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Leveraging GPGPU Computing in Grid and Cloud Environments: First Results from the Mobrain Competence Center

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The MoBrain CC (https://mobrain.egi.eu) has been designed with the aim to allow scientists access to the best e-Science environments from micro to macro scales. It builds on solid basis and expertise provided by the N4U, WeNMR and INSTRUCT initiatives. The aim of MoBrain is to lower barriers for scientists to access modern e-Science solutions to investigate and simulate life science processes. To this end, MoBrain has focused on the development of accelerated computing solutions as well as of cloud-based approaches for specific applications in Structural biology.
In this presentation I will describe our effort in leveraging GPGPU computing using both grid and cloud resources, focusing on two applications developed in our laboratory for exhaustive search automated fitting of 3D structures into cryo-EM density (Powerfit software, http://github.com/haddocking/powerfit) and for assessing the conformational space consistent with a few distance restraints in the case of biomolecular complexes (DisVis, http://github.com/haddocking/disvis). Both applications have been packaged in Docker containers. These containers were used both in grid and cloud contexts. For the grid scenario, computations could be successfully submitted with gLite to GPGPU supporting CREAM-CE. Cloud testing is an ongoing activity in the INDIGO-DataCloud project to which we also participate. Our initial results show that the use of Docker containers, both in grid and cloud scenarios does not lead to any significant performance loss compared to running directly on bare metal.
We are currently developing user-friendly web-portals for those application that will leverage the GPGPU capabilities of grid and cloud computing. These will ultimately be offered through the West-Life virtual research environment portal.

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