Milipeia usage by portuguese scientists

Pedro Alberto

Centro de Física Computacional
Laboratório de Computação Avançada
Universidade de Coimbra

UNIVERSIDADE DE COIMBRA

CENTRO DE FÍSICA COMPUTACIONAL

Bem vindos à página da Milipeia

O cluster Milipeia é composto por:

- **Hardware**
  - 2 nós de gestão Sun Fire X4100:
    - 2x processadores Opteron 275 (double core @ 2.2 GHz);
    - 8 GB RAM;
    - 2 discos SAS de 36 GB.
  - Sun 3511 StorEdge:
    - 6 TB de disco;
    - 2 ligações de 1 Gbs fibre-channel a cada nó de gestão.
  - 130 nós de computação Sun Fire X4100:
    - 2x processadores Opteron 275 (double core @ 2.2 GHz);
    - 8 GB RAM;
    - 1 disco SAS de 36 GB.
- **Software**
  - O sistema operativo: CentOS 4.4.
  - Sistema de gestão de processos/scheduler: Torque (2.1.7)/Maui (3.2.6p19).
  - Allocation management: Gold (2.13).
  - Gestão de ambiente do utilizador: Environment Modules (3.2.5).
  - Compiladores GNU, Intel e Pathscale.

Equipamento financiado pelo PNRC (Programa Nacional de Re-equipamento) sob a égide da FCT (Fundação para a Ciência e Tecnologia) e co-financiado pelo Programa POCI2010, FEDER.

FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

Ciência.Inovação 2010 Programa Operacional Ciência e Inovação 2010

- CentOS, Torque/Maui, GNU, Intel and Pathscale compilers, mpich2
- Application software and libraries: FFTW, lapack, acml, mkl, cernlib, gromacs, namd, siesta, vasp, gamess, octopus, etc
- Access is by scientific projects submission
- Last call in February 2010

Scientific projects

- 33 projects (3M cpu-hours granted over 6.140.000 requested)
- PIs from 7 Universities and research institutions like LIP, I3N, CESAM and ITN
- collaborators all over Portugal and abroad

Scientific projects (a sample)

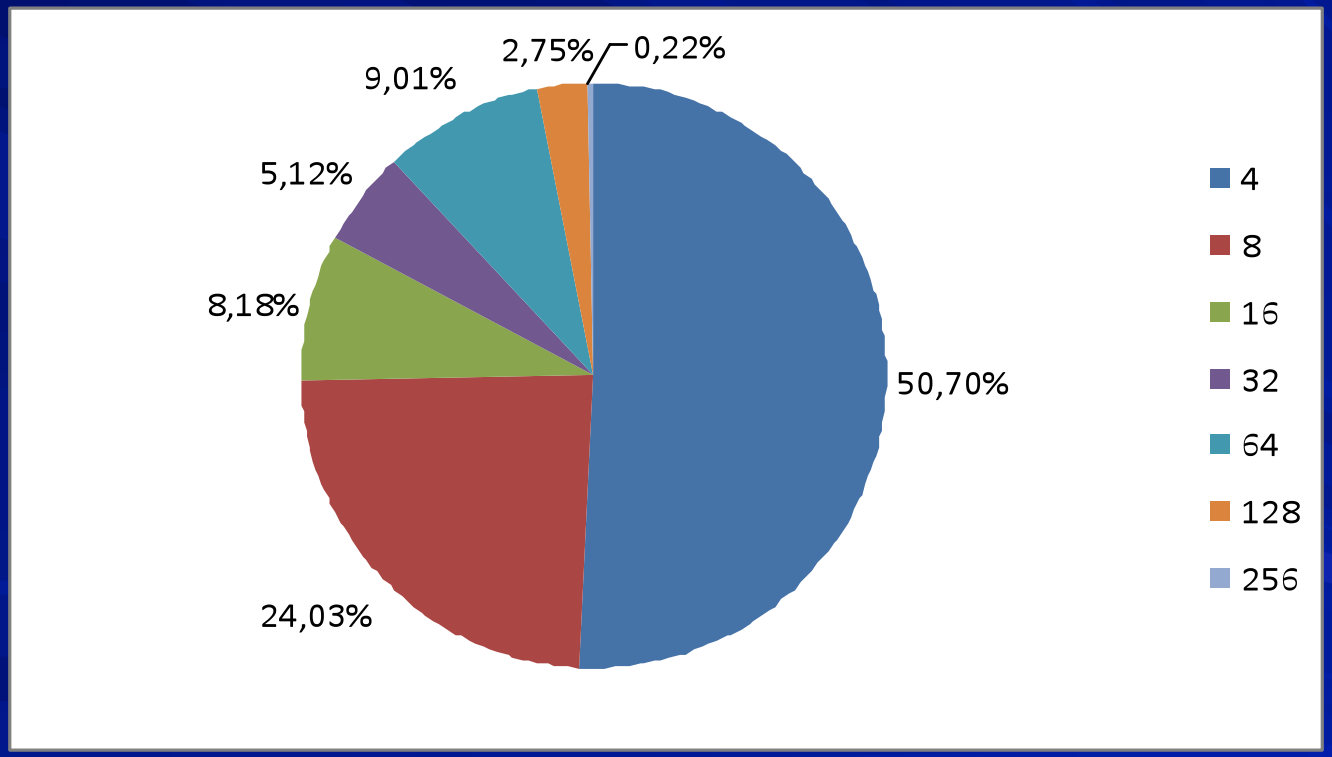
- Adaptive numerical strategies for simulating multiscale problems
- Large-scale parallel Monte Carlo simulations for Ocean Colour applications
- Analysis of atmospheric aerosols using Chemical Transport Model
- Dynamic Black Holes in generic space-times
- Interaction of High Velocity Clouds with the Disks of Galaxies
- Electronic structure and excitations
- Lattice QCD
- Neutron and Proton Radiobiology at ICNAS
- MD simulations of proteins: towards a better understanding of amyloid diseases
- Increasing the accuracy of the computational rational drug-design methods

Milipeia Usage

- 10/2009-5/2010:
  - **90 %** of the machine occupied on average
  - Waiting jobs for 580 cores on average
- Used by post-graduate students in U Coimbra courses and final year projects
- Average of 20 core/job

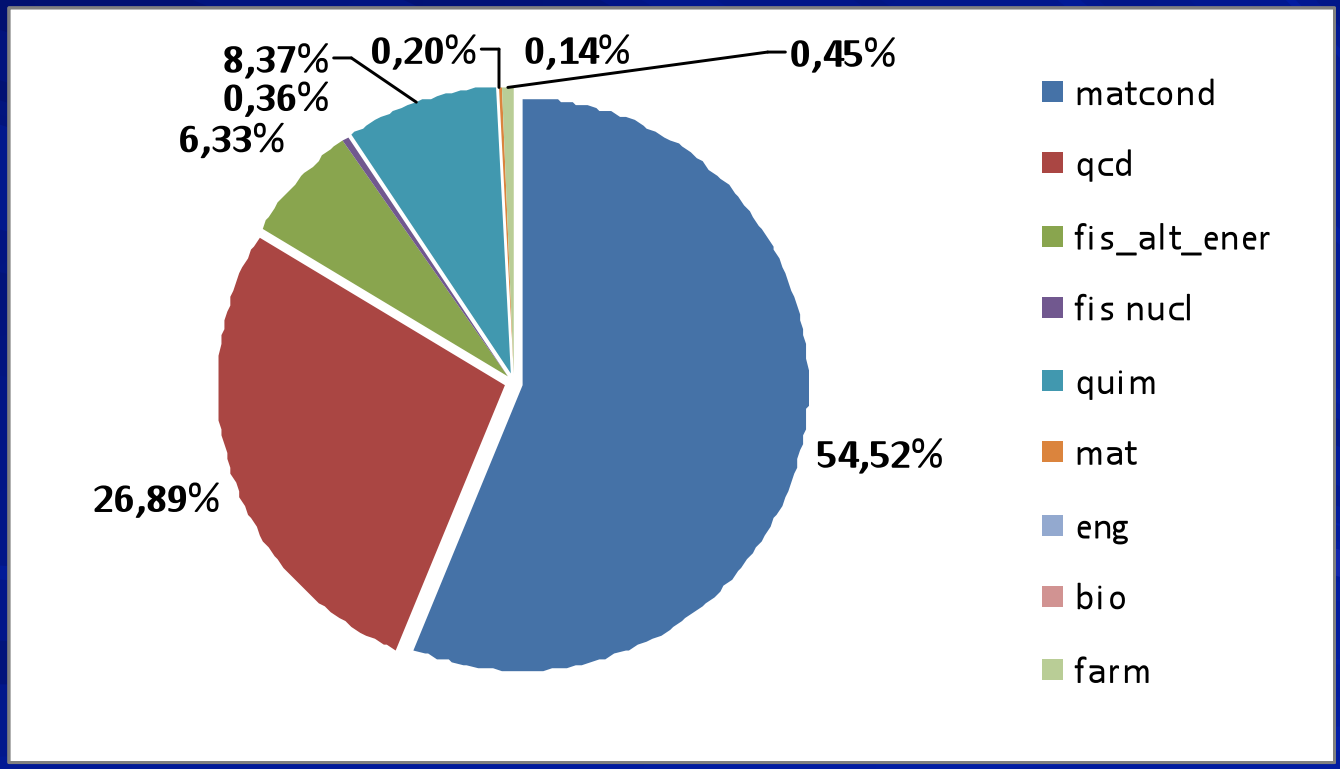
Milipeia Usage (last year)

Fraction of jobs/# cores



Milipeia Usage (last year)

Usage percentage per scientific domain



Thank you!