# IS-ENES – WP3

# D3.8 - Report on Training Sessions


**Abstract:**

The deliverable D3.8 describes the organization and the outcomes of the tutorial meetings on the Grid Prototype designed within task4 of the NA2 work package. The training events aimed mainly at increasing the interest and knowledge related to grid technologies; familiarizing users with the Grid Environment and its features through an active hands-on approach; introducing a user-friendly tool for executing and monitoring ensemble experiments through the v.E.R.C. portal. Seven tutorials have been organized among the main climate centers in Europe. In particular, the tutorials have been organized at: CMCC, BSC, IPSL, DKRZ and INGV. The Grid infrastructure used for the tutorial exploited three computing nodes made available by CMCC, DKRZ and BSC. The tutorials were targeted mainly to users with a medium skill level on climate modeling and basic knowledge on grid computing and shell programming. Several fruitful feedbacks have been acquired from the audience for improving the Grid Prototype.


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# Table of Contents

# Index of Tables

# Introduction

Users as well as developers of Earth System Models rely on an infrastructure, consisting of high-end computing, data storage and network resources to perform complex and demanding simulations. In the past, mainly local resources and infrastructures were used. However, the increasing requirements on computing capability and capacity as well as on data storage facilities often exceed the possibilities of single centers. An ensemble simulation consists of many individual runs, which require intensive computational power and produce huge amount of data to be post-processed and archived in a production environment. In Europe, there is the need to deploy and develop technologies in order to provide climate scientists with virtual proximity to distributed computing resources and data.

The IS-ENES (InfraStructure for the European Network for the Earth System Modelling) is an FP7-Project (March 2009-February 2013) funded by the European Commission under the Capacities Programme, Integrating Activities. It has developed the ENES v.E.R.C. ("virtual Earth-System modelling Resource Centre"), an information and collaboration portal to present all the services, tools and data available to the community in a coherent way to foster the exchange of information and the collaboration within the community.

The NA2 task of this project aims at the set up and deploy an e-infrastructure providing climate scientists with the needed virtual proximity to distributed data and distributed compute resources. So, CMCC have planned and developed a grid prototype used for prototyping and testing a distributed environment for running ensemble experiments. A detailed description of the prototype can be found in deliverable D3.4 "Report on design and deployment of Grid portal and development environment".

## Glossary of Acronyms

| Acronym | Definition |
|---|---|
| GRB | Grid Resource Broker [1] |
| CompSs | Comp Super scalar [4][5] |
| CMCC | Euro Mediterranean Center on Climate Change |
| DKRZ | Deutsches Klimarechenzentrum |
| BSC | Barcelona Supercomputing Center |
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*Table 1: Glossary of Acronyms*

# Tutorials Organization

## Aims

Within the Task4 of the NA2 work package a prototypal grid infrastructure for climate application has been designed and deployed among the resource centers involved in the project. Namely, DKRZ, BSC and CMCC have provided the user with the access to part of their computing resources. The Grid Prototype is detailed in deliverable D3.4. A web interface can be used to access the grid infrastructure and it concerns two types of applications: running ensembles of multi-model experiments and monitor the execution of the whole experiment with both an overview snapshot over all of the members and detailed information on each single member. The task established also a first interaction with and configuration of Grid environments straightforward and thus to improve the uptake of Grid technology on a larger scale.

The prototype ESM Grid Environment exploited already available grid services, namely: GRB services, CompSuperscalar and Globus middleware. An integrated workbench framework to access the power of existing Grid infrastructures has been provided. The web-based aims at providing tools to customize Grid users' applications, to manage Grid resources and to support the development cycle of new Grid applications. With the help of this workbench not only Grid application users but also resource providers and application developers will be supported in their interactions with the Grid environment. The training events aims mainly at increasing the interest and knowledge related to grid technologies; familiarizing users with the Grid Environment and its features through an active hands-on approach; introducing a user-friendly tool for executing and monitoring ensemble experiments through the v.E.R.C. portal.

The tutorials are targeted mainly to users with a medium skill level on climate modeling. Even if no other prerequisite are required to attend the tutorial, a basic knowledge on grid computing and shell programming can be useful.

## Structure

### Tutorial on Prototype of Grid Environment for Earth System Models

The grid environment prototype allows exploiting already available grid services, namely GRB services and Globus middleware. A web services based system allows the brokering and scheduling of jobs in a distributed environment, supporting different grid middleware (such as Globus or directly through SSH/SCP). The grid infrastructure used for tutorials is made of three computing sites at DKRZ in Germany, CMCC in Italy and BSC in Spain. The configuration for each sites is as follow: DKRZ provides a node with 32 cores Power6 with LoadLeveler local scheduler; CMCC provides a node with 32 cores of Power6 processors with LSF local scheduler; BSC provides 8 nodes with a total of 32 cores of PPC processors with SLURM as local scheduler.

A grid portal has been planned and implemented by the CMCC and it represents the access point to the infrastructure. It allows the job submission and monitoring of ensemble climate experiments. Moreover, information of the job status has been enriched with details on the experiment, knowing, at run time, the progress of each ensemble member, involved resources, etc.

The prototype has been tested on a case study related to a global coupled ocean-atmosphere general circulation model (AOGCM) named HRT159 developed at CMCC. The model test case is composed by ECHAM5 at T159 resolution, NEMO at 2° coupled with OASIS3. Anyway for the tutorial we used a toy model.

The grid portal is one of the services provided by v.E.R.C.: https://verc.enes.org/computing/job-submission-and-monitoring-portal.

During the tutorial the grid portal and the related technologies will be described presenting also a user-friendly tool for executing and monitoring climate change ensemble experiments.

Considering existing grid infrastructures and services, the tutorial will show how this tools has the potentiality to efficiently exploit part of the European HPC ecosystem for real computational science experiments.

The tutorial cover the following topics:

- An introduction to the Grid technology
- Which requirements must the grid infrastructure meet for the climate applications
- The GRB services and software architecture
  - Grid Prototype Infrastructure: design overview
  - Grid Portal
    - Experiment submission
    - Runtime monitoring
- A case study: the ensemble experiment
  - Description of the experiment
  - Configuration of the experiment
  - Running of the experiment
- Description of the IS-ENES testbed and its Grid sites
- Hands-on section

## Tutorial on CompSs

The tutorial on the COMPSs framework has been directed to software developers interested in the optimization of the execution of their applications in grid environments. In the tutorial example applications have been made available to the attendants and a specific session has been dedicated to the analysis of specific use cases as needed by the participants.
As basis for the tutorial two samples applications have been used; a first example application for multimodel ensemble mean of surface temperature has been ported to COMPSs. Another example application implements a workflow that orchestrates the execution of HRT159 models in grid environments. This example has been used also to demonstrate the integration with the GRB scheduler; the Grid Portal invokes directly the parallel application written with COMPSs for the ensemble experiment. The log file produced by the tasks are then moved to the Grid Portal for monitoring.
Detailed operational steps have been defined as follow:

- Adaptation of the current portal submission interface to enable the execution of a batch job through COMPSs instead of multiple jobs (parameter sweep) managed by the portal. This task is directed to administrators and in the tutorial has been explained to make it clear the underlying mechanisms to execute the applications through the GRB portal.
- Development of a COMPSs application able to launch the model (hrt159.sh script) running on the gateway has to be added
- The COMPSs main application, wrapping the user code, has to be invoked with the following arguments: *-n tot_num -u user -o pathlog_portal*

where *tot_num* is the total number of members belonging to the ensemble experiment, *user* is the user login on the portal and *pathlog_portal* is the path on the portal where the experiments logs have to be saved.
The user training includes the following steps:

- A toy model deployment on the provided virtual machine simulating the presence of real compute nodes.
- Writing of the run script executing the toy model
- The model execution and monitoring through the grid portal

The complete tutorial includes the following topics:

- Introduction to the COMPSs framework
- COMPSs and the IS-ENES Grid infrastructure.
- Case studies: HRT159 an high resolution coupled model and data aware post-processing. COMPSs here is used as orchestrator of independent executions of the model (parameter sweep) and not as optimizer of the single model execution.
- Demo of the execution of eScience use cases ported to COMPSs. These use cases include the execution of bioinformatics, biology workflows composed of computational intensive tasks working on files.
- Hands-on
  - Simulation set-up using a toy model
  - Submission and monitoring
- Collection of requirements from users

## Venues

**Location**: Ugento (LE), Italy – In conjunction with CMCC Annual Meeting 2012
**Tutorial's title**: CompSs
**Date**: 11/06/2012
**Number of attendees**: 10
**Attendees expertise**: *3 computer scientists; 7 model developers*
**Comments and feedbacks received**:
The auditors consider the CompSs really powerful but they express relevant doubts on the effort required to include a new coupled model in the infrastructure. The model must be ported and installed on all of the computing nodes before accessing the portal; than a CompSs application must be written using the specific CompSs programming environment. On the other hand, the programming environment provided by CompSs can be used to specify more complex experiments and to define dependencies among the tasks in a workflow.

**Location**: Madrid, Spain – in conjunction with HPCS2012 conference
**Tutorial's title**: Prototype of Grid Environment for Earth System Models
**Date**: 02/07/2012
**Number of attendees**: 15
**Attendees expertise**: 3 climatologists, 12 computer scientists
**Comments and feedbacks received**:
Audience participation and also Q&A session have been very good.
Many feedbacks have been received with regard to the architecture of the grid prototype.
Several questions regarded the grid data scheduler. In particular, some people asked us:

1) what are the scheduling policies adopted by the GRB scheduler during the distribution of the ensemble jobs on various resources.

   We have explained that GRB uses simple heuristics such as: Min-Min, Max-Min and Sufferage.

2) how a new site can be configured/added in the grid prototype.

   We have described the grid configuration procedure with the additional possibility to use the grid portal for adding a new resource, in particular the grid scheduler and the working directory used by the GRB for stage-in and stage-out of data.

3) does the system support the workflow jobs?

   The answer has been that GRB supports batch (including MPI), parameter sweep and acyclic workflow jobs. A version that supports also cyclic workflow has been implemented by CMCC in the PROGENIA enactment engine, in another project called ProGenGrid which demo was presented in the same conference. So for major details, people have been invited to follow the demo.

Regarding the job monitoring, the climatologists have found the implemented interface very useful, with the possibility to visualize the progress of the experiments.
Several questions have regarded the performance of the system.
We have answered that performance depends on the availability of the resources hence by the queue policies, etc.
During the hands-on session, 13 users have submitted a job with a number of members that ranges from 20 to 45 members of the coupled model.
Several questions regarded the significance of the fields of the interface ("with step"). We have explained that this parameter represents the interval between the ensemble members.
The evaluation of the results, visualized by the interface, has been interactive with the users and the feedback very good.
At the last presentation, we have received an email by the session handler, with the compliments for the tutorial.

**Location**: Barcelona Supercomputing Center BSC, Barcelona Spain
**Tutorial's title: Prototype** of Grid Environment for Earth System Models
**Date**: 05/07/2012
**Number of attendees**: 10

**Attendees expertise**: 7 climatologists, 3 computer scientists
**Comments and feedbacks received**:
People have provided valuable feedback on the application and technology.
We have received positive feedback with regards to the grid portal, in particular for the grid configuration and credential managements.
Several people have made questions on the following arguments:

1) System Architecture. In particular:

   a) what are the features of the gateway and if it is a constraint at the system.

      The answer has been that the gateway machine has been inserted in the system for avoiding installing added software on the front-end node of the supercomputing machine. All of the software required by the gateway are installed on a virtual machine with clear advantages w.r.t the portability of the gateway for accessing to new sites.

   b) what are the scheduling policies used by the GRB.

      The answer has been: simple heuristics such as: Min-Min, Max-Min and Sufferage.

   c) what are the GRB libraries and if we foresee the extension for supporting Cloud infrastructure.

      The answer has been that GRB supports several libraries for the management of the credentials, data stage-in and stage-out, the data structures used in the scheduler.

   d) What is the information service used in GRB?

      The answer has been that GRB supports the iGrid information service [2][3], a relational IS that retrieves the main data used for the scheduler (CPU load, memory, etc.). A description about this component has been provided.

2) Grid portal. In particular:

   a) What are the parameters used for the submission of a job (toy and coupled model).

      The answer has regarded the definition of each field of the GUI. In particular for the coupled model, a configuration file must be created. Feedbacks have been given in order to create this file.

   b) What are the main features of the monitoring page?

      The answer has regarded the possibility to visualize the progress of the experiment, taking into account the geographic position of the resource used for each member. Details for each member have been explained in particular the simulated days/months.

   c) How configure an interface for another application?

      The answer has been related to the necessity to implement another page, written in C (CGI). The GRB has a default page where is possible to configure a generic application but it has been not used in the project.

3) Comparison with other tools.

   An important feedback has been given by people of IC3, involved in the implementation of another tool for the submission of ensemble jobs, named Autosubmit.
   In particular, by the discussion are emerged the main differences between tools and in particular they asked us how to add one of their node at the grid infrastructure.

During the hands-on session, 10 users have submitted a job with a number of members that ranges from 30 to 100 members of the toy and coupled model.
The evaluation of the results, visualized by the interface, has been interactive with the users and the feedback very good.

**Location**: IPSL, Paris France
**Tutorial's title**: CompSs
**Date**: 14th November 2012
**Number of attendees**: 6
**Attendees expertise**: 3 climatologists, 3 computer sciences
**Comments and feedbacks received (from Marie Alice Fujols)**:
We appreciated the presentation and the hands-on.

We asked a lot of questions and received answers. Interactions were productive.
We installed only one PC as we received instructions to install the virtual machine only on Monday 12th.
We are not convinced by the fact that only a toy (echo $date_of_simulation) was included in the demonstration. It's far from a distributed environment for ensemble simulations. To go further, we estimated the time of work : 6 months for one engineer at IPSL to describe IPSL runtime environment (including ensembles runs and post-processing) into the software.
We still have to evaluate other solutions and this will take some time.

**Location**: INGV Bologna, Italy
**Tutorial's title**: Prototype of Grid Environment for Earth System Models
**Date**: 16/01/2013
**Number of attendees**: 8
**Attendees expertise**: 2 system administrators; 6 climate modelers
**Comments and feedbacks received**:
The main comments regards the easiness on using the web interface for defining the experiment. Before starting an ensemble experiment through the gird portal, some preparatory phase must be accomplished by the user; he must create a parameter file for each member of the ensemble. If the experiment includes more than 20 members, this phase could be tedious and error prone. The auditors suggested to develop a web page dedicated to the definition of the parameters for the experiment.
The attendees found the monitoring interface really powerful
During the hands-on session all of the users were able to easily submit and monitor an experiment made of up to 50 members using the pre-deployed coupled model. A face-to-face tutorial has been requested to deploy a new coupled model in the grid environment. The coupled model, already tested and compiled in the CMCC supercomputing center, has been included into the grid environment and the user successfully submitted some sample tests.

**Location**: DKRZ Hamburg, Germany
**Tutorial's title**: CompSs
**Date**: 14/01/2013
**Number of attendees**: 6
**Attendees expertise**: all climatologist
**Comments and feedbacks received**:
The auditors consider the CompSs really powerful but they express relevant doubts on the effort required to include Fortran applications in the infrastructure. The model must be deployed on all of the computing nodes before accessing the portal; than a CompSs application must be written using the specific CompSs programming environment. On the other hand, the programming environment provided by CompSs can be used to specify more complex experiments and to define dependencies among the tasks in a workflow.

**Location**: DKRZ Hamburg, Germany
**Tutorial's title**: Prototype of Grid Environment for Earth System Models
**Date**: 14/01/2013
**Number of attendees**: 8
**Attendees expertise**: 2 computer scientist; 6 climate modelers
**Comments and feedbacks received**:
The auditors commented about the fault tolerance mechanism and the data management. The Grid Environment presented already includes some basic mechanism to improve the fault tolerance; in case of failure of a computing node, the member executing on the that node is re-submitted on a different node of the grid. The whole experiment is not affected on such failure. Indeed the others members, belonging to the experiment, can be simulated regardless of the failure and re-submission of few of them. The grid system will transparently take care of resubmission and monitoring of those members that were running on failure nodes.
Regarding the data management, the current version of the prototype manages on the input file transferring the data from the storage node to the executing node, but does not include any transfer of the output files. When the experiment terminates, the user has to gather the output files from the computing nodes involved by the experiment. In the next version of the prototype the output will be sent to the data node specified by the user and a link to that data node will provided directly from the monitoring page of the grid portal.

# Conclusion

The overall evaluation of the grid environment can be considered positive. Never the less the tools is still lacking on several key aspects. The integration with the services for data management is strictly required: the user can be burden for the copy of the output from each computing nodes. The produced output files should be automatically transferred to data nodes for archiving, data analysis and visualization.
Even if the grid infrastructure has been already tested with a real coupled model named HRT159, deeper tests, using higher resolution models, are needed to prove the robustness, reliability and efficiency of the grid solution. A higher resolution model imply not only a much higher demand of computational power, but imply also bigger amount of data to be transferred in the distributed environment and this could be the real bottleneck of the grid infrastructure.
Moreover the definition of the ensemble experiment must be improved with more user-friendly web interface.
In the next phase, the infrastructure will be improved with the deployment of several other climate coupled models. The idea is to create different Virtual Organizations in which the users of the same group share the same models. The infrastructure will also grant the access for guest users that can execute a toy model for demo purposes. Hence, when a user asks for registration to the v.E.R.C. portal, a guest account for job submission will be automatically created. A user who want use an advanced model should request an account to a VO configured by its administrator for the test of the model on the resources.
Several grid technologies and some previous experiences demonstrate how the execution of an entire climate workflow could be considered and included in the prototype. Pre-processing, post-processing and visualization tasks can be connected with dependencies constraint and executed on a distributed environment through several already available grid services.
Moreover the integration between GRB and CompSs produced a tools that includes advantages from both technologies. The powerful of expressiveness provided by the CompSs programming environment is merged with the high level grid services provided by the GRB.

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