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
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