[ONSITE] PerMedCoE/BioExcel: Introduction to HPC for Life Scientists

Objectives

Objectives: High-performance computing (HPC) is a fundamental technology used to solve a wide range of scientific research problems. Many important challenges in science such as protein folding, drug discovery, and tumour evolution, all depend on simulations, models and analyses run on HPC facilities to make progress.

This course introduces HPC to life science researchers, focusing on the aspects that are most important for those new to this technology to understand. It will help you judge how HPC can best benefit your research, and equip you to go on to successfully and efficiently make use of HPC facilities in future. The course will cover basic concepts in HPC hardware, software, user environments, filesystems, and programming models. It also provides an opportunity to gain hands-on practical experience and assistance using an HPC system (MARENOSTRUM) through examples drawn from the life sciences, such as biomolecular simulation (GROMACS) and multicellular simulations (PhysiCell).

The course is organised and funded by PerMedCoE - the HPC/Exascale Centre of Excellence in Personalised Medicine (https://permedcoe.eu/) and BioExcel - the Centre of Excellence for Computational Biomolecular Research (http://bioexcel.eu) using the HPC infrastructure at the Barcelona Supercomputing Centre.

Requirements

Prerequisites: Familiarity with basic Linux commands (at the level of being able to navigate a file system). You may find a Linux online course such as https://swcarpentry.github.io/shell-novice/ useful if you are less familiar with Linux.

No programming skills or previous HPC experience is required.

Participants will need to bring their own laptop to the course. Further instructions will be provided after registration.

Learning Outcomes

On completion of the course, we expect that attendees will be able to:

Explain the drivers and motivation to use HPC
Identify HPC hardware - Building blocks and architectures
Define Parallel computing - Programming models and implementations
Use HPC systems

- Access
- Batch schedulers & resource allocation
- Running jobs
- Dealing with errors
- Using libraries
- Performance

Academic Staff

Image not found or type unknown

Course convenors: Daniel Thomas López (EMBL-EBI, PerMedCoE), Marta Lloret Llinares (EMBL-EBI, PerMedCoE)

Lecturers: Jose Carbonell (BSC, PerMedCoE), Francisco Javier Conejero (BSC, PerMedCoE), Berk Hess (KTH, BioExcel), Szilárd Páll (KTH), David Vicente (BSC, PerMedCoE), Alessandra Villa (KTH, BioExcel, PerMedCoE), Thaleia Ntiniakou (BSC).

Materials

Image not found or type unknown

The materials used in the training use the licence Creative Commons CC BY 4.0.

Further information

Image not found or type unknown

All PATC Courses at BSC do not charge fees.

A limited number of **grants** will be available for this event. If you would like to be considered for a grant:

- Check the information in the PerMedCoE grants document.
- Complete the registration form for the course.
- Email Marta Lloret Llinares after the submission of your application explaining why you should be considered for a grant.

Sponsors:
- BSC
- PerMedCoE (www.permedcoe.eu) is funded by the European Union's Horizon 2020 Programme under grant agreement 951773.
BioExcel is funded by the European Union Horizon 2020 programme under grant agreements 823830, 675728, and Horizon Europe programme under grant agreement 101093290.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

---

Source URL (retrieved on *6 Oct 2024 - 14:57*): https://www.bsc.es/es/education/training/other-training/onsite-permedcoebioexcel-introduction-hpc-life-scientists