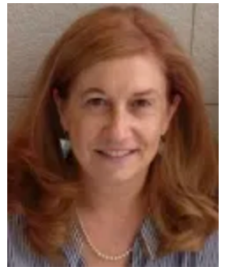
After today...

- 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), heterogeniety
- 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



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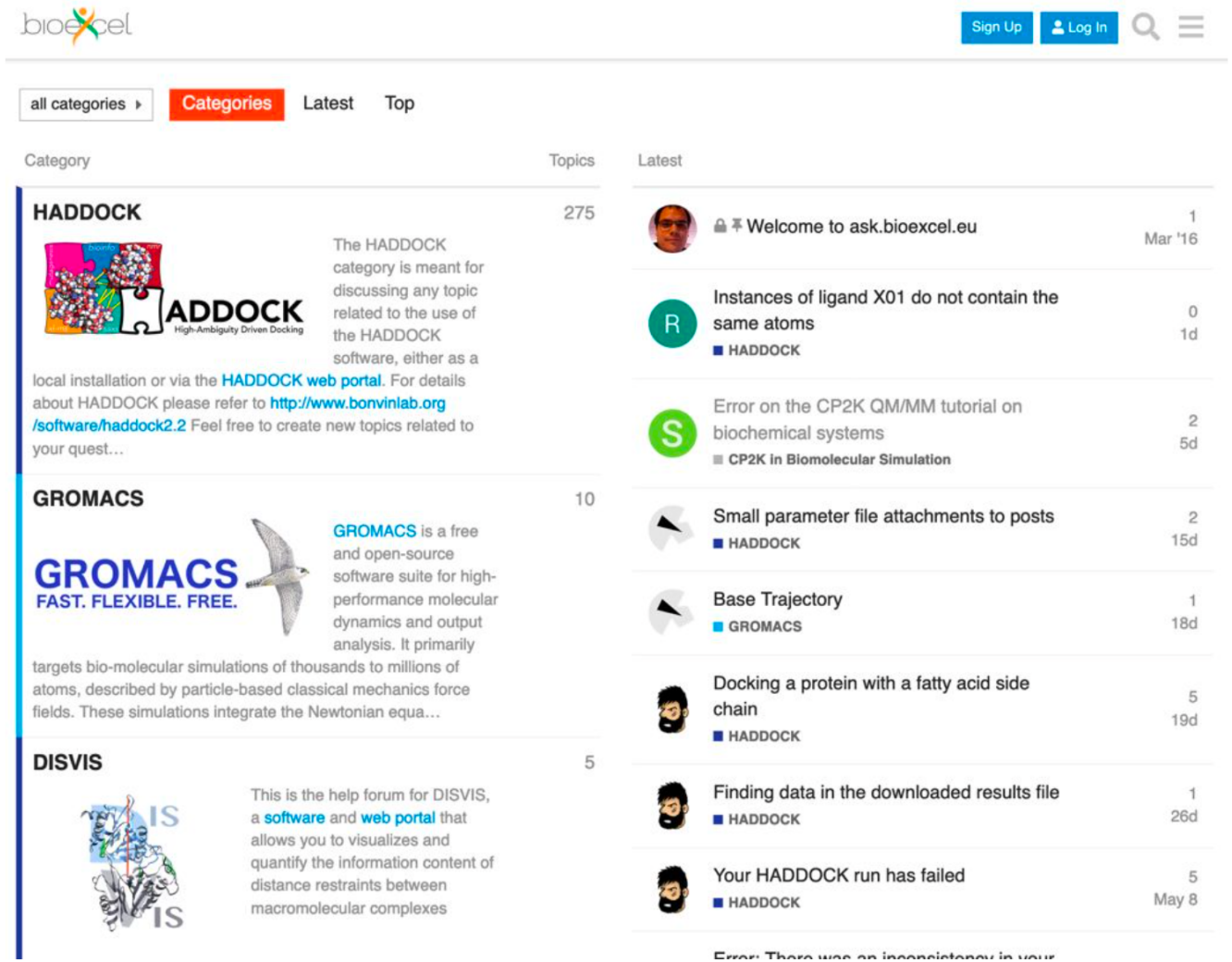
(co-organiser)

Support Forums http://ask.bioexcel.eu



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Centre of Excellence for Computational Biomolecular Research

UNIVERSITY OF JYVÄSKYLÄ

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Horizon 2020
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Thank you for attending!