

Powering Biomolecular Research through Advanced Modelling and Simulation

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

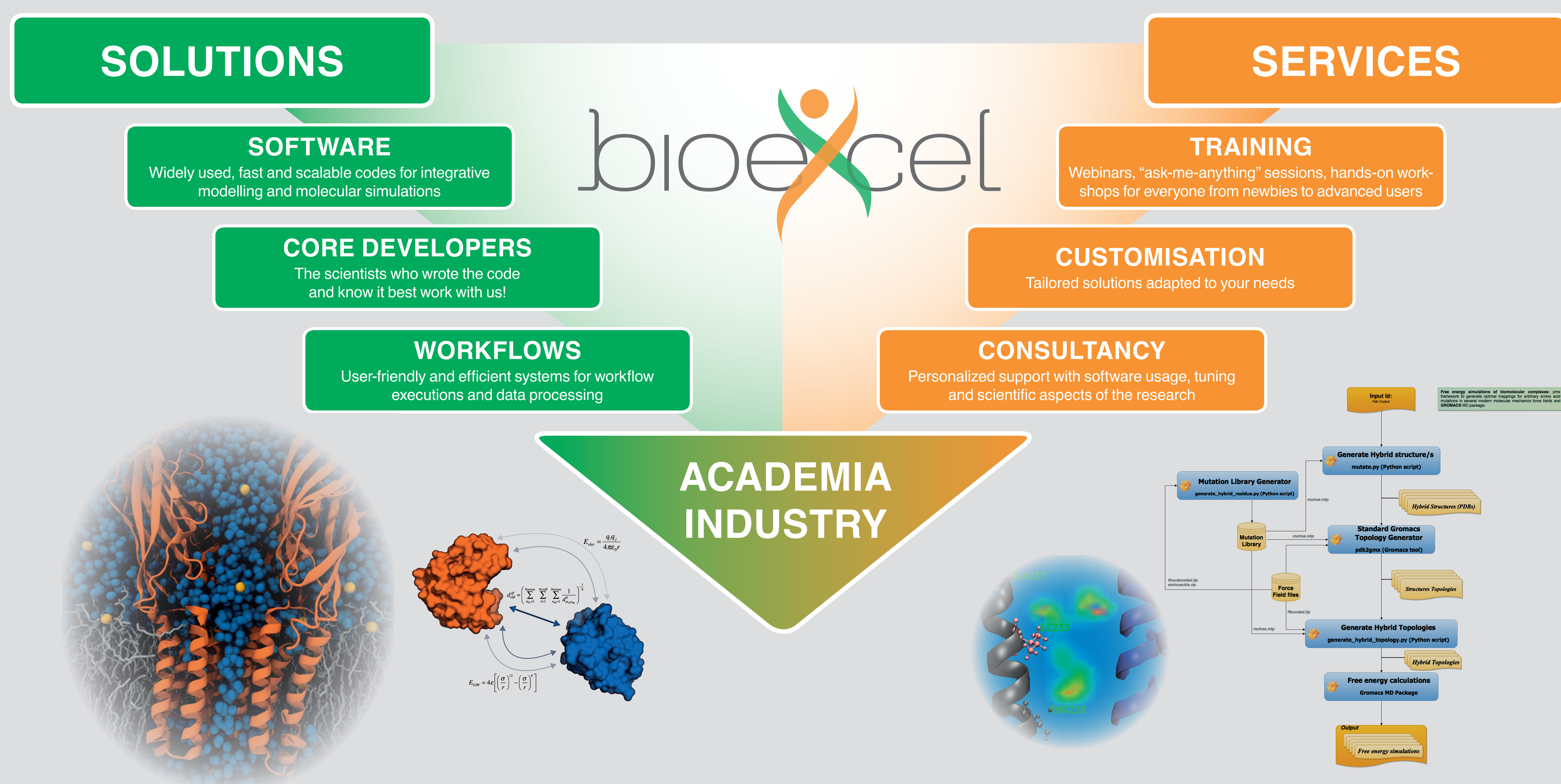
of maturity in widely used codes and platforms, but taking full advantage of these requires training and guidance by experts. The services ecosystem required for that is presently inadequate, so a suitable infrastructure needs to be set up in a sustainable way.

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.

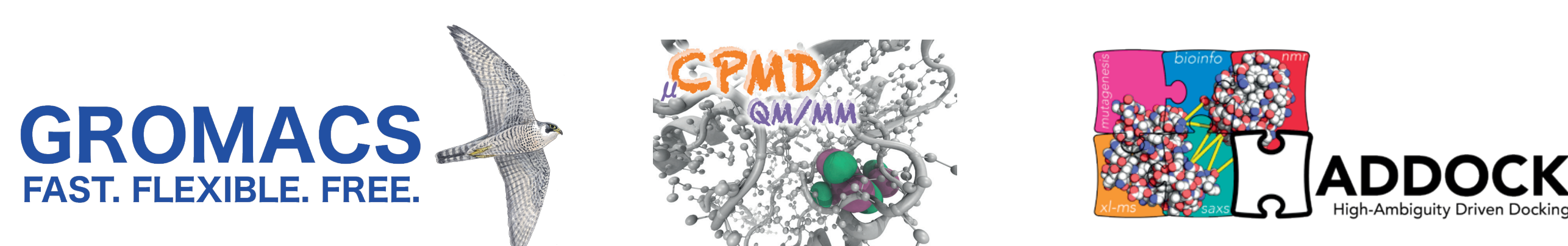
User-driven research and development

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.



Key Software



Key Workflows and Platforms



Partners

