Powering computational biomolecular research

The BioExcel Center of Excellence supports academia and industry with the usage of advanced techniques for high-end computing.

Are you an end user of our applications?
Do you develop related software?
Are you a resource provider?

Get in touch with us to learn more about the various ways that BioExcel can improve your work:

www.bioexcel.eu

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Excellence in Scientific Software
Improve the performance, efficiency and scalability of selected software packages of high importance for biomolecular Life Sciences research on next-generation HPC systems

Key Software
CPMD
GROMACS
HADDOCK

Excellence in Usability
Improve the usability of ICT technologies for biomolecular researchers, both in academia and industry
According to user needs, efficient workflow environments with associated data handling and integration of simulation and analysis codes will be devised.

Key Workflows & Platforms
Open PHACTS
COMPss
Galaxy PROJECT
KNIME
Apache Taverna

Excellence in Support
Promote best practices and train end users to make the best use of both the software and computational infrastructure
Supporting academia and industry with the usage of advanced techniques for high-end computing

Much of the current Life Sciences research relies on intensive biomolecular modelling and simulation. As a result of this, both academic and industrial researchers are facing significant challenges when it comes to applying best practices for optimal resource usage and workflow productivity, and to finding a faster path to achieve results.

High-performance computing (HPC) and high-throughput computing (HTC) techniques have now reached a level of maturity in widely used codes and platforms, but taking full advantage of these requires training and guidance by experts. The services ecosystem required for that is presently inadequate, so a suitable infrastructure needs to be set up in a sustainable way.

The BioExcel Center of Excellence (CoE) 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.

User driven research and development
The BioExcel CoE actively engages with a number of interest groups, formed by members of academic and industrial communities, which lay the foundation of the long-term basis for user-driven governance of the center:

- academic and non-profit end users,
- industrial end users,
- software vendors and academic code providers,
- non-profit and commercial resource providers, and
- related international projects and initiatives.