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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

Learning Outcomes: Setup, execute, and analyze standard simulations in HPC environment

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.

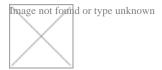
Please download and carefully read the following **instructions** regarding the logistics participants enrolling online PATC at BSC are expected to follow.

Academic Staff

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Course Convener: Josep Gelpi

Materials



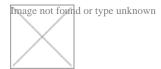
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• For further details, please contact BSC?CNS patc [at] bsc [dot] es

Further information



All PATC Courses at BSC do not charge fees.

In the context of virtual meetings, the Organiser may facilitate live webstreaming and audio recording. You have the option to opt out of inclusion in recordings by contacting our Education&Training team.

<u>CONTACT US</u> 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

Sponsors: BSC and PRACE 6IP project are funding the PATC @ BSC training events. If you want to learn more about PRACE Project, visit the website.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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