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Objectives

The course will make the attendants familiar with simulation technologies used in Life Sciences and their specific adaptation to HPC environment

Detailed outline:

Introduction to biomolecular simulation Coarse-grained and atomistic simulation strategies Automated setup for simulation

HPC specifics: Large scale parallelization, use of GPU's Storage and strategies for large scale trajectory analysis

Requirements

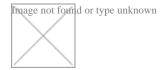
Prerequisites: Basic knowledge of structural bioinformatics Basic knowledge of parallelization strategies. Material will be provided during the course, students are welcome to provide their own use cases.

Please download and carefully read the following **instructions** regarding the logistics participants enrolling online PATC at BSC are expected to follow.

Learning Outcomes

Setup, execute, and analyze standard simulations in HPC environment

Academic Staff



Course Convener: Josep Gelpi, BSC Life Sciences - INB Computational Node 2 Group Manager

Materials



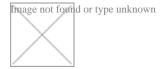
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• For further details, please contact BSC?CNS patc [at] bsc [dot] es

Further information



PLEASE BRING YOUR OWN LAPTOP.

NOTE: PATC courses do not charge fees

Recommended Accommodation: Please follow the link for map of some local hotels.

CONTACT US for further details about MSc, PhD, Post Doc studies, exchanges and collaboration in education and training with BSC.

For further details about Postgraduate Studies in UPC - Barcelona School of Informatics (FiB), visit the website.

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