Dear NGI Representative

In this short letter we would like to present basic ideas behind Chemical and Material Science and Technology Specialised Support Centre (CMST SSC)– an initiative aiming to support chemical and material science community on the grid. The idea of CMST SSC has their beginning in Computational Chemistry Cluster of Excellence in EGEE on the basis of solid group of research laboratories lead mainly by ACC Cyfronet AGH and University of Perugia. Over the years of EGEE projects all the partners of the Cluster greatly contributed to the development of computational chemistry on EGEE Grid. As one of the results vast number of commercial and freely available software packages can be accessed via Compchem, Gaussian Turbomole and VOCE VOs on EGEE Grid. This has greatly attracted our community to the Grid making it third EGEE power consumer.

The central motivation for instituting CMST SSC among continuous user's support for the community members, building and maintaining basis services and high level middleware tools and targeted web portals/dashboards is that of stimulating discovery and transforming the way simulations are performed, data handled and codes interfaced through collaborative endeavours on the Grid. For this purposes the various activities will be aimed at:

- supporting the members of CMST community in implementing and using an environment for 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 libraries of codes/software packages relevant to CMST as a 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;

These activities will result in collection of software packages geographically distributed, a workflow manager, a central (web-based) interface for accessing and composing some computer programs and applications as web services and prototype of QoS and QoU together with a system of credit award among others.

In the era of National Grid Initiatives it is of concern of CMST SSC to assure certain level of resources for our community. Therefore we rely on each NGI support for CMST VOs. In exchange we offer our knowledge and expertise for NGI's and their users. In the tables below you will find both the partners forming CMST SSC as well as research laboratories that expressed their support for the idea of CMST SSC. If there are no SSC supporters from your country please contact your local chemical and material science community and pass on this message.

Should you have any further questions concerning CMST SSC please do not hesitate to contact us.

On behalf of CMST SSC,

Mariusz Sterzel (m.sterzel@cyfronet.pl)
Antonio Laganà (lag@dyn.unipg.it)

Participants:

University of Perugia, Dept of Chemistry	Italy
ACC Cyfronet AGH	Poland
National Center for Biomolecular Research	Czech Republic
IT Center for Science ltd	Finland
Ente nazionale energie alterantive	Italy
Consorzio Interuniversitario CINECA	Italy
Theoretical chemistry and computational grid applications	Switzerland
Foundation for Research and Technology Hellas, Inst. Electronic structure and lasers	Greece
Democritos, ICTP, Trieste	Italy
University of Barcelona	Spain

Supporting laboratories:

Austria	University of Vienna	Hans Lischka
Austria	University of Vienna	Wilfried Gansterer
Austria	University of Innsbruck	Maximilian Berger
Austria	University of Vienna	Matthias Ruckenbauer
Belgium	University of Ghent	Michel Waroquier
Croatia	Rudjer Bošković Institute, Zagreb	Zvonimir Maksić
Croatia	Department of Physics, University of Zagreb	Goranka Bilalbegovic
Czech Republic	Czech Academy of Sciences, Prague	Jiri Pittner
Czech Republic	National Centre for Biomolecular Research	Jan Kmunicek, Jaroslav Koca
Czech Republic	Loschmidt Laboratories	Jan Kmunicek, Jiri Damborsky
France	ENSCP Chimie ParisTech 11, Paris	Carlo Adamo
France	Dept. of Phys., Univ. Rennes, Rennes	Jean M. Launay
France	University of Toulouse	Stefano Evangelisti
France	University of Lille	Valerie Vallet
France	University Pierre et Marie Curie, Paris	Rodolphe Vuilleumier
Germany	Research Center Jülich	Thomas Müller
Germany	Humboldt University Berlin	Vlasta Bonačić-Koutecký
Germany	University of Heidelberg	Hans Dieter Meyer
Germany	University of Heidelberg	Horst Köppel
Germany	Zuse-Institut, Berlin	Thomas Steinke
Germany	FAU Erlangen-Nürnberg	Tim Clark
Greece	University of Thessaloniki	Evangelia Varella
Hungary	Eötvös Loránd University, Budapest	Péter G. Szalay
Hungary	Chem. Res. Center, Hungarian Academy of Sciente, Budapest	Gyorgy Lendvay
Hungary	University of Budapest	Mihaly Kállay
Hungary	University of Pannonia, Vezprem	Lajos Fodor
Italy	University of Pisa	Maurizio Persico
Italy	IMIP, Bari	Domenico Bruno

Italy	University of Bologna	Gian Luigi Bendazzoli
Italy	University of Ferrara	Renzo Cimiraglia
Italy	SISSA, Trieste	Paulo Carloni
Italy	Department of Chemistry, University of Bari	Fabrizio Esposito
Italy	Department of Physics, University of Perugia	Massimiliano Alvioli
Italy	INFN, Perugia	Leonello Servoli
Italy	University of Naples	Michele Pavone
Italy	University of Padoa	Laura Orian, Gianpietro Sella
Italy	University of Milan, Bicocca	Ugo Cosentino
Italy	University of Pisa	Alberto Coduti, Alessandro Ferretti
Italy	University of Naples	Mauro Causà, Luisa Caracciolo
Italy	University of Padoa	Andrea Vittadini
Italy	University of Pisa	Susanna Monti
Italy	University of Modena	Cristina Menziani
Netherlands	University of Amsterdam	Evert-Jan Meijer
Norvegia	University of Tromsø	Kenneth Ruud
Spain	Dept. Phys. Chem, Univ. Basq. Country, Vittoria	Ernesto Garcia
Spain	Centro de Supercomputaciòn de Galicia, Santiago de Compostela	Aurelio Rodriguez
Spain	University of Valencia	Josè Sanchez-Marin
Spain	Universidad de Sevilla	Antonio M. Márquez Cruz
Spain	Universidad de Sevilla	Javier Fernández Sanz
Spain	Universidad de Barcelona	Margarita Alberti
Spain	CSIC	Octavio Roncero
Sweden	Dept. of Chem., Univ. Goteborg, Goteborg	Gunnar Nyman
Switzerland	ETH Zürich	Hans Peter Lüthi
Switzerland	University of Berne	Samuel Leutwyler
Switzerland	Swiss National Supercomputing Centre, Manno	Mario Valle
Switzerland	ETH Zürich	Martin Brändle
Switzerland	University of Zurich	Juerg Hutter
Switzerland	Swiss Center for Scientific Computing	Peter Kunszt
Switzerland	ETH Zurich	Michele Parrinello
Switzerland	SIB; Ludwig Inst. for Cancer Research	Olivier Michielin
UK	University of Cambridge	Peter Murray Rust
UK	Imperial College London	Henry Rzepa
UK	University of Cambridge	Michiel Sprik