

Introduction for Simulation Environments for Life Sciences @ BSC

Wednesday 11 March 2020 - Thursday 12 March 2020

Barcelona BSC Campus Nord

Agenda

Day 1

Session 1

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

Session 2

14.00h – Simulation Setup (FB)
15.30h – Break
16.30h – Setup and Analysis Hands On (PA)
18.00h – Adjourn

Day 2

Session 3

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

Session 4

14.00h – Trajectory visualization and analysis (PA)
16.00h – Break
16.30h – Report writing (FB, PA)
18.00h – End of the course

PD: Pablo Dans (IRB-Barcelona)

PA: Pau Andrio (BSC)

FB: Federica Battistini (IRB-Barcelona)