enable distributed decision-support systems that could integrate all the required sources for process design activities, whether available in-house or from external sources, in a unified environment and make available vast computing power to tackle computationally intense problems. Such systems could significantly improve the design efficiency. We have set up a prototype Grid for integrated process and molecular design to demonstrate the potential of Grids in the Computer-Aided Process Engineering (CAPE) arena. The design problem makes an ideal candidate to investigate the potential of Grid technologies, to identify implementation difficulties and to highlight technology shortcomings. The prototype integrates a number of software resources (computer-aided molecular design (CAMD) tools, data mining tools for the analysis of molecular design information, process synthesis tools, web mining tools) and data repositories (in-house and web databases) required in the different design stages. The prototype also facilitates distributed Grid computing to tackle the computationally demanding process synthesis calculations. The user interface is a web portal designed under consideration of the design workflow and its possible variations. We will focus on the architecture of our prototype Grid and discuss its implementation together with the problems we faced and the lessons learned in the process. An application in integrated CAMD and process synthesis in liquid-liquid extraction will be presented.

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