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Title: *HPDA for Biomolecular Research: The BioExcel Case*

Abstract

BioExcel is the European Centre of Excellence for provisioning support to academic and industrial researchers in the use of high-performance computing (HPC) and high-throughput computing (HTC) in biomolecular research. The BioExcel was established to provide the necessary solutions for long-term support of the biomolecular research communities: fast and scalable software, user-friendly automation workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code and personalized consultancy support. The talk will first introduce a quick overview of the BioExcel activities, and then will present the progress on the design and development of reproducible computational biomolecular workflows tackling real scientific problems. These workflows are based on the biobb library, powered by PyCOMPSs, and will combine HPC and Data Analytics.