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

There are facilities for Neutrons, X-rays, NMR that are maintained; *independent* from the research using it; is scientific software should be part of the European Cyber Infrastructure

- Solutions at the EU level are needed; software crosses boundaries and local solutions are inefficient
- Researchers should pay for the software; otherwise it is of no value; it gets supported now
- Research funding is not supporting consolidation; awareness is growing at the national level (UK, NCF)

A possible model

- Identify the key development team
 - Well within the science community
 - Support from the Cyber I:
 - Maintenance code
 - Implementation novel algorithms
- HPCN centers:
 - Distribute the codes over the grid
 - Support system (how to implement the code on the local machine)
 - Testing and porting codes
- At the European level

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