The following section contains subtasks established to accomplish proposal objectives concerning computational chemistry development for third part of EGEE project.

Subtask ID	CC1	**Start Month**	1	**End Month**	24
Subtask Name	Cluster Management				

CYFRONET	**M.Sterzel**	3	3				

Goals

This subtask has in charge the management of the whole CC cluster. It supervises activities of all other subtasks and must assure continuous contacts and flow of information within the cluster.
The goals pursued through this subtask can be summarized as follows:

- Manage interactions with the EGEE/NA4 and with the EGEE Project Office.
- Monitor and coordinate activities of all other subtasks and the progress of each of them.
- Set up tools and services to foster the collaborative work within the cluster.
- Organize cluster meetings, both face-to-face and remote (through collaboration tools). This will be done in tight contact with EGEE/NA4.
- Produce reports and other documentation requested by EGEE/NA4 SC and by the Project Office.

Benefits

A good management of the cluster is mandatory to guarantee that all activities are carried out in a coherent manner. This is achieved by constant monitoring of each subtask to maintain the focus on the main objectives of the cluster. The cluster manager plays also the role of unique referent for EGEE/NA4 SC and for the Project Office and this is another advantage.

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC1-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	Number of people who join and contribute to the cluster
M-CC1-2	Status of the cluster at month 3	Number and type of collaboration tools set up within the cluster
M-CC1-3	Status of the cluster at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	
M-CC1-4	Check status of the cluster at month 12 (EGEE User Forum IV, Spring 2009)	Number and type of collaboration tools set up within the cluster
M-CC1-5	Check status of the cluster at month 18 (EGEE 09 Conference, Autumn 2009)	

M-CC1-6	Closing meeting (April 2010)	Number and type of collaboration tools set up within the cluster

Subtask ID		CC2	**Start Month**	1	**End Month**	24	
Subtask Name		Management of VOs supporting computational chemistry users					
UNIPG	**O. Gervasi**	2	4				
	A. Constantini	1					
Cyfronet	M. Sterzel	1					

Goals: In pursuing the main objectives of the cluster (porting of applications to the Grid and development of tools and services for the benefit of the chemical community as well as of other disciplines) it is very important for developers to rely on a pool of guaranteed Grid resources. These resources are made available through one or more VOs (Virtual Organizations) created on top of the EGEE Grid infrastructure. Right now several VOs were set up for users from chemistry domain. Some VOs are of general type like CompChem, some like GAUSSIAN are related to specific chemical packages supported by EGEE. It is very important to mantain tight coordination of all these VOs to optimize the number and kind of shared resources.

Benefits: The most important benefits coming from a good management of chemistry-related VOs are:

a) Constant monitoring of the creation of new chemistry-related VOs (purpose and the corresponding community of users);

b) Maximization of the number and type of resources available in each specific VO making in this way the CC cluster attractive not only for increasing number of chemists but also for users from other science disciplines who utilise chemical packages for their research.

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC2-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	None.
M-CC2-2	Status of the management at month 3	Number of active chemistry related EGEE VOs. For each of them: a) number of shared resources; b) number of available resources; c) number of registered users; d) list of software packages used
M-CC2-3	Status of the management at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	Number of active chemistry related EGEE VOs. For each of them: a) number of shared resources; b) number of available resources; c) number of registered users; d) list of software packages used
M-CC2-4	Check status of the management at month	Number of active chemistry related EGEE VOs. For each of them: a)

	12 (EGEE User Forum IV, Spring 2009)	number of shared resources; b) number of available resources; c) number of registered users; d) list of software packages used
M-CC2-5	Check status of the management at month 18 (EGEE 09 Conference, Autumn 2009)	Number of active chemistry related EGEE VOs. For each of them: a) number of shared resources; b) number of available resources; c) number of registered users; d) list of software packages used
M-CC2-6	Closing meeting (April 2010)	Number of active chemistry related EGEE VOs. For each of them: a) number of shared resources; b) number of available resources; c) number of registered users; d) list of software packages used

Subtask ID		CC3	**Start Month**	1	**End Month**	12	
Subtask Name		Extension of Charon GUI on top of gLite middleware					
CESNET	**J. Kmunicek**	5	5				
Goals: The main goal of this task is to extend existing functionality of Charon GUI by predefined set of options required for seamless research work in grid environment in a graphical, highly useable and reliable way.							
Benefits: Highly customizable GUI's with possibility of skin or language change are especially useful for users accustomed to integrated environments. Such users have very limited knowledge about command line tools therefore availability of Charon GUI on the Grid, with tools making the job management easier, greatly smoothes user's adoption on Grid platform.							
Milestones and Metrics to gauge Progress							
M-ID	**Milestone Description**			**Metrics**			
M-CC3-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008			List of planned features			
M-CC3-2	Status of the development at month 3						
M-CC3-3	Status of the development at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)						
M-CC3-4	Month 12 (EGEE User Forum IV, Spring 2009) – end of the task			a) List of VO for which CEL GUI was installed; b) Number of users			

		utilizing package; c) List of features developed
M-CC3-5	EGEE 09 Conference, Autumn 2009)	
M-CC3-6	Closing meeting (April 2010)	

Subtask ID		CC4	**Start Month**	1	**End Month**		12
Subtask Name		Extension of Wien2K workflow					
UIBK	**M. Berger**	5	5				

Goals: This task will mainly focus on reduction of overhead accompanying Wien2K workflow execution on EGEE Grid. Execution test revealed low applicability of workflow execution for short time jobs.

Benefits: Reduction of overhead accompanying execution of short time jobs is important for all Grid activities. The knowledge concerning parameters lowering overhead will not only make execution of short jobs worthwhile, but it will also significantly increase the Grid effectiveness.

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC4-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	
M-CC4-2	Status of the development at month 3	
M-CC4-3	Status of the development at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	
M-CC4-4	Month 12 (EGEE User Forum IV, Spring 2009) – end of the task. Provision of ready to use package;	List of parameters which have influenced workflow overhead;
M-CC4-5	Check status of the cluster at month 18 (EGEE 09 Conference, Autumn 2009)	
M-CC4-6	Closing meeting (April 2010)	

Subtask ID	CC5	**Start Month**	1	**End Month**	12
Subtask Name	Development of ECCE port on gLite infrastructure				

KTH	**O. Vahtras**	5	5				

Goals: The main aim of this task is to bring *Extensible Computational Chemistry Environment* (ECCE) graphical interface to EGEE infrastructure. Apart excellent tool for building/visualizing chemical structures the planned functionality will involve:

- Job submission
- Job retrieval
- Job monitoring
- Dataserver on Fireman catalogue

Benefits: ECCE belongs to problem solving environments that support entire assortment of scientific computational problem-solving activities ranging from problem formulation via simulation execution to solution visualization. The package is operational from 1997 and used by chemists on workstations as an environment for conducting research. The gLite port of ECCE will not only bring existing users to the Grid platform but also attract new ones looking for similar solutions.

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC5-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	List of features planned
M-CC5-2	Status of the development at month 3	
M-CC5-3	Status of the development at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	
M-CC5-4	Month 12 (EGEE User Forum IV, Spring 2009) – end the task and provision of: ready to use package;	a) List of features implemented; b) List of the sites where the package was installed
M-CC5-5	Month 18 (EGEE 09 Conference, Autumn 2009)	
M-CC5-6	Closing meeting (April 2010)	

Subtask ID	CC6	**Start Month**	1	**End Month**	12
Subtask Name	Development of grid license models – preparation of documentation concerning software porting.				

Cyfronet	**M.Sterzel**	2	6				
KTH	O. Vahtras	1					
CESNET	J. Kmunicek	1					
UIBK	M. Berger	1					

UNIPG	A. Lagana	1					

Goals: The main aim of this task is to provide complete, ready for use, set of procedures which if applied during porting of licensed (commercial or not) software on the Grid will resolve issues concerning software license(s)

Benefits: Availability of such procedures should speed up entire process of porting of licensed software to the Grid, which becomes more and more popular. Previous experience suggests that approx. 80% time spent on porting procedure is related to solutions concerning license requirements. Ready to use procedures will also avoid duplication of work during software porting

Milestones and Metrics to gauge Progress

M-ID	Milestone Description	Metrics
M-CC6-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	Definition of list of typical license models required by software used by Grid users
M-CC6-2	Status of the procedures at month 3	None
M-CC6-3	Status of the procedures at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	List of procedures for freely available software
M-CC6-4	Publication of the procedures on NA4 web pages. Month 12 (EGEE User Forum IV, Spring 2009)	Procedures for commercial packages (for which grid port already exists)
M-CC6-5	Month 18 (EGEE 09 Conference, Autumn 2009)	
M-CC1-6	Closing meeting (April 2010)	

Subtask ID	CC7	**Start Month**	1	**End Month**	24
Subtask Name	Development web portal for chemists				

Cyfronet	**M.Sterzel**	9	30				
	T. Szepieniec	13					
	D. Harezlak	8					

Goals: The main aim of the task is to provide convenient user-data-centric environment for chemical computation using Grids and build portal-like framework for quick application adaptation on grids that results with application- and data-oriented 'extensions' for specific application. The tools integrated with the portal will not only allow easy job preparation, submission and management but also automation of common tasks performed to accomplish computational investigations and visualization of results.

Benefits: The most important advantage of offering easy extendable portal with set of tools for chemist is automation of common tasks performed by community members

during research conduction. The portal will not only help existing user speed up their work but also attract new ones for whom command line interface is to difficult to use, who are accustomed to the GUIs which come with many chemical software packages.

Milestones and Metrics to gauge Progress		
M-ID	**Milestone Description**	**Metrics**
M-CC7-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	Definition of portal futures and software packages it will support
M-CC7-2	Status of the development at month 3	None
M-CC7-3	Status of the development at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	None
M-CC7-4	Check status of the development at month 12 (EGEE User Forum IV, Spring 2009) – presentation of prototype with plug-in to Gaussian package, poster	
M-CC7-5	Check status of the cluster at month 18 (EGEE 09 Conference, Autumn 2009)	
M-CC7-6	Closing meeting (April 2010) – production version with plug-ins to two more chemical packages in addition to Gaussian. Demonstration an EGEE User Forum V	List of software packages supported, list of features implemented.

Subtask ID		CC8	**Start Month**	1	**End Month**		24
Subtask Name		Development of grid port of parallel version of chemical software packages					
UNIPG	**A. Lagana**	1	8				
	C. Manuali	2					
	O. Gervasi	1					
	A. Constantini	2					
Cyfronet	M. Sterzel	2					
Goals: The key point of this task is to provide parallel version of the most frequently used chemical software packages for the users.							

Benefits: Parallel version of chemical software packages is highly expected due to nature of chemical jobs, which are long-running with high demands for memory. Availability of parallel version of most frequently used chemical packages will not only speed up computations but also make some computations possible (those which will not fit in due to hardware limitations)		
Milestones and Metrics to gauge Progress		
M-ID	**Milestone Description**	**Metrics**
M-CC8-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	Preparation of list of the already ported package for which parallel version is needed
M-CC8-2	Status of the porting at month 3	
M-CC8-3	Status of the porting at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	
M-CC8-4	Check status of the cluster at month 12 (EGEE User Forum IV, Spring 2009)	List of parallel version of chemical packages ported to the Grid
M-CC8-5	Check status of the cluster at month 18 (EGEE 09 Conference, Autumn 2009)	
M-CC8-6	Closing meeting (April 2010)- preparation of the documentation concerning software porting and its publication on NA4 web pages.	List of parallel version of chemical packages ported to the Grid

Subtask ID	CC9	**Start Month**	13	**End Month**	24		
Subtask Name	Expansion of the segment of EGEE Grid available for users from chemistry domain						
UNIPG	**A. Lagana**	3	4				
Cyfronet	M. Sterzel	1					
Goals: The key point of this task is to provide enough computational resources for users from chemistry domain. This is necessarily to keep constant ratio between increasing number of community members and available computational resources.							
Benefits: Certain level of computational resources will increase overall user satisfaction, as the total time required to perform computational tasks will be reduced, especially along with utilization of parallel version of chemical packages. Moreover the increase of computational resources will make Grid platform more attractive for new users directly leading to community increase.							
Milestones and Metrics to gauge Progress							
M-ID	**Milestone Description**			**Metrics**			
M-CC9-1	Kick-off at month 1. All Hands			None			

	meeting; Orsay (Paris), 9-10 June 2008	
M-CC9-2	Status of the cluster at month 3	None
M-CC9-3	Status of the cluster at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	None
M-CC9-4	Check status of the task at month 12 (EGEE User Forum IV, Spring 2009) – start of the negotiations concerning resource allocation for chemical users	
M-CC9-5	Check status of the task at month 18 (EGEE 09 Conference, Autumn 2009)	List of sites/processors for certain VOs
M-CC9-6	Closing meeting (April 2010)	List of sites/processors for certain VOs

Subtask ID		CC10	**Start Month**	1	**End Month**		24
Subtask Name		Execution efficiency testing					
UNIPG	**A. Constantini**	2	6				
	C. Manuali	1					
	O. Gervasi	1					
Cyfronet	M. Sterzel	2					

Goals

All applications ported in Grid shall be tested to verify the success of the gridification process and application developers usually carry out this task. Therefore the activity of this task will mainly focus on execution efficiency of chemical software on certain sites. Studies concerning this topic has been partially done during EGEE-II project and revealed that execution efficiency highly depends on given site configuration, especially during parallel execution. Therefore this subtask will carry our its activity in close connection with CC8 (Grid port of parallel version of chemical software on the Grid.

Benefits

The accurate testing activity performed by this subtask will verify that chemical applications and newly developed tools and services ensure their robustness and reliability on the Grid

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC6-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	
M-CC6-2	Status of the task at Month 3	
M-CC6-3	Status of the task at month 6 (EGEE 08	

	Conference, Istanbul, 22-26 September 2008)	
M-CC6-4	Check status of the task at month 12 (EGEE User Forum IV, Spring 2009) Start of the task at Month 13.	
M-CC6-5	Check status of the task at month 18 (EGEE 09 Conference, Autumn 2009)	Number of applications tested, number of sites used during software tests
M-CC6-6	Closing meeting (April 2010)	Number of application tuned and number of sites where tuned software packages were installed

Subtask ID		CC11	**Start Month**	1	**End Month**		24
Subtask Name		First line support for users, training and dissemination					
UNIPG	**A. Constantini**	1	2				
Cyfronet	M. Sterzel	1					

Goals: Users accustomed to clusters or SMP machines experience many issues related to their traditional way of thinking when switching to the Grid. Therefore training and dissemination plays an important role in helping users adopt on new infrastructure and abandon their habits. It is also necessarily to quickly react in case of user problems in order not to discourage users to new computational platform.

Benefits: Once trained, users are able to exploit the advantages of the Grid technology in an efficient way. Users well trained and satisfied of the suite of tools, services and of the amount of resources available in EGEE will attract new ones and extending this way the chemical community utilizing grid rsources.

Milestones and Metrics to gauge Progress

M-ID	**Milestone Description**	**Metrics**
M-CC6-1	Kick-off at month 1. All Hands meeting; Orsay (Paris), 9-10 June 2008	
M-CC6-2	Status of the task at Month 3	List of users whom the team has helped, list of talks, seminars or trainings given
M-CC6-3	Status of the task at month 6 (EGEE 08 Conference, Istanbul, 22-26 September 2008)	List of users whom the team has helped, list of talks, seminars or trainings given
M-CC6-4	Check status of the task at month 12 (EGEE User Forum IV, Spring 2009) Start of the task at Month 13.	List of users whom the team has helped, list of talks, seminars or trainings given
M-CC6-5	Check status of the task at month 18 (EGEE 09 Conference, Autumn 2009)	List of users whom the team has helped, list of talks, seminars or trainings given
M-CC6-6	Closing meeting (April 2010)	List of users whom the team has

		helped, list of talks, seminars or trainings given

Future perspectives concerning computational chemistry after EGEE-III

Computational chemistry as well as other science disciplines on EGEE Grid has put a lot of effort to build stable and reliable computational infrastructure. Therefore to preserve the EGEE achievements the EGI and consequently NGI's should adopt this infrastructure as a base for further development. Therefore we expect tools and services developed for EGEE as well as VOs set up to support chemist on the grid to be preserved by EGI/NGI's. This will assure that all chemical software packages ported already to the Grid will run without any change after transition from EGEE-III to EGI.

In addition computational chemistry as well as other disciplines using chemical software look forward for seamless support for calculations requiring long time computational jobs (i.e. running for weeks or even months), intensive support for parallel execution chemical jobs (thorough MPI or any other implementation) or bulk submission of computational jobs to prevent applications developers to have to wrap standard commands in sets of custom scripts to deal correctly with jobs preparation, submission, processing and possible resubmission. Moreover, to make the researchers life easier it would be great to have a unique, official way how to deal with the licensing of software packages (commercial or not) to be used within Grid environment. This is of particular importance as almost all software packages used by chemical community are affected by license restrictions.