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ScalaLife - Improving the efficiency and scalability of Life Science Software

Wednesday, 28 March 2012 14:00 (30 minutes)

Advances in HPC have transformed computational Life Science into an indispensable tool for both theoretical and experimental research. Peta- and upcoming exa-scale systems offer great possibilities for simulations and data processing. As usual software development is playing catch-up to hardware advances, even more so in the Life Science domain where computer engineering expertise is lagging relative to other fields. The ScalaLife project focuses on improving the scalability and efficiency of Life Science software and spreading the best practices among the community. The project began work with 4 codes for molecular simulations – DALTON and ERGO (quantum mechanics), GROMACS (molecular dynamics) and DISCRETE (discrete molecular dynamics), thus covering a wide range of time-scales of physical processes. Through the collaboration with PRACE, several improvements to DALTOAN and GROMACS have been achieved, including new parallelization schemes, and the usage of GPUs and even FPGAs. In this talk we will present the experiences gained by working with these packages and the results will also be reported in two PRACE white papers.

Presenter: APOSTOLOV, Rossen

Session Classification: PRACE Workshop