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GPGPU-enabled molecular dynamics of proteins on a distributed computing environment

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As part of the activities of the MoBrain Competence Center within the EGI-Engage project, we have implemented services for the use of molecular dynamics (MD) simulations on biological macromolecules (proteins, nucleic acids) based on the AMBER suite and taking advantage of GPGPU architectures within a grid computational infrastructure.
The rationale for this development is to improve upon the tools already provided within the WeNMR gateway [1], which allow for MD-based refinement of macromolecular structures derived from NMR spectroscopy data as well as for unrestrained (i.e. without experimental data) MD simulations. These services are available via the AMPS-NMR portal, which has been using the EGI computational infrastructure for almost five years [2]. The portal allows a large range of users that are not computer-savvy to apply successfully state-of-the-art MD methods through completely guided protocols. The current protocols are only designed to work with CPUs. Transitioning to GPGPU services would result in a significant reduction of the wall time needed for calculations, thereby enabling a higher throughput of the portal. Alternatively, one could run simulations for larger, more complex molecular systems or could sample molecular motions more extensively in order to obtain information on various biologically relevant time scales.
For the above reasons, we thus decided to extend the capabilities of the AMPS-NMR portal so that it would provide access to both CPU and GPGPU resources, depending on the requirements of the specific calculation requested by the user and taking into account also resource availability. To achieve this it is necessary to modify the submission pipeline that underlies the portal as well as to implement different versions of the AMBER suite. Some changes to the software code were necessary in order to achieve the best treatment of NMR-based experimental restraints during MD simulations. A further hurdle was the lack of an approach generally agreed upon to expose GPGPU resources on the EGI grid environment. To address this middleware limitation, we endeavored to contribute to testing the implementation of different queuing systems within EMI.
In this contribution, we show the initial results of the above work. We also demonstrate an example biological application that is only possible on GPGPU systems.

[1] Wassenaar TA, et al. WeNMR: Structural biology on the Grid. J. Grid. Computing 10:743-767, 2012
[2] Bertini I, Case DA, Ferella L, Giachetti A, Rosato A. A Grid-enabled web portal for NMR structure refinement with AMBER. Bioinformatics. 27:2384-2390, 2011

Primary authors: GIACHETTI, Andrea (CIRMMP); ROSATO, Antonio (CIRMMP)

Presenters: GIACHETTI, Andrea (CIRMMP); ROSATO, Antonio (CIRMMP)

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