BioExcel-3: BioExcel-3 Centre of Excellence for Computational Biomolecular Research

Description

Life Science is turning into a data-driven and HPC dependent research field. BioTeam/Hyperion s 2022 estimates show that 95% of Life Science projects are being dependent on HPC. The rapid response to Covid-19 showed how an EU collaboration between pharma industry, Life Science researchers and supercomputing centres resulted in several newly identified hits now undergoing clinical trials. Life Science is already delivering actual drug candidates within a year by using HPC in general, and BioExcel codes in particular (1000s of papers citing GROMACS or HADDOCK for SARS-CoV-2 simulations).The Centre of Excellence for Computational Biomolecular Research (BioExcel) was established in 2015, and funded again in 2018, to helpaccelerate this development. The BioExcel-3 strategy to achieve significant impact relies on (i) ensuring that the most widely used European codes provide high performance, efficiency, scaling, reliability and quality to meet academic and industrial needs; (ii) identifying user needs to prioritise development of features with high scientific impact & performance/porting requests for deployment on EuroHPC resources; (iii) providing state-of-the-art training program for next-generation EU workforce on exploitation of ensemble algorithms, AI approaches, and convergence of HPC, HTC and HPDA; (iv) being the preferred EU partner for international organisations; (v) providing sustainable business paths for companies that need commercial support or want to fund development of specific features; and (vi) operating under an open governance model that provides transparency for the community and EC to be confident BioExcel makes the right priorities based on user and HPC needs.BioExcel-3 will grow and sustain the Life Science HPC community in Europe. Our success will be measured by our ability to support codes andtrain scientists who produce almost 10,000 scientific papers and numerous industrial projects every year. Biomolecular Life Science, Drug Discovery, Biotechnology, Exascale, HPC, Automation and Data Integration

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