

The European Theoretical Spectroscopy Facility and the role of standards



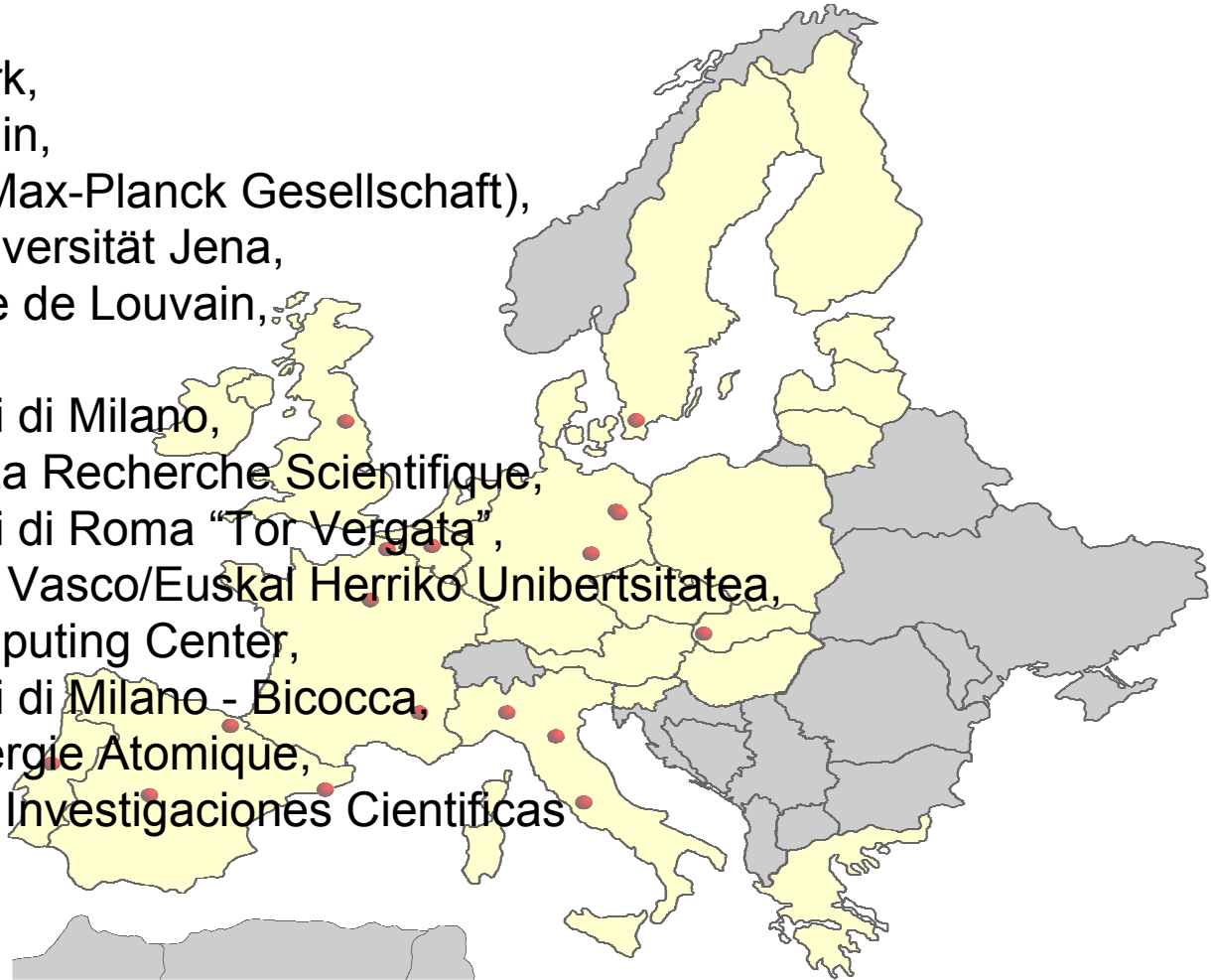
**4th e-Infrastructure Concertation Event
Sophia-Antipolis, 5th-6th December 2007**



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Consortium members

- The University of York,
- Freie Universität Berlin,
- Fritz-Haber Institut (Max-Planck Gesellschaft),
- Friedrich-Schiller-Universität Jena,
- Université Catholique de Louvain,
- Lunds Universitet,
- Università degli Studi di Milano,
- Centre National De La Recherche Scientifique,
- Università degli Studi di Roma "Tor Vergata",
- Universidad del País Vasco/Euskal Herriko Unibertsitatea,
- Barcelona Supercomputing Center,
- Università degli Studi di Milano - Bicocca,
- Commissariat à l'Energie Atomique,
- Consejo Superior de Investigaciones Científicas



Project objectives

- **Networking:** develop the operation of the ETSF for a broad community of researchers working in the field of spectroscopy through the maintenance of theory and code “beam-lines” and dedicated communications.
- **Service Provision:** facilitate wide access to ETSF theoretical and numerical tools by carrying out User projects in close collaboration with supercomputer centres and delivering services such as training and e-documentation.
- **Joint Research:** create, collect and connect knowledge to keep ETSF services at the forefront of knowledge with new theory and code developments for the description of complex systems and phenomena, to set up a knowledge data base and to enhance software portability.



Work plan outline

- WP1 "Consortium Management".
- WP2 "Foresight for Improvement": strategic development planning for software and associated improvements.
- WP3 "Improving Communications, Dissemination, and Widening Understanding".
- WP4 "Implementing ETSF User Projects".
- WP5 "Promoting Code Availability".
- WP6 "Delivering External Training".
- WP7 "Development of Theory, Software and User Support".
- WP8 "Software Portability and interoperability".
- WP9 "ETSF e-Libraries".



Standards related work

- Flexible and portable file format for data exchange
 - electronic structure and crystallographic data
 - software-specific extensions
- ETSF I/O library (licence: LGPL)
 - implementation of the file format
 - stable and currently being deployed
 - fully documented (web standards), with tutorials
- Pseudopotential data exchange
 - interconversion utility
 - participation to the design of a XML format (in progress)
- Designing programming standards

