[ONLINE] PATC: Short course on HPC-based Computational Bio-Medicine @ BSC

Tuesday, February 15, 2022 - Friday, February 18, 2022

Scientific Program

Agenda and topics

Tuesday 15th of February 2022

HPC-basics track
10:00-14:00hs CET. “First steps in the HPC environment”. This training provides information and tutorials about how to access and perform basic actions on a supercomputer. This session covers a wide range of topics: some theoretical aspects such as the description of the processor architecture, the several levels of code parallelization, and practical aspects such as the batch scheduler usage, compilation and optimization guidelines towards good performance achievements.

Wednesday 16th of February 2022

Molecular medicine track
10:00-11:00hs CET “Introduction to Computer-Aided Drug Design (CADD)”. The subject of my presentation is application computer-aided drug design (CADD) methods in drug design. CADD is the application of computer modelling techniques to drug design process. I will provide a brief overview of these CADD approaches illustrated by the examples taken from real drug discovery campaigns. In my presentation, I will cover the basic theory behind these methods and describe various techniques like virtual screening, homology modeling, docking, structure- and ligand- based drug design, fragment-molecular orbital (FMO) quantum mechanics analysis of protein-water-ligand interactions, GPCR modeling, structure-activity analysis (SAR) and artificial intelligence/deep learning.
11:30-14:00hs CET “Molecular Medicine”. This workshop in molecular medicine aims to provide participants with a theoretical understanding of the importance of the relationship between human microbiomes – the microorganisms present in and on the human body – and human health and with the practical opportunity to use state of the art computational resources to run a metagenomics pipeline. Using marker gene abundance data and the QIIME2 computational workflow, the identity of the different bacterial taxa present in Next Generation Sequence data obtained from medically-relevant microbiome samples will be obtained and the statistical significance of the experimental hypothesis determined.

Thursday 17th of February 2022

Computational Mechanics track
10:00hs-11:55hs CET “Fluid-Structure Interaction methods for biomechanics”. During this hands-on course, different approaches for modelling fluid-structure interaction (FSI) couplings will be explored. The working principles of both boundary-conforming and immersed methods will be introduced in order to understand the benefits of using one or another in diverse applications. Relevant aspects of high-performance computing (HPC) will also be discussed during the course. Practical exercises will be carried out using Alya, a multi-physics HPC code developed at BSC designed from scratch to run efficiently on supercomputers. We will be running simulations on Marenostrum 4, BSC's supercomputer, in order to get familiarised with an HPC server environment.
12:05-14:00hs CET “Zoom in on blood - Using supercomputers for blood flow simulations”. 1 mm^3 of human blood, that is less than a single drop, contains about 5 million cells. The interaction and deformation of these cells give rise to the unique properties of blood. Modern biomedical research (e.g. on drug delivery, effect of various diseases such as diabetic cells or sickle cell disease) builds on this information. Unravelling detailed biomechanical and rheological processes in flowing blood requires an accurate modelling of these deformable cells and the surrounding fluid on microscopic level. In this lecture an open-source package (www.hemocell.eu) will be discussed that on one

hand allow us to model the behaviour of single cells accurately, and on the other hand can scale up to the level of large flows with millions of cells.

Friday 18th of February 2022

Metabolic and multiscale modeling track

10:00-10:45hs CET. ""A brief introduction to large-scale constraint based metabolic modeling and analysis". Constraint-based reconstruction and analysis (COBRA) is a promising methodology for modeling of the chemical processes in living organisms. It can be used to accurately simulate the metabolic output and predict growth of bacteria and microbe communities, and to find various information about genes and enzymes that influence the metabolism. In the talk, we will describe the mathematical rationale behind the COBRA methods and show hands-on examples of common analyses, their inputs and outputs, and the outcomes reachable by large-scale application of the methods. The methods will be showcased using COBREXA.jl, a new HPC-enabled software package for running large metabolic modeling and analysis workflows.

11:00-14:00hs CET. "The use of multiscale modelling to build a virtual patient from the cell-level up" Multiscale modelling is a versatile methodology that can reconcile cell intracellular events (such as mutation or drug effects) with cell population effects (such as cancer phenotypes or clonal heterogeneity formation). These models are helping researchers address the diseases at the cell level by enabling the study of the consequences of mutations and genomic alterations in specific signalling and metabolic pathways of the different cell types, the modelling of the temporal evolution of the complete tumour and its microenvironment and the prediction of the response to different drugs.In this talk, we will introduce the basics of multiscale modelling (Metzcar et al., 2019), the use of Boolean-logic-based models of signalling pathways (Stoll et al., 2017), and the simulation of tumour evolution with agents representing cell types (Ghaffarizadeh et al., 2018). Specifically, we will present tools to tailor a Boolean model to a given patient's data (Béal et al., 2019; Montagud, Béal, et al., 2021) and simulate the interplay of genetic and environmental perturbations in the context of cancer cells' resistance to drugs (Letort et al., 2019; Ponce-de-Leon et al., 2022). Finally, we will present recent advances in using such tools in pre-exascale high-throughput computing clusters to simulate cancer tumours of millions of cells and simulate thousands of patients in optimised analysis pipelines that go from patients' genomic information to simulation results (Montagud, Ponce-de-Leon, et al., 2021; Saxena et al., 2021).