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# **PATC: Introduction to Simulation Environments for Life Sciences**

# **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.

### 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



#### 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.

**Sponsors:** BSC and PRACE 5IP project are funding the PATC @ BSC training events. If you want to learn more about PRACE Project, visit the <u>website</u>.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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