

## Enabling JChem on the Grid

Nowadays researchers in biotechnology and at pharmaceutical industries are supported by many chemical software development platforms and desktop applications. JChem is one example of such key software platforms, which is a java based suite of integrated programs and toolkits for many cheminformatics tasks. Its components include chemical database engines, chemical structure editor and visualization tools, physicochemical property predictors and other tools for chemical structure manipulation. In collaboration with MTA SZTAKI's Application Porting Centre distributed computing infrastructure (DCI) support was added to the JCHEM framework to increase its processing power. Our project work addressed all issues how to combine a highly specialized chemical software development platform with a stand-alone DCI focused application development environment; namely with gUSE - grid User Support Environment. On one side the developed solution provides for JChem framework users a native application programming interface to launch time-consuming tasks transparently on the available grid and cluster infrastructure. On the other side the work has exploited the new remote access API and application specific interfaces of gUSE. To demonstrate and test our solution we have created a workflow based grid application that enables the JCHEM software environment to do Markus searches against large datasets on gLite middleware with the help of the parameter study feature of the WS- PGRADE Portal. As a result, our solution lets JChem users to use their custom Markush searching tasks with parameter values on their local machines, and use DCIs to execute such tasks. Thus even with moderate large datasets end users were able to achieve significant speedup in chemical structure search by the DCI-enabled version of JChem comparing to single multi-core computers.

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