Biochemistry

Supercomputer

High Performance Computing

Numerical simulations

Astronomy

Materials

Optics

Parallel computing

Exoplanets

Big data

Networks

Chemistry

Image processing

Mathematics

Complex systems

Supramolecules

Polymers

Tensor calculations

Superabsorber

Drug design

Genetic algorithm

Biology

DESCRIPTION

HPC is a key step in present development of both new technologies and fundamental science but is also essential for the analysis of large amount of data. The PTCI platform proposes to the user an access to high-performance computing (HPC) equipment combined with a high level technical support. Our service includes the estimation of the hardware requirements and an assistance to optimize the software performances on our facilities. Our cluster is dedicated to general purpose job and handle many concurrent jobs from several users with varying requirements. The PTCI is part of the shared infrastructure of the Fédération Wallonie-Bruxelles CÉCI (Consortium des Équipements de Calcul Intensifs).

EXPERTISE

The PTCI has an expertise for the management of HPC equipment and for the installation and optimization of codes dedicated to particular applications, including the license management. The fields of expertise of the University research teams involved in the PTCI are very broad: Chemistry, Mathematics, Physics, Astronomy, Material Science, Polymers, Optics, Algorithmic, Biology,...

EQUIPMENT

The main cluster (Hercules) comprises more than 900 cores spread across 65 compute nodes including multi-core nodes (from 12 to 24 cores) with 24 to 128 GB of RAM and GPGPU. All the nodes are interconnected by a Gigabit Ethernet network and have access to several shared storage systems for a total capacity of 100 TB. Two hardware-accelerated interactive visualization nodes provide a way to remotely run 3D accelerated application. More than 100 softwares are installed, including most of the general programming languages, home-made codes developed for particular applications, major scientific codes under license or visualization tools. As part of the CÉCI shared infrastructure, the PTCI gives also access to larger HPC facilities.
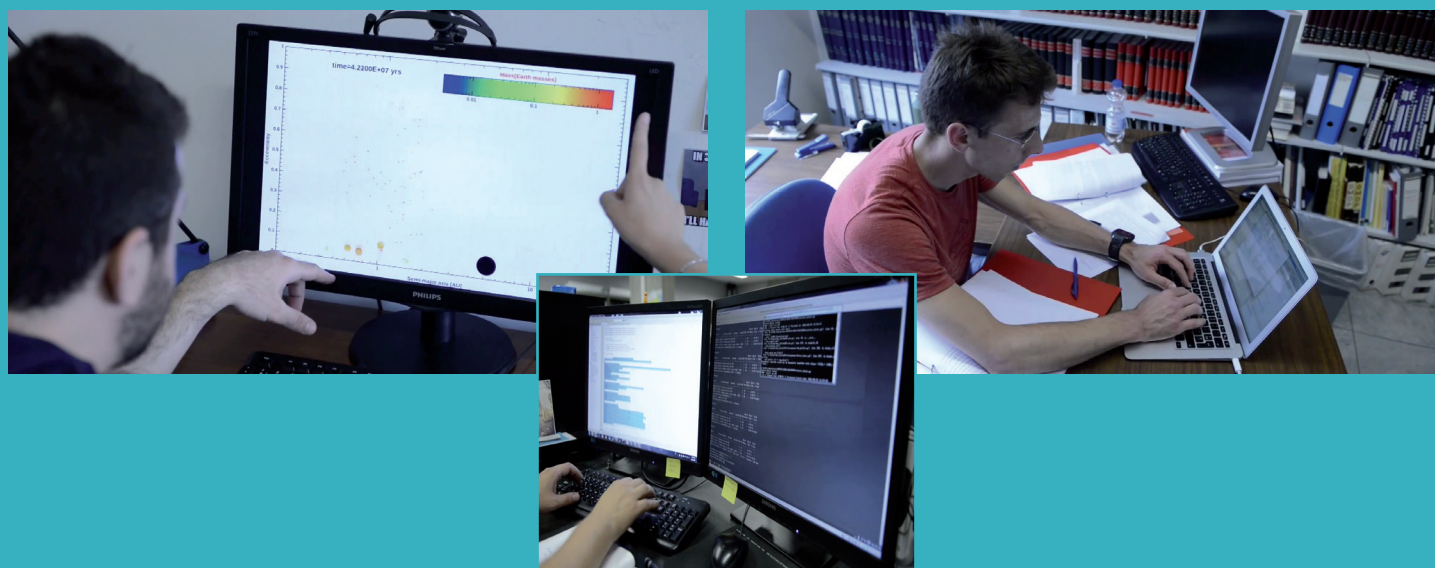
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