PATC Course: 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**

**Course Convener:**

Josep Gelpi
Registration for this course will be opened at a later date.

**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 4IP 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

---