CECAM, Lyon
(Centre Européen de Calcul Atomique et Moléculaire)

- Activities:
  - 20-25 workshops
  - 5-10 tutorials
- Research:
  - Posdocs/sabbaticals
- Coordination
  - ESF programs: SIMU (SimBioMa) – Psi-k
  - EU programs (Marie Curie)

Current support

- Belgium: FNRS and FWO
- France: CNRS, CEA, ENS-Lyon
- Germany: DFG
- Greece: FORTH
- Italy: CNR
- The Netherlands: NWO and UvA
- Spain: Min. of Science and Culture
- Suisse: FNS
- United Kingdom: EPSRC

CECAM's scientific mandate

Particle based computer simulations of (Bio) materials: *from electrons to polymers*

- *Electronic structure calculations:* (Psi-k)
  - ESF program supported by 20 European countries
  - Approximately 800 active groups (>2000 scientists)
- *Molecular Simulations*: (Simu)
  - ESF program supported by 16 European countries
  - Approximately 500 active groups (>1500 scientists)
- Characteristics
  - Europe is leading in this domain
    - Development of novel algorithms
    - Mayor computers codes are from European groups
  - Very heavy users of HPCN

Example of codes

- VASP (Hafner and Kress, Vienna)
  - Electronic structure calculations
  - 400 User groups
  - 300 publications each year

- FLAPW-code Wien 2000 (Vienna)
  - Electronic structure calculations
  - 800 User groups
  - 600 publications each year

- CPMD-code Juerg Hutter (Zuerich)
  - Car-Parrinello molecular dynamics
  - 200 User groups
  - 150 publications each year

"Scientific software is an essential integral part of the European Cyber infrastructure"

- Computational methods have become so advanced it is not possible anymore that every scientist writes is own code.

- Groups rely on the availability of very sophisticated software for their research;

- This software needs to be
  - maintained,
  - ported to new machines,
  - novel algorithms have to be implemented.

"Development of novel algorithms is an integral part of the European Cyber infrastructure"

- Is it desirable to *separate* research and infrastructure?
  - Only if there is a direct link between state of the art research and those that maintain the codes, Europe will maintain a competing position.

"The European Cyber Infrastructure should have instruments to secure academic software"

At present academic software *evaporates* as soon as the thesis has been written, only in accidental cases the software is rescued.

Make a EU rescue plan:

– Establish procedures to identify academic software that will become part of the cyber-infrastructure

– Provide long term (5+5 years) support for software development of these.

– Collaboration with HPCN centers

Support needed

- Maintain code:
  - Tests on all available compilers
  - Distribution of codes
  - Scientists want to stay in charge/on top of the development
- Grid:
  - Programs have very different efficiencies on different machines;
  - Research Councils agencies give support for the "local" machine;
  - Trading mechanisms: win-win situation the infrastructure is such that the Grid finds the "best" EU computer

Workshop on a european cyberinfrastructure

12-13 July 2005

Accademia dei Lincei (Roma)

Proposal for a European Cyberinfrastructure for Atomistic Simulations of Hard, Soft, and Biological Matter

http://abaddon.phys.uniroma1.it/index.php/Main/WorkshopLincei