

# **[ONSITE] PerMedCoE/BioExcel: Introduction to HPC for Life Scientists**

**Tuesday, March 7, 2023 - Wednesday, March 8, 2023**

**Edifici Vèrtex, Campus Nord, UPC**

## **Agenda**

Day 1: Tuesday 7 March 2023

09:00 - 09:45 Welcome, introductions and expectations  
09:45 - 10:05 LECTURE: Introduction to High Performance Computing (HPC)  
10:05 - 10:30 PRACTICAL: Connecting to MareNostrum  
10:30 - 11:00 Break  
11:00 - 11:20 LECTURE: HPC Architectures  
11:20 - 12:00 PRACTICAL: Overview of the MareNostrum system and modules  
12:00 - 12:20 LECTURE: Batch systems and parallel application launchers  
12:20 - 13:00 PRACTICAL: Batch Systems and MareNostrum Slurm Scheduler  
  
13:00 - 14:00 Lunch break  
14:00 - 14:30 LECTURE: Computational Building Blocks (software + hardware)  
14:30 - 15:00 LECTURE: Parallel Programming Models (OpenMP, MPI)  
15:00 - 15:30 PRACTICAL: PhysiCell, OpenMP, MPI  
15:30 - 16:00 Break  
16:00 - 16:45 PRACTICAL: PhysiCell, OpenMP, MPI  
16:45 - 17:45 Women in science session: From the Top Secret Rosies to women in HPC  
17:45 - 18:30 Drinks and nibbles

Day 2: Wednesday 8 March 2023

9:00 - 9:05 Welcome  
9:05 - 9:45 Mapping computation to HPC hardware: molecular simulation  
9:45 - 10:30 Practical: GROMACS simulations on multicore CPUs  
10:30 - 11:00 Break  
11:00 - 11:45 Practical: GROMACS simulations on multi node clusters  
11:45 - 12:15 GPU accelerators and heterogeneous architectures  
12:15 - 12:55 Practical: GROMACS simulations on GPUs  
13:00 - 14:00 Lunch break  
14:00 - 14:30 LECTURE: Introduction to PyCOMPSs programming model  
14:30 - 15:00 PRACTICAL: PyCOMPSs  
15:00 - 15:30 LECTURE: PerMedCoE Building Blocks and Workflows  
15:30 - 16:00 Break  
16:00 - 16:30 PRACTICAL: PerMedCoE Building Blocks and Workflows  
16:30 - 17:00 Course wrap-up, final questions & feedback