

After today...

- ARCHER2 accounts under ta025 will keep access until June 1st
 - Download any data *before* June 1st
- 1000 CU compute time available (1000 node hours)
 - ARCHER2 downtime expected in May – use sooner rather than later
- Course feedback survey (registration page on PRACE website)
- Recordings will appear on youtube.com/bioexcelcoe

Best Practices in QM/MM Simulation of Biomolecular Systems

Challenges

research question

the scope of QM/MM simulations

starting structure

x-ray/NMR/Cryo-EM/homology model

tautomers (protons), heterogeneity

Hamiltonian

force field and level of quantum chemistry theory

size of QM and MM regions

QM/MM boundary

QM/MM interactions

validation

soft- and hardware

sampling

static or dynamics

collective variables / reaction coordinates

convergence



Maria João Ramos



Adrian Mulholland



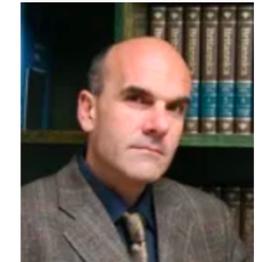
Maria Khrenova



Ulf Ryde



Carme Rovira

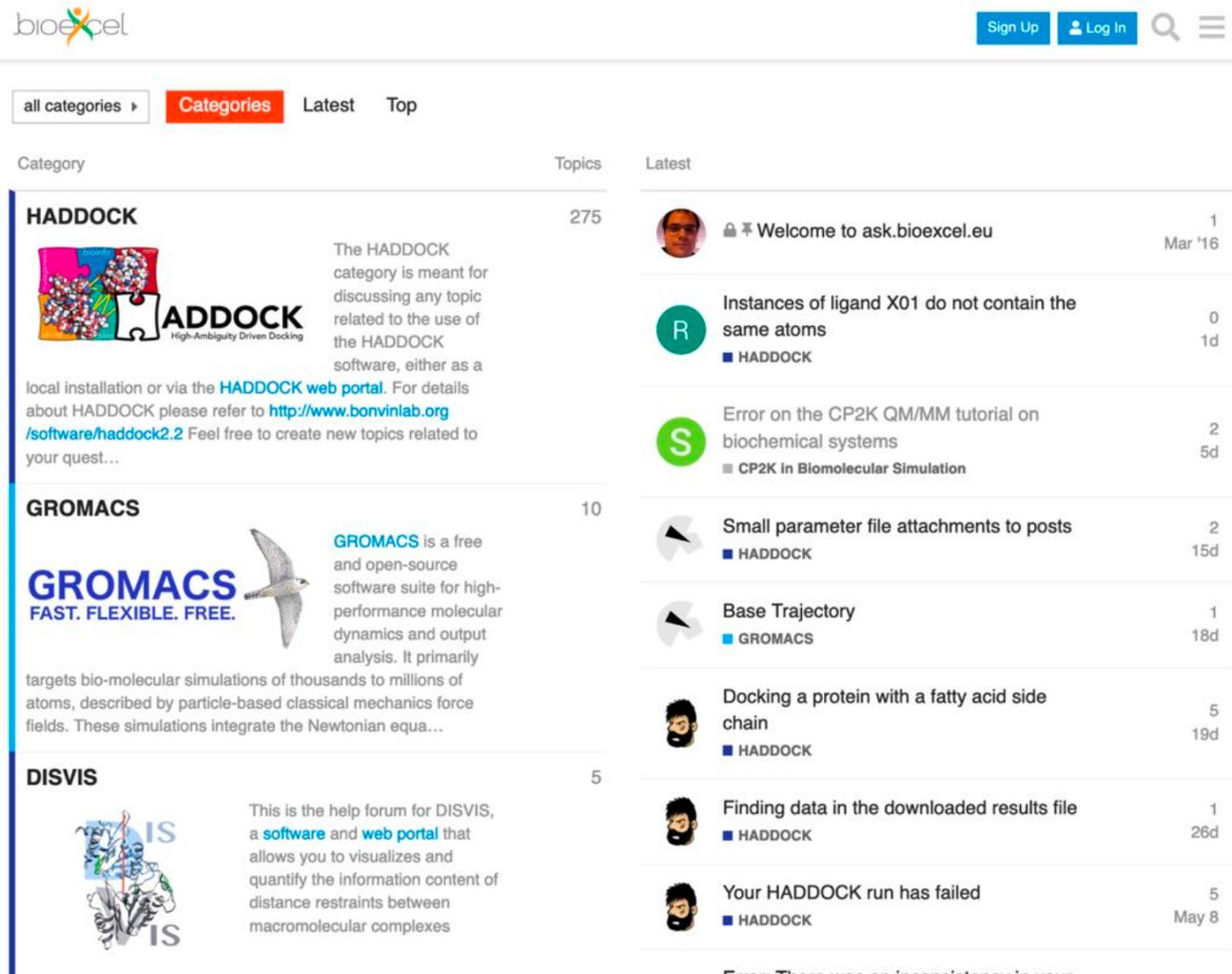


Janez Mavri



Gerrit Groenhof
(co-organiser)

Support Forums <http://ask.bioexcel.eu>



The screenshot shows the bioexcel support forums interface. At the top, there is a navigation bar with the bioexcel logo, a search icon, and buttons for 'Sign Up' and 'Log In'. Below the navigation bar, there are filters for 'all categories', 'Categories', 'Latest', and 'Top'. The main content area is divided into two columns: 'Category' and 'Latest'.

Category

Category	Topics
HADDOCK  <p>The HADDOCK category is meant for discussing any topic related to the use of the HADDOCK software, either as a local installation or via the HADDOCK web portal. For details about HADDOCK please refer to http://www.bonvinlab.org/software/haddock2.2 Feel free to create new topics related to your quest...</p>	275
GROMACS  <p>GROMACS FAST. FLEXIBLE. FREE.</p>  <p>GROMACS is a free and open-source software suite for high-performance molecular dynamics and output analysis. It primarily targets bio-molecular simulations of thousands to millions of atoms, described by particle-based classical mechanics force fields. These simulations integrate the Newtonian equa...</p>	10
DISVIS  <p>This is the help forum for DISVIS, a software and web portal that allows you to visualize and quantify the information content of distance restraints between macromolecular complexes</p>	5

Latest

Topic	Replies	Time
 Welcome to ask.bioexcel.eu	1	Mar '16
 Instances of ligand X01 do not contain the same atoms ■ HADDOCK	0	1d
 Error on the CP2K QM/MM tutorial on biochemical systems ■ CP2K in Biomolecular Simulation	2	5d
 Small parameter file attachments to posts ■ HADDOCK	2	15d
 Base Trajectory ■ GROMACS	1	18d
 Docking a protein with a fatty acid side chain ■ HADDOCK	5	19d
 Finding data in the downloaded results file ■ HADDOCK	1	26d
 Your HADDOCK run has failed ■ HADDOCK	5	May 8

Error: There was an inconsistency in your

Thank you for attending!

