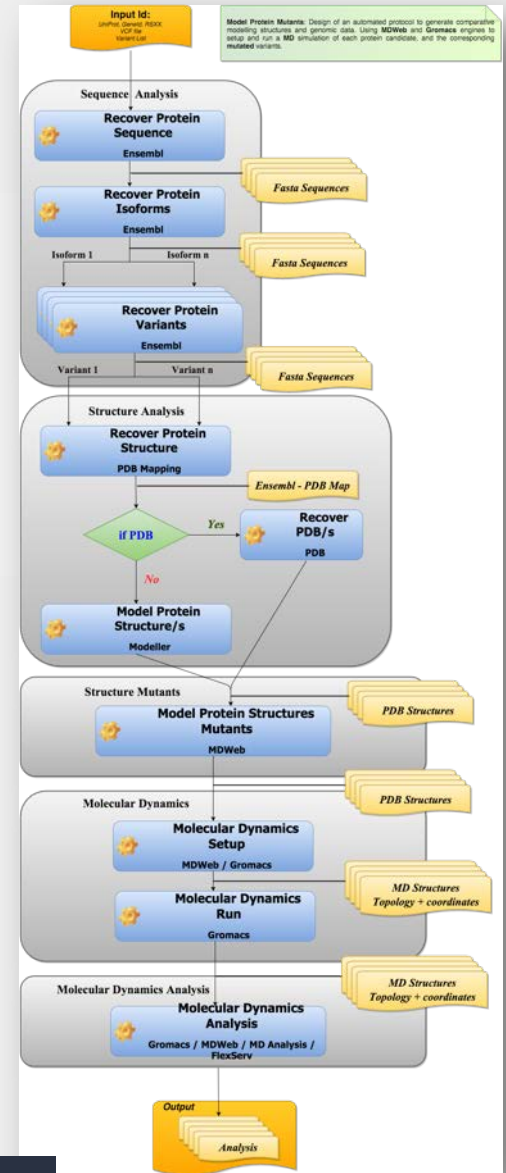
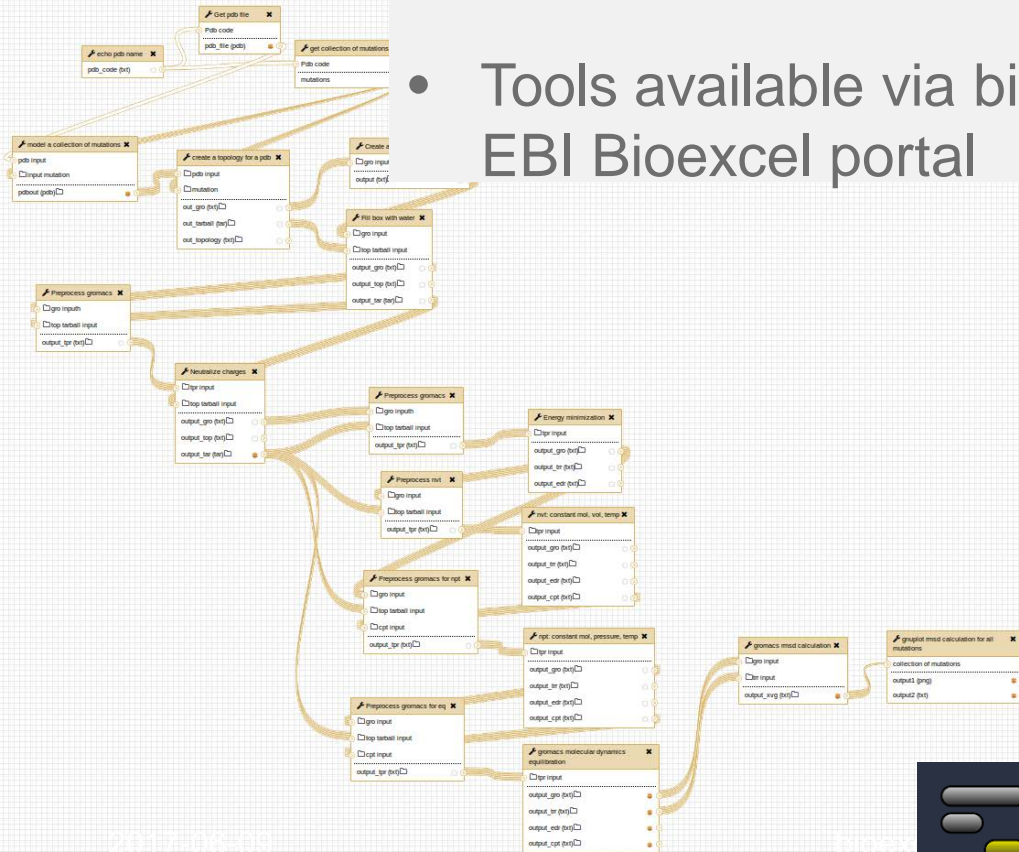


Usability

- First prototype workflows based on use cases (protein mutation)
- Tools available via bio.tools; EBI Bioexcel portal



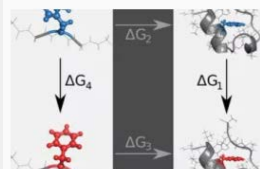
Community Engagement

- 7 Active Interest Groups
- Successful webinar series
- Successful training program
- Scientific publications

Home » Publications

Publications

Below is a list of related publications by the partners of the BioExcel consortium. We strive to publish as Open Access, or to provide green open access preprints where gold open access is not possible. Please let us know if you are unable to access any of our publications.



pmx Webserver: A User Friendly Interface for Alchemy Edit

10 May, 2017 in Publications by Mirren White

This paper describes the pmx webserver, part of the BioExcel community. The paper was published in February 2017 in the Journal of Chemical Information and Modelling. Abstract With the increase of available computational power and improvements in simulation algorithms, alchemical molecular dynamics based free energy calculations have developed into routine [...]



Accelerated cryo-EM structure determination with parallelisation using GPUs in RELION-2 Edit

9 May, 2017 in Publications by Mirren White

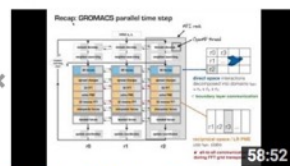


BioExcel Center of Excellence for Computational Biomolecular Research

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Video material developed by the center of excellence.

Uploads



BioExcel Webinar Series #6:
Optimizing cluster and simulation...
195 views • 8 months ago



BioExcel Webinar Series #5:
QM/MM approaches in CPMD
242 views • 11 months ago

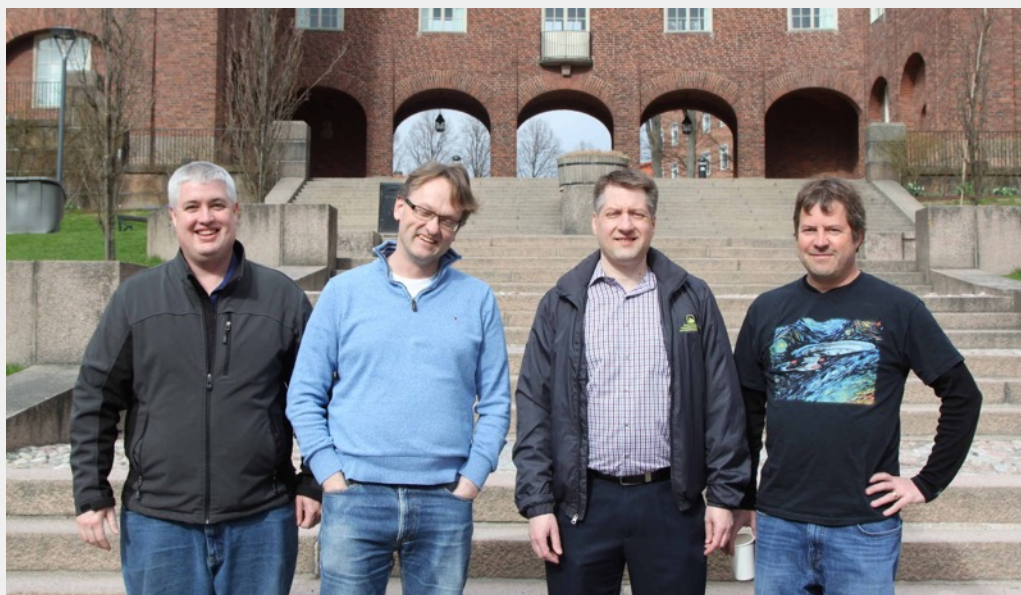


BioExcel Webinar Series #4:
Mutation free energy calculation...
287 views • 11 months ago



BioExcel Webinar Series #3:
Atomistic Molecular Dynamics...
256 views • 1 year ago

PRACE/BioExcel Spring School



We organized the first ever workshop with the core developers of the 3 most widely used MD codes and visualization application – GROMACS, AMBER, NAMD and VMD

<https://events.prace-ri.eu/event/502/>

Summary

- Centers of Excellence (CoE) are an effective way of supporting scientific communities on their path towards the exascale
 - Needs long-term commitment
 - Critical mass
- Life Sciences and molecular modeling are a prime user group of HPC
- Serious software development efforts needed
 - Including rationalization of software packages