Day 1 (Feb. 13)

**Session 1 / 9:00am – 1:00 pm (4 h lectures)**

9:00-9:15 Welcome (Mariano Vázquez, BSC)

9:15-11:00 Introduction to HPC in Computational Modelling (Marco Verdicchio, SURFsara)

11:00-13:00 Compilation and Optimization in the HPC environment (Okba Hamitou, Bull)

13:00-14:00 Lunch Break

**Session 2 / 2:00pm – 6:00 pm (4 h lectures)**

14:00-16:00 Zoom in on blood - Using supercomputers in hemodynamics (UvA) (Gábor Závodszky, UvA)

16:00-18:00 PlayMolecule: Cloud-based Applications for Molecular Discovery (João Damas, ACELLERA, Adrià Perez, UPF)

Day 2 (Feb. 14)

**Session 3 / 9:00am – 1:00 pm (4 h lectures)**

9:00-11:00 Hands on Image Registration with pFIRE (Phil Tooley, USFD)

11:00-12:00 Parallel algorithms for Computational Mechanics (Ricard Borrell, BSC)

12:00-13:00 HPC Multi-scale computational modelling using Alya Red (Jazmín Aguado-Sierra, BSC)

13:00-14:00 Lunch Break

**Session 4 / 2:00pm – 6:00 pm (2 h lectures, 2 h practical)**

14:00-15:00 Introduction to Computer-Aided Drug Design (CADD) and GPCR Modelling (Dr Alexander Heifetz, EVOTEC)

15:00-16:00 Innovations in HPC-training for medical, science and engineering students (Andrea Townsend-Nicholson, UCL)

16:00-18:00 Molecular Medicine: Hands On (Andrea Townsend-Nicholson, UCL)

Day 3 (Feb. 15)
Session 5 / 9:00am – 1:00 pm (4 h lectures)

9:00-10:00 Data Visualization for Researchers (Guillermo Marín, BSC)

10:00-12:00 Visualization applied to 2D/3D scientific datasets (Paul Melis, SURFsara)

12:00-13:00 Integrating Computational Biology and Soil Metagenomics: An Undergraduate Study (Mariana Pereira da Costa, UCL)

13:00-14:00 Lunch Break

Session 6 / 2:00pm – 4:00 pm

14:00-16:00 Visit to MareNostrum

END of COURSE

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