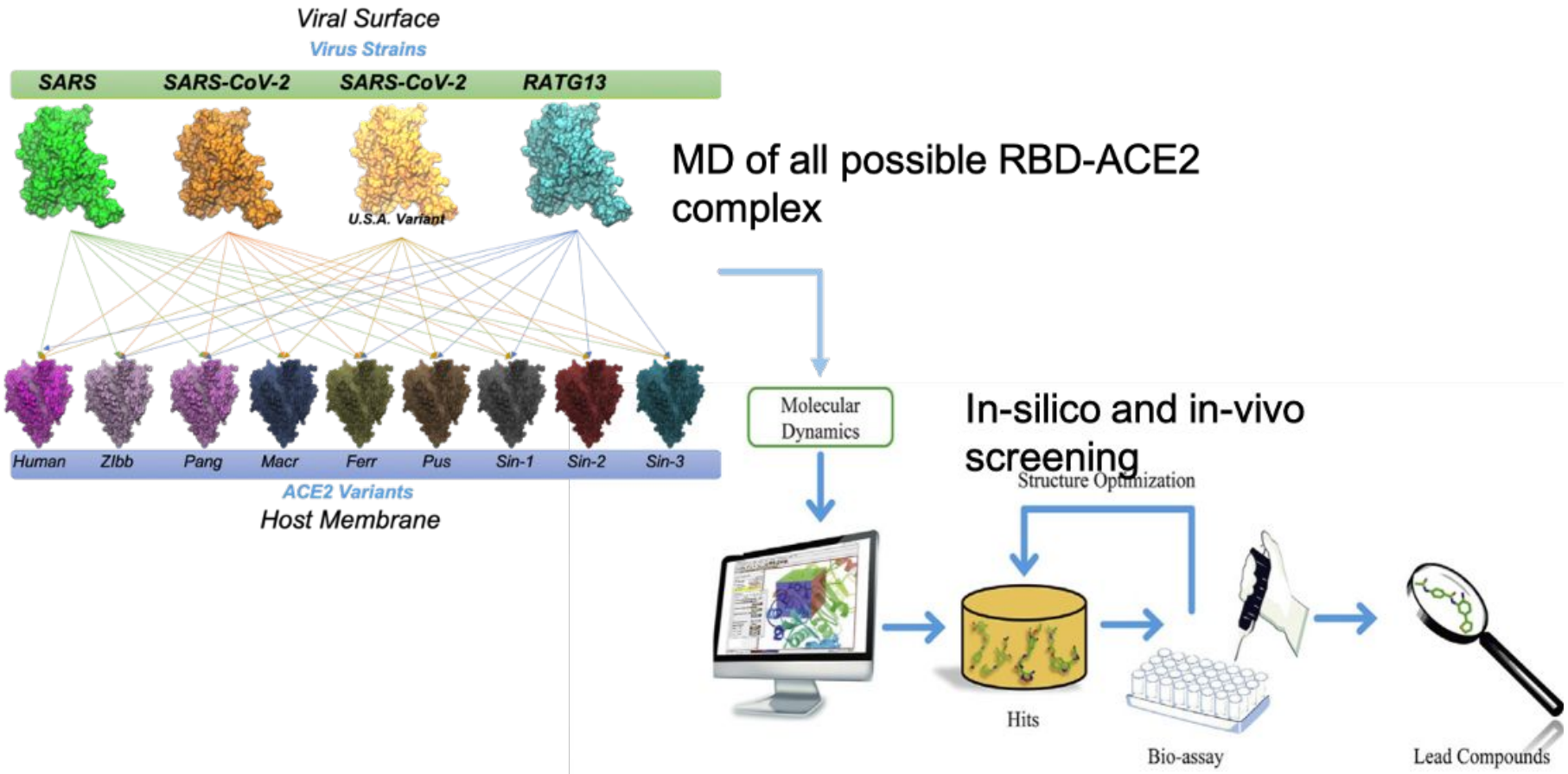
BioExcel Centre of Excellence

Driving Computational Biomolecular Research in Europe

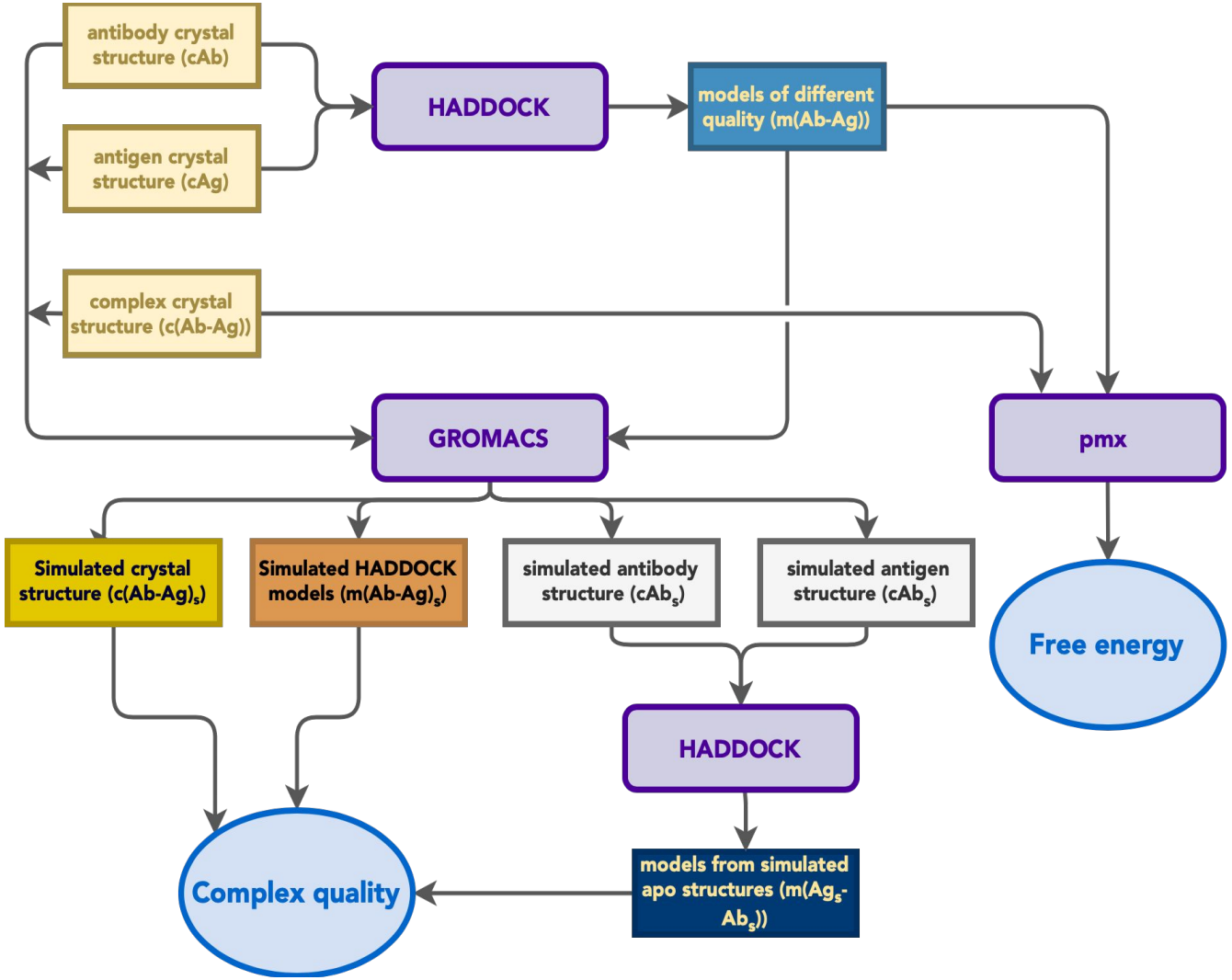
Rossen Apostolov

rossen@bioexcel.eu

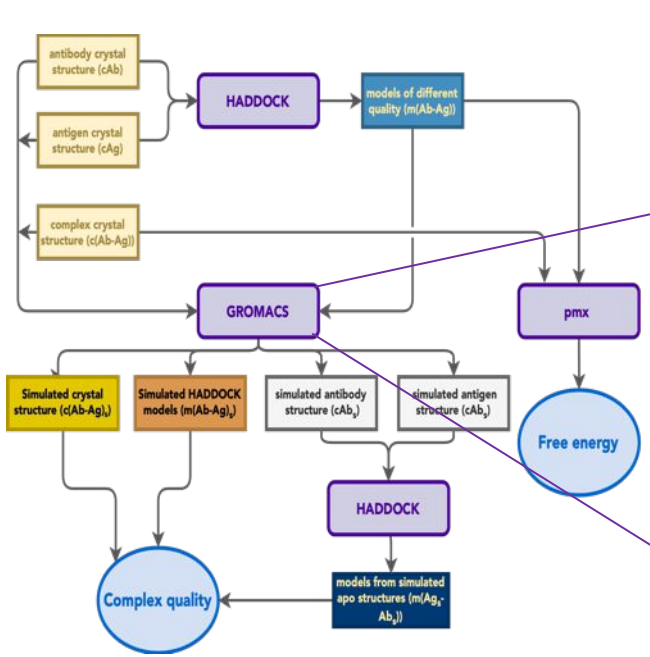
COVID-19 drug screening

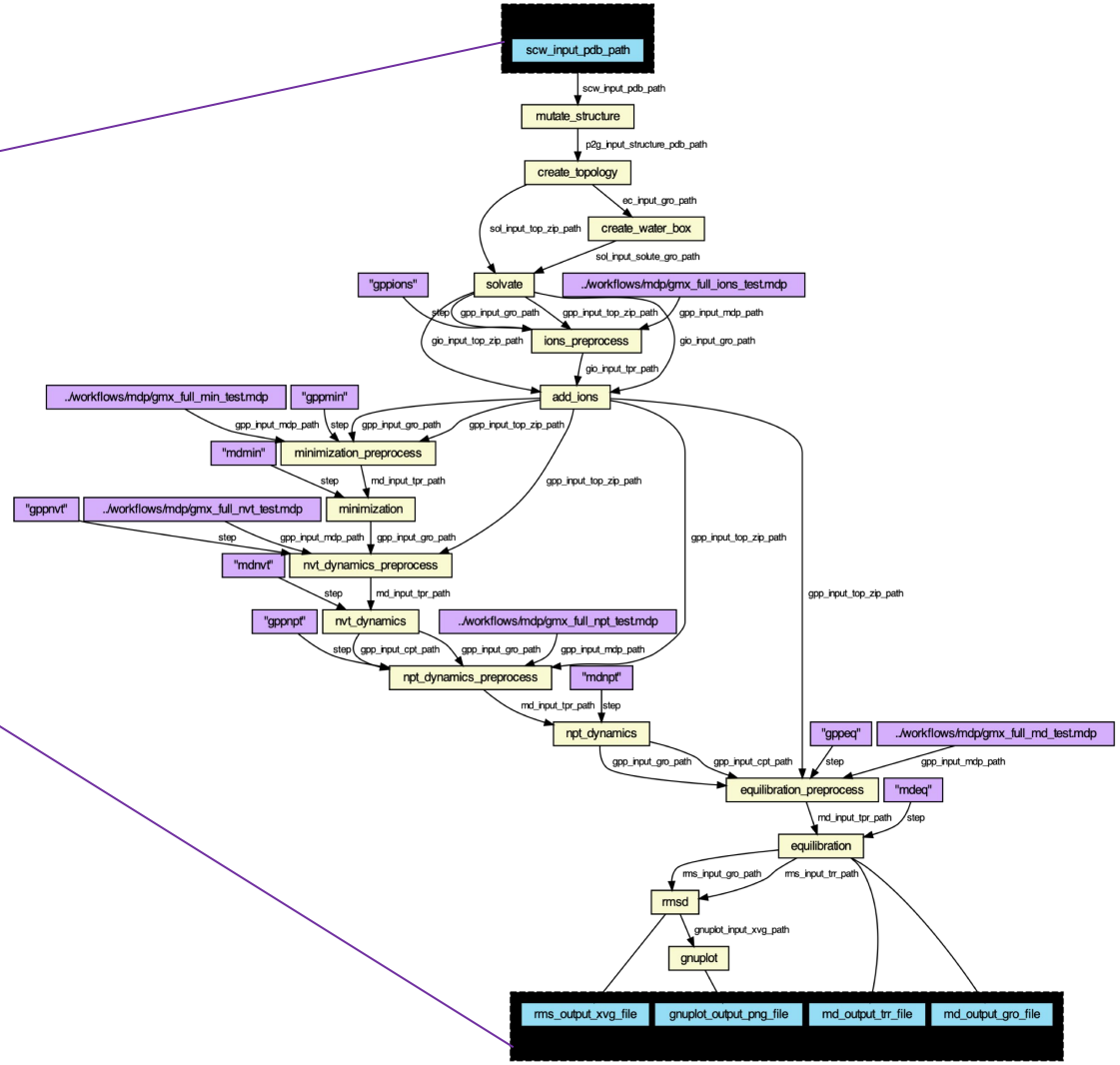


Antibody Design



Antibody Design





Summit: 2,400,000 cores

Piz Daint: 387,000 cores

Beskow: 67,000 cores

Sunway: 10,700,000 cores

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Centre of Excellence for Computational Biomolecular Research

BioExcel Partners

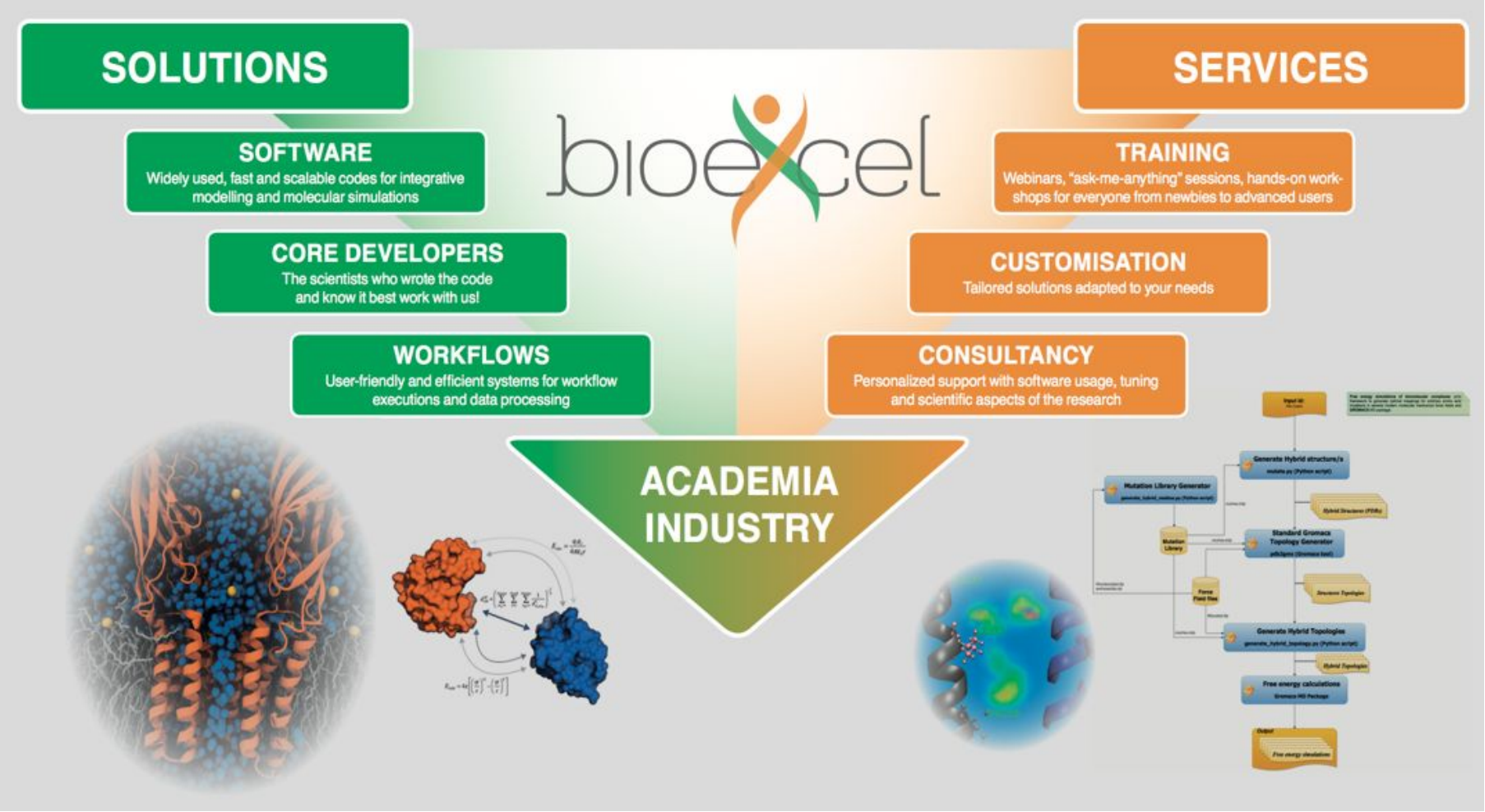
Utrecht University

UNIVERSITY OF JYVÄSKYLA

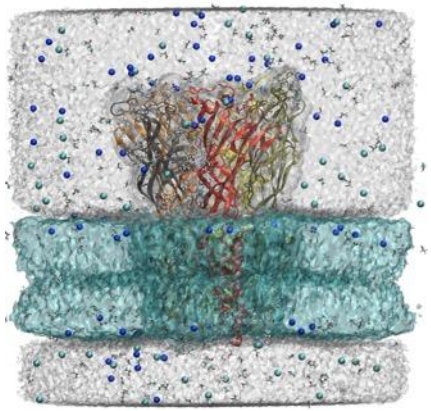
Horizon 2020
European Union Funding
for Research & Innovation

BioExcel is funded by the European Union Horizon 2020 program under grant agreements 675728 and 823830.

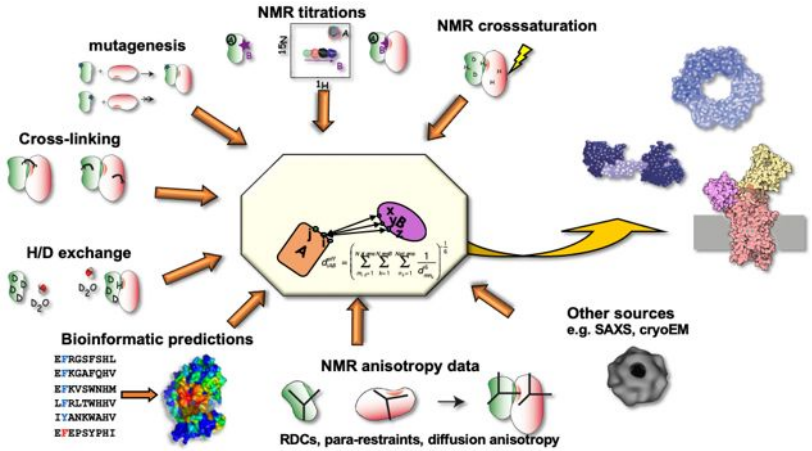
The European hub for biomolecular modeling and simulations



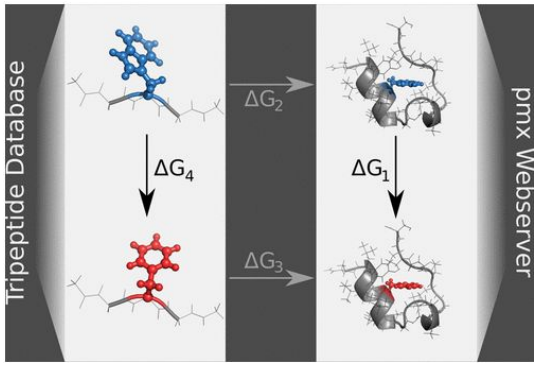
Core Applications



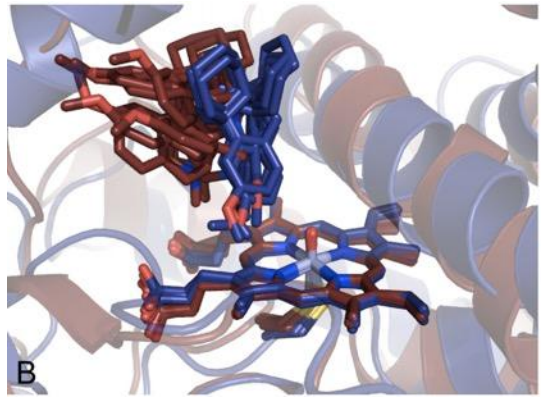
MD with GROMACS



Integrative modelling with HADDOCK



FE with PMX



Hybrid QM/MM with CP2K

Workflows - Usability and Automation

- Make research computing easier to use by biomolecular researchers, both in academia and industry
- Devise efficient workflow environments with associated data integration

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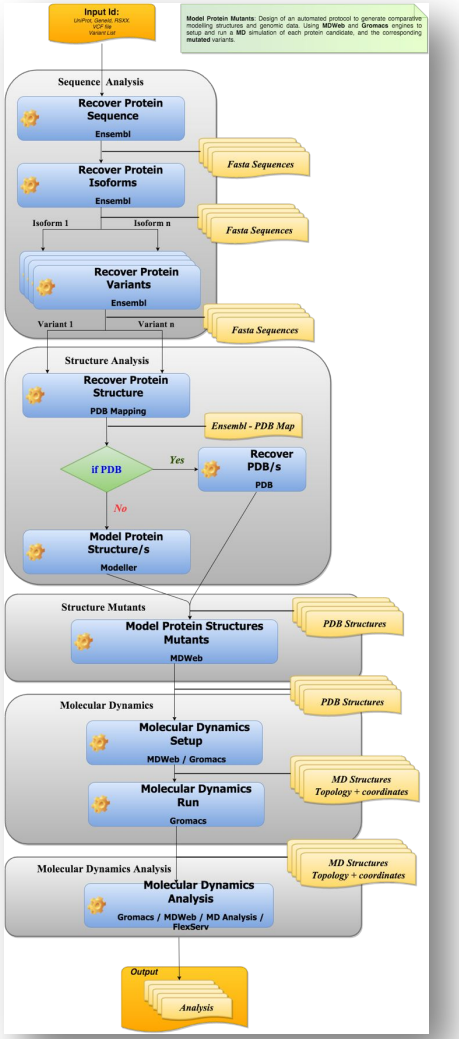
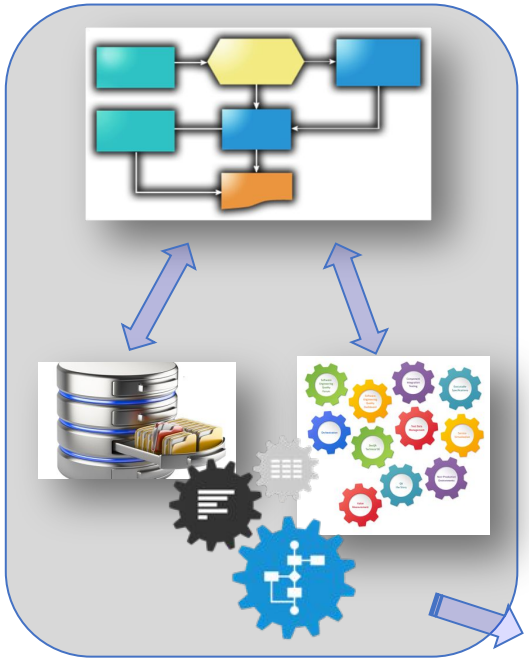
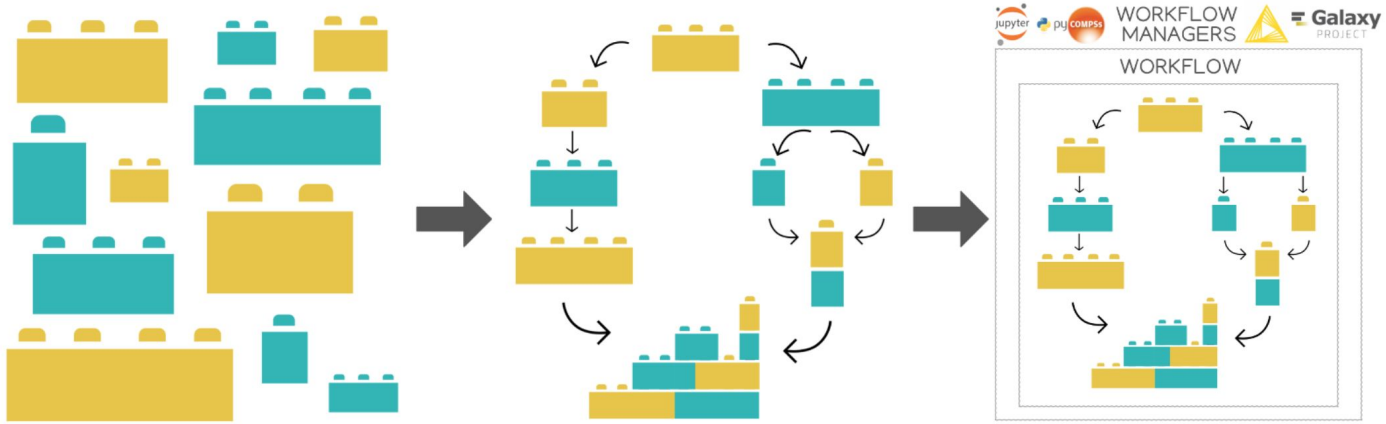
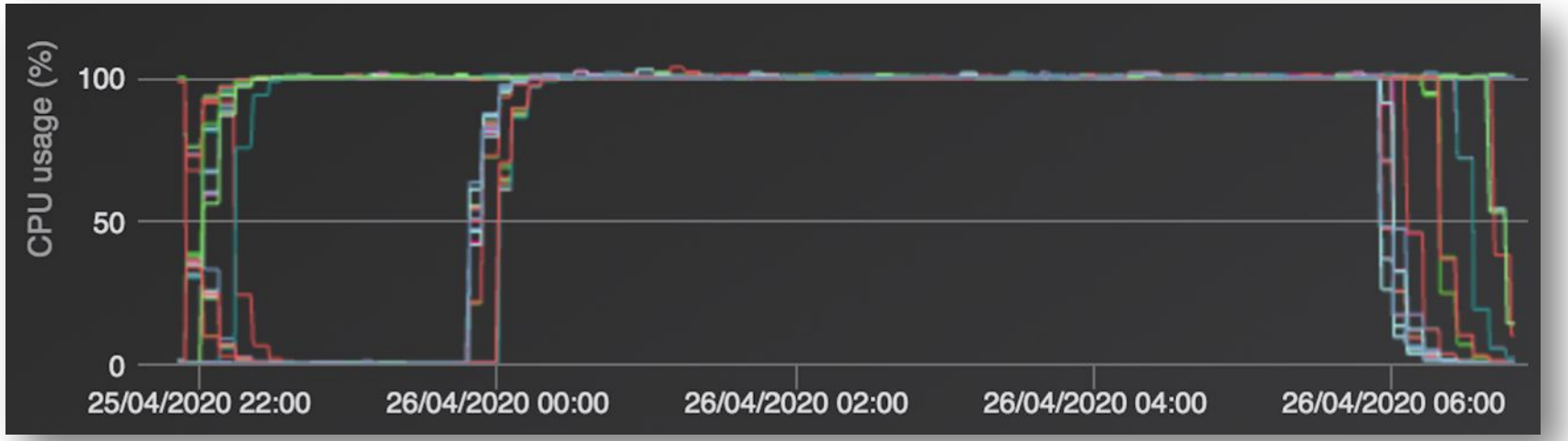


Exascale ready workflows



Workflows Optimization for exascale





✔ *Used in COVID-19 studies*

Supporting Academia and Industry

janssen

Supporting the Pharmaceutical Industry: BioExcel experts visit Janssen's R&D site in Belgium

29 Apr, 2018 *In Featured / Latest News / Success stories by Ian Harrow*

BioExcel continues its direct support to industry through site visits. In early March we were pleased to participate in an exciting day of collaborative talks hosted by Janssen at their research site in Beerse, Belgium.

The morning comprised of presentations by Janssen's Computational Chemistry group, led by Herman van Vlijmen who emphasized that now is an exciting time for computational drug design. Principal scientist, Dr Gary Tresadern covered their interests and needs for molecular dynamics (MD) and free energy (FE) calculations applied to molecular design and virtual screening for drug discovery projects. Important challenges are keeping abreast of the latest methodologies and validation of molecular dynamic predictions in a timely manner. Post-doctoral scientist, Dr Laura Perez presented her recent work on free energy perturbations (FEP) applied to the public 3D structure phosphodiesterase 2 (PDE2) published recently: Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Pérez-Benito L, Keränen H, van Vlijmen H, Tresadern G. Sci Rep. 2018 Mar 20;8(1):4883. DOI: 10.1038/s41598-018-23039-5. Recent collaboration with BioExcel partner, Dr Vytautas Gapsys on GROMACS (bioexcel.eu/software/Gromacs) and PMX (bioexcel.eu/software/pmx) applied to PDE2 has demonstrated encouraging results.

Supporting the Pharmaceutical Industry: BioExcel experts visit UCB's R&D site in Belgium

October 8, 2018 Ian Harrow

BioExcel continues its direct support to industry through site visits. In late May we were pleased to visit UCB's research site in Braine D'Alleud, Belgium for an exciting day of in depth discussions.

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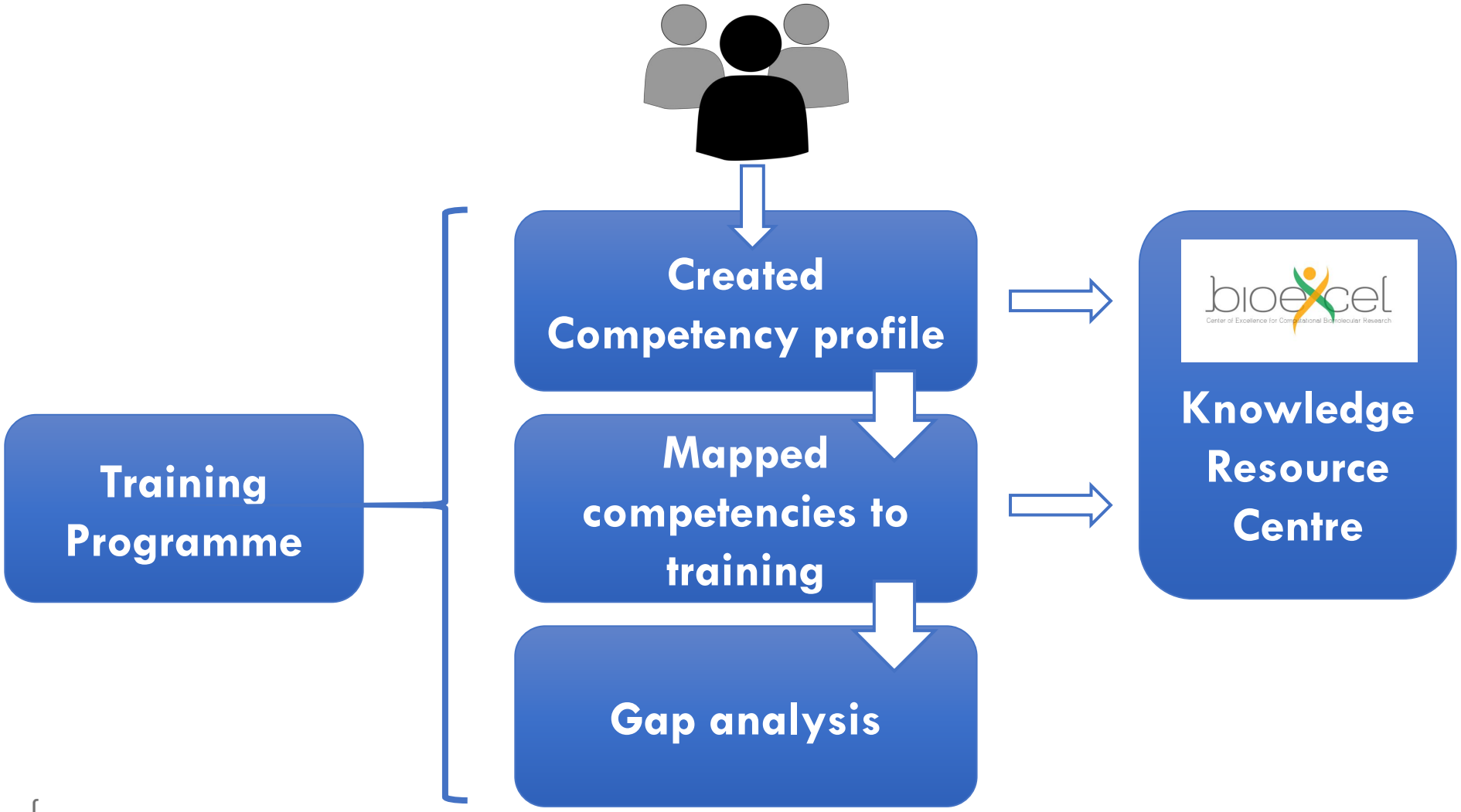
Training Program based on needs analysis



Training events and courses

COMMON WORKFLOW LANGUAGE

Reproducible analyses with Common Workflow Language

29 Apr, 2020 @ 13:00 – 15:30 – Online [...]

archer2

Preparing to run biomolecular QM/MM simulations with CP2K using AmberTools Online

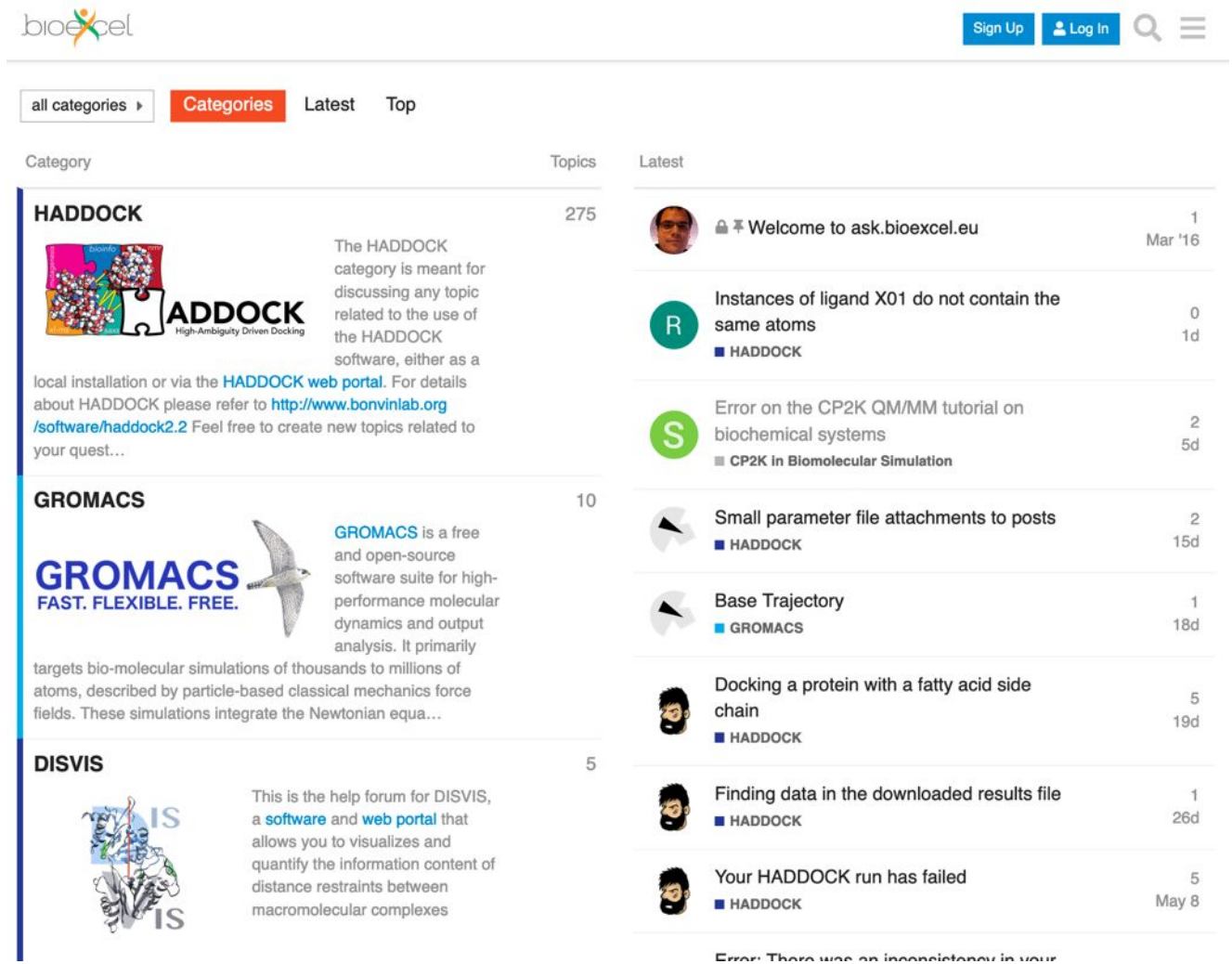
09 Jun, 2020 @ 13:00 – 16:00 – Online [...]

Remote BioExcel Summer School on Biomolecular Simulations

22 Jun, 2020 – 26 Jun, 2020 @ All Day – Online [...]

Webinar Series http://bioexcel.eu/webinars

Support Forums http://ask.bioexcel.eu



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