

Chemical and Material Science and Technology SSC

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CESNET

ACC Cyfronet AGH

SSC Workshop,

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- **Supporting the members of the CMST community in implementing and using an environment of shared hardware and software resources on the grid**
- **Adopting models and standards for molecular and material knowledge allowing a reuse of quantum chemistry data and codes for an easy connection of different packages**
- **Implementing on the grid libraries of codes relevant to CMST as web services for use by the community**
- **Designing and developing tools for evaluating quality of services (QoS) and quality of users (QoU) in CMST web services**
- **Build a credit system as part for constructing a grid economy able to reward people contributing to the SSC sustainability.**

- **A collection of CMST programs geographically distributed on heterogeneous platforms to be used either on an individual or on a shared basis**
- **A central (web based) interface for accessing and composing some computer programs and applications as web services**
- **A workflow manager finalized to the handling of a grid empowered simulation**
- **A prototype QoS and QoU evaluator of the services and the users of the CMST SSC**
- **A repository for QC data complying with the model and standards of QC5**
- **An agreement with the owners of some widely CMST programs for supporting shared usage and/or common formats**

- **Local Coordinator** (from each research institute, research group or project). Local coordinators form Management Board (MB)
- **SSC Chair** nominated by MB
- **Planning Board** - appointed by the MB to develop strategic initiatives and make recommendations to the MB about future developments.
- **Front Desk** - is the technical unit responsible for several activities concerning consulting, integration of MMST community resources with the grid infrastructure or assistance for application porting including integration of grid services necessarily to utilize the application in grid environment.
- **User Support**
 - Direct User Support
 - Technical Support
 - Documentation
 - Grid Program exchange database
- **In general we'll follow one of the proposed SSC governance models**

- **Effort estimation - approx 14 FTEs:**
 - The SSC Chair and its deputy(s): 1.5-2 FTE
 - Front Desk - 2-3 persons responsible for several activities including SSC contact points, consulting, integration of resources, etc. 2-2.5 FTE
 - User's Support teams
 - Direct User Support - first line support for users including dissemination and trainings - 2-3 FTE
 - 0.5 FTE for coordination of Documentation specific to MMST community
 - Technical Support - responsible for all the services specific to MMST community 2-3 FTE
 - Grid Program Exchange - a technical unit responsible for domain's software database creation 2.5-3 FTE

Part. no.	Participant organization name	Part. short name	Country
1	University of Perugia, Dept of Chemistry	UNIPGCHIM	Italy
2	Cyfronet	CYFRONET	Poland
3	National Center for Biomolecular Research	NCBR	Czech Rep.
4	IT Center for Science ltd	CS C	Finland
5	Ente nazionale energie alterantive	ENEA	Italy
6	Consorzio Interuniversitario CINECA	CINECA	Italy
7	Theoretical chemistry and computational grid applications	UZH	Switzerland
8	Foundation for Research and Technology Hellas, Inst. Electronic structure and lasers	FORTH	Greece
9	Democritos, ICTP, Trieste	DEMOCRIT	Italy
10	University of Barcelona	UBQP	Spain

- **Support from 60+ institutes and research groups and several NGI's (see accompanying document for details)**

- **WP1: Implementation and support for utilities and soft.**
- **WP2: DFT - development of models**
- **WP3: Validation of codes as web services**
- **WP4: Design Quality evaluation criteria and tools for Services and users**
- **WP5: Credit system establishment**
- **WP6: Implementation of CMST repository data**
- **WP7: Design & implementation of tools and workflows**
- **WP8: Establishment of links with European software owners**
- **WP9: Dissemination**
- **WP10: Project management**

- **Join forces with MSSSC**
- **Get support from more NGI's**