

CiGri - CIMENT GRID

A Grenoble GRID for Monte Carlo simulation

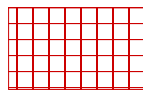
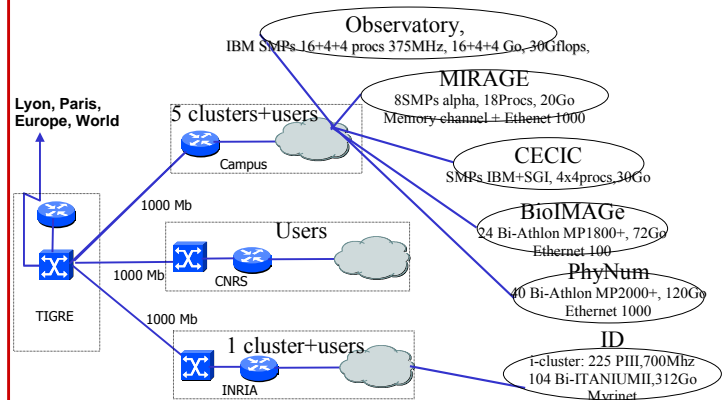
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IMAG, Grenoble Observatory and IPMMC

Contact: Laurent.Desbat@imag.fr, CiGri is hosted at IMAG-UJF
http://cigri.ujf-grenoble.fr, http://ciment.ujf-grenoble.fr, http://www-sop.inria.fr/aci/grid/public/acigrd.html

PRESENTATION

- Starting date: Dec 2002. Duration: 24 Months
- Objective: building a Grenoble GRID based on distributed local computing clusters from the CIMENT project (Intensive Computing, Modeling, Numerical and Technological Experiments)
- Development of a Middleware for the submission and the administration of Monte Carlo jobs on a Metropolitan GRID
- Validation on Monte Carlo computing from the Grenoble university scientific community
 - * Material Science: Crystal grow, SiC grow,...
 - * Astronomy: Planet dynamics, Interstellar environment (quantum chemistry),...
 - * Geophysical science: seismic, wave propagations,
 - * Biology et medicine: Genetics, medical imaging and modeling...
- Participation to larger GRID projects

CiGri is based on the CIMENT cluster network



Our GRID context:

- + Dedicated distributed computing clusters
- + Cluster idle time used for GRID

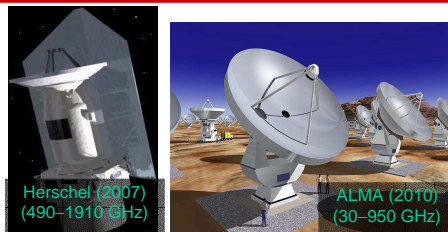
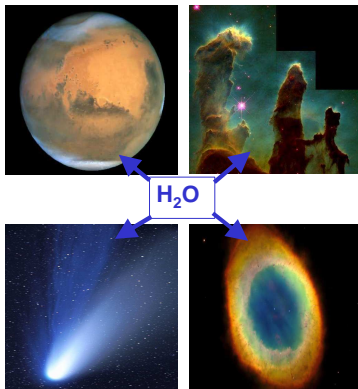
GRID mode on Phynum, I-cluster and Observatory: **15000 computing hours (equivalent 733MHz PIII) within 8 days**

A mean of 78 equivalent 733MHz PIII, computers allocated to the GRID computing

Cluster GRID use:

- I-cluster: from 0 to 80 %
- Phynum: from 0 to 20 %
- Observatory: day=18 computers, night=24 computers

FIRST RESULTS



Quantum chemistry application
Water is everywhere in the universe.
Preparation of observational analysis for the next generation of telescopes: study of H₂O collision excitation.
10⁶ geometries = 200 000 hours on a 1GHz PC (9D hyper surface sampling)

Noga J., Valiron P., « Explicitly Correlated Coupled Cluster R12 Calculations », *Computational Chemistry: Reviews of Current Trends Vol. 7, 2002*, 131,

Development of a light environment for Monte Carlo job submission based on scripts and job distribution programs: srun (sequential), prun (parallel), grun (grid)
Standard tools: NFS, ssh, PBS
Simple but relative efficient algorithms for some fault tolerance

Perspectives

- Specification of multi-parametric jobs,
- Scheduling of a huge job number
- Data base for jobs, computers and users management
- Modular software architecture

PARTNERS

Laboratories

Techniques de l'Imagerie de la Modélisation et de la Cognition (TIMC-IMAG, Medical imaging and Modeling)
Informatique et Distribution (ID-IMAG, Distributed Computer Science)
Laboratoire de Physique et Modélisation des Milieux Condensés (LPMMC, Numerical Physics)
Laboratoire d'AstrOphysique de Grenoble (LAOG, astrophysics)
Laboratoire de Modélisation et Calcul (LMC-IMAG - MIRAGE, environment and climate computing)
Centre d'Expérimentation du Calcul Intensif en Chimie (CECIC, Chemical Computing)

University and research organizations

CNRS, INPG, INRIA Rhône-Alpes, UJF
IMAG, Observatoire de Grenoble, IPMMC
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