

[ONLINE] PATC: Introduction to Simulation Environments for Life Sciences @ BSC

Monday, March 14, 2022 - Tuesday, March 15, 2022

Scientific Program

Tentative Agenda

Day 1

Session 1

09.00h – Welcome & Introduction
10.30h – Break
11.00h – Atomistic MD Algorithm
11.45h – Algorithm improvements & HPC
12.30h – Break

Session 2

14.00h – Simulation Setup
15.30h – Break
16.30h – Setup and Analysis Hands On

Day 2

Session 3

09.00h – Simulation DBs and Data Management
10.30h – Break
11.00h – Coarse Grained MD
12.00h – Application Examples
13.00h – Break

Session 4

14.00h – Trajectory visualization and analysis
16.00h – Break
16.30h – Report writing
18.00h – End of the course