The HADDOCK WeNMR Portal: Combing gLite, DIRAC4EGI and Crowd Computing. Cloud Next?

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Content:
The HADDOCK web portal [1] is a widely used scientific portal for the modelling of biomolecular interactions. It is part of the computational workflows and services offered by the WeNMR project (www.wenmr.eu) [2] that make efficient use of the European Grid Infrastructure (EGI). The HADDOCK interface hides the complexity of the workflows and grid submission from users by providing them with friendly interfaces matching the level of expertise of the user. Each user submission translates into several hundreds individual grid jobs that are handled by the complex workflow beyond the portal. To date HADDOCK counts over 4600 registered users worldwide and has resulted in the last year in over 6'000'000 grid job submissions.

In its initial WeNMR grid-enabled implementation, the portal was only making use of standard gLite-based submission and retrieval of jobs via a user-interface based on robot certificates. In collaboration with the "DIRAC4EGI" team we implemented early 2014 a DIRAC client, adapting very easily the submission machinery of the portal to DIRAC. At about the same time HADDOCK went crowd computing: In collaboration with the International Desktop Grid Federation (IDGF) team we ported and validated the HADDOCK computational engine, the CNS software, into a Linux virtual machine for BOINC. This effectively enabled the HADDOCK portal to send jobs to IDGF resources using the same gLite-based mechanism as for regular EGI resource. More than one year into this triple operation mode, results indicate a very efficient and reliable submission process. The DIRAC4EGI service in particular shows a very efficient job rate, while having access to IDGF resources opens the world of crowd computing. In the future, we are aiming at porting HADDOCK to the cloud as a way of providing a self-contained server to potential commercial users.

URLs
http://haddock.science.uu.nl/enmr/services/HADDOCK
http://www.wenmr.eu

References:


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