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The HADDOCK WeNMR portal: From gLite to DIRAC submission in three hours

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The HADDOCK web portal is a widely used scientific portal for the modelling of biomolecular interactions. It makes uses of the EGI grid infrastructure for job submission. Users interact through a user-friendly web interface. 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 3600 registered users worldwide and has resulted in the last year in over 860'000 grid jobs for a total of over 150 CPU years (normalised CPU time (kSI2K) - source EGI accounting portal).

Until recently, the grid-enabled portal was only making use of standard gLite-based submission and retrieval of jobs via a user-interface. In collaboration with the "DIRAC 4 EGI"team we implemented in a few hours a DIRAC client, adapting very easily the submission machinery of the portal. The first tests indicate a very efficient submission process, with a larger number of jobs being handled within a defined time window compared to standard gLite-based submission. The DIRAC client also has the advantage that it does not require any local EMI middleware installation, which reduces the burden of local system administrators.

With the DIRAC service in place, we now have a clone of our HADDOCK portal, which is expected to increase its overall output and directly benefit our end user community.

Wider impact and conclusions

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URL(s) for further info

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

Description of work

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