

BioExcel2: Centre of Excellence for Biomolecular Research 2

Description

Life Sciences have become increasingly digital and this is accelerating. Computational techniques play key roles in processing, analysis and generating new knowledge from experiments, even in replacing them. This has been enabled due to tremendous advances in techniques such as docking and molecular simulations at both atomistic and quantum levels to which world-leading European research and software are contributing. Pushing computational capabilities towards Exascale will advance the area, enabling researchers to tackle increasingly complex questions related to biomolecules' function, mechanisms, dynamics and interactions. This will impact on our daily life, in health, for the development of new drugs and efficient drug delivery methods, in biotechnology, environment, agriculture, food industry and education. To exploit this great computational power, in academia and industry, significant efforts on software efficiency, scaling, usability and education are needed. This is the mission of the BioExcel Centre of Excellence for Computational Biomolecular Research launched in 2015 with EC support. It has made significant contributions by focusing on highest-impact European codes, workflows and an extensive, international education program. BioExcel-2 will continue and expand this work, with a focus on Exascale impact, improved usability, expanded training and commercial applications, while strengthening its user-driven governance. Specifically it will:

- Push performance, efficiency, scalability and usability of the selected software packages towards Exascale in a co-design manner, contributing to the EuroHPC vision
- Support convergence of HPC, HTC, and HPDA with workflows combining simulations with data management and analytics
- Support and enlarge the user community by providing support, workforce development, continued training, guidance, and best practices
- Develop a sustainable and open community centre with user-driven governance and clear KPIs.

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