Excellence in Scientific Software

Improve the performance, efficiency and scalability of selected software packages of high importance for bio-molecular Life Sciences research on next-generation HPC systems

Key Software

CPMD QM/MM

GROMACS
FAST. FLEXIBLE. FREE.

HADDOCK
High-Ambiguity Driven Docking

Excellence in Usability

Improve the usability of ICT technologies for biomol-ecular researchers, both in academia and industry

According to user needs, efficient workflow environ-ments with associated data handling and integration of simulation and analysis codes will be devised.

Key Workflows & Platforms

Open PHACTS

COMPSs

Galaxy PROJECT

Open for Innovation
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
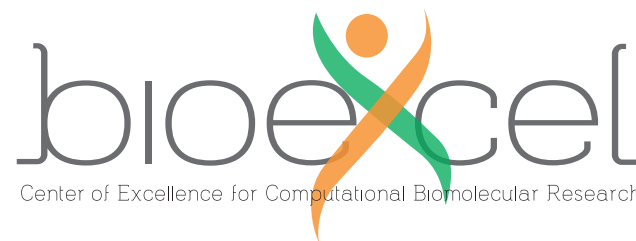
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bioexcel

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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bioexcel
Center of Excellence for Computational Biomolecular Research

Powering computational biomolecular research

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

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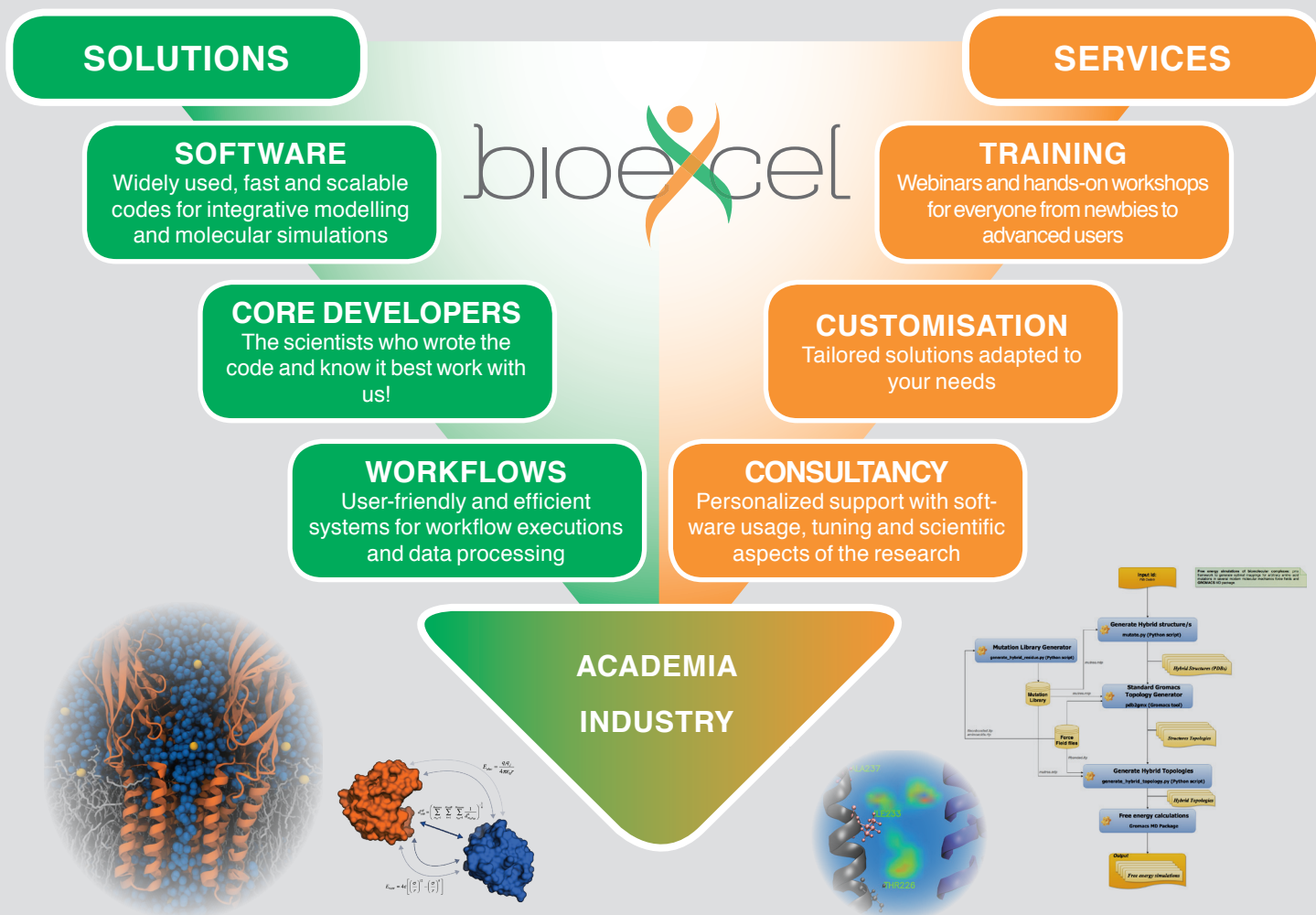
High-performance computing (**HPC**) and high-throughput computing (**HTC**) techniques have now reached a level of maturity in widely used codes and platforms, but taking full advantage of these requires training and guidance by experts. The services ecosystem required for that is presently inadequate,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

SOLUTIONS

SERVICES

SOFTWARE
Widely used, fast and scalable codes for integrative modelling and molecular simulations

TRAINING
Webinars and hands-on workshops for everyone from newbies to advanced users

CORE DEVELOPERS
The scientists who wrote the code and know it best work with us!

CUSTOMISATION
Tailored solutions adapted to your needs

WORKFLOWS
User-friendly and efficient systems for workflow executions and data processing

CONSULTANCY
Personalized support with software usage, tuning and scientific aspects of the research

ACADEMIA

INDUSTRY

Partners

bioexcel.eu