

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

Description

Life Science is becoming increasingly dependent on data-driven and HPC research. BioTeam/Hyperion's 2022 estimates show that 95% of Life Science projects are 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 research 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 it received funding again in 2018, to help accelerate this trend of HPC in Life Sciences. The BioExcel-3 strategy strives to:

- (i) ensure that the most widely used European codes provide high performance, efficiency, scaling, reliability and quality to meet academic and industrial needs;
- (ii) identify user needs to prioritise development of features with high scientific impact & performance/porting requests for deployment on EuroHPC resources;
- (iii) provide state-of-the-art training program for the next-generation EU workforce on exploitation of ensemble algorithms, AI approaches, and convergence of HPC, HTC and HPDA;
- (iv) be the preferred EU partner for international organisations;
- (v) provide sustainable business paths for companies that need commercial support or want to fund the development of specific features; and
- (vi) operate under an open governance model that provides transparency for the community and allows the EC to be confident that BioExcel is prioritising based on user and HPC needs.

BioExcel-3 will grow and sustain the Life Science HPC community in Europe. Success will be measured by our ability to support codes and train scientists who produce almost 10,000 scientific papers and numerous industrial projects every year related to Biomolecular Life Science, Drug Discovery, Biotechnology, Exascale, HPC, Automation and Data Integration.

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