

PRACE Spring School – HPC for Life Sciences – in collaboration with BioExcel Center of Excellence

10 April (day 1)

08:30-09:00 Registration

09:00-09:15 Welcome [**Michaela Barth**]

09:15-10:00 BioExcel Center of Excellence training program [**Vera Matser**]

10:00-10:30 Coffee break

10:30-12:00 Molecular visualisations with VMD [**John Stone**]

12:00-13:00 Lunch

13:00-14:30 Hands-on VMD

14:30-15:00 Coffee Break

15:00-17:00 Hands-on VMD

11 April (day 2)

09:30-10:30 HPC Simulations with NAMD - [**Jim Phillips**]

10:30-11:00 Coffee break

11:00-12:00 HPC Simulations with NAMD

12:00-13:00 Lunch

13:00-14:30 Hands-on NAMD

14:30-15:00 Coffee Break

15:00-17:00 Hands-on NAMD

12 April (day 3)

09:30-10:30 HPC Simulations with GROMACS [**Erik Lindahl**]

10:30-11:00 Coffee break

11:00-12:00 HPC Simulations with GROMACS

12:00-13:00 Lunch

13:00-14:30 Hands-on GROMACS

14:30-15:00 Coffee Break

15:00-17:00 Hands-on GROMACS

18:00 Social Event Dinner

13 April (day 2)

09:30-10:30 HPC Simulations with AMBER [**Tom Cheatham**]

10:30-11:00 Coffee break

11:00-12:00 HPC Simulations with AMBER

12:00-13:00 Lunch

13:00-14:30 Hands-on AMBER

14:30-15:00 Coffee Break

15:00-17:00 Hands-on AMBER