**First CMMST VT teleconference - 19/02/2013**

Scheduled time 10:00 – 11:00 CET

The teleconference was hosted by the EGI Webex system

AGENDA

1. Welcome and acknowledge all participants  
    \* Apologies received  
    \* Note any absent members.  
    \* Brief outline of aims of this meeting.
2. Introduction  
    \* Presentation by Chair (slides included beneath)
3. Participants introductions:  
    \* Name, organisation and position.  
    \* The role you expect to play in this VT.
4. Discussion  
    \* Task assignment
5. Emerging Issues and Actions
6. AOB
7. Details of next meeting and presentations.

CONNECTION INFORMATION

**To join the online portion of the Personal Conference meeting with a computer**  
 1. Go to

[https://egi.webex.com/egi/j.php?ED=22867647&UID=129638627&PW=NM2NlZDBjZjhl&RT=MiMyMg%3D%3D](https://egi.webex.com/egi/j.php?ED=22867647&UID=129638627&PW=NM2NlZDBjZjhl&RT=MiMyMg%3D%3D" \t "_blank)  
 2. If a password is required, enter the Meeting Password: 30326451  
   
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MINUTES

Meeting started at 10:05

**Item 1.** Welcome and Apologies

*Attending*: Antonio Laganà (**AL**) – IT – VT Leader, Gergely Sipos (**GS**) – EGI.eu, Richard MCLennon (**RM**) EGI.eu, Alessandro Costantini (**AC**) IGI, Daniele Cesini (**DC**) IGI, Fermin Huarte (**FH**) ES, Jelena Tamuliene (**JT**) EGI.eu, Peter Annousek (**PH**) CZ, Remco Havenit (**RH**) NL, Stavros Farantos (**SF**) GR, Michele Ceotto (**MC**) IT, Ernesto Garcia (**EG**) ES, Akos Benksura (**AB**) HU;

*Apologies*: Mariusz Sterzel PL, Sergio Maffioletti CH, Peter Oliver UK, Marco Verdicchio FR, Gyorgy Lendvay HU

**Item 2.** Introduction

AL started the teleconference by presenting the material (slides) uploaded in the Indico page.

<http://indico.egi.eu/indico/conferenceDisplay.py?confId=1310>

whose articulation is sketched below:

* The VT projects and the CMMST VT
* How to establish a Virtual Research community
* Tasks and Milestones of the CMMST VT
* Information on the preliminary meeting
* Volunteers for VT tasks leaders
* Planning activities for tasks 1
* Plan of future WebEx conferences
* Administrative aspects (if any, by Richard McLennan)

**Item 3.** Participants present themselves and their role in the VT

**AL**: University of Perugia, VT Leader , member of the board of IGI (Italian Grid Infrastructure) and of its User Support and Training Units, Expert in Computational chemistry and concurrent computing

**GS**: EGI.EU representative

Technical Outreach Manager at EGI.eu (the coordinating institute of the European Grid Infrastructure) in charge of promoting existing tools and services to scientific communities, coordinating the development of new user-facing tools and facilitating interactions between software developers, service providers and user communities.

Contribution to M1 in carrying out the investigation planning document with the list of technical and non-technical topics that the project should investigate

**RM**: EGI.EU representative

Expert in project management, giving administrative support to the VT

**DC**: Italian Grid Infrastructure representative

Support in services and resources usage. Contribution to tasks 1 and 2

**FH**: University of Barcelona

Expert in reaction dynamics; computational chemistry program developer; EGI grid user

**EG**: University of Vittoria

Expert in reaction dynamics; skills in the massive usage of EGI grid. Contribution to tasks 1

**RH**: University of Groeningen

Expert in theoretical chemistry and supercomputers calculations: Erasmus Mundus TCCM Master member

**SF**: University of Crete

Expert in classical, semiclassical and quantum chemistry; algorithm developer for the interaction between HTC/HPC resources; EGI grid user

Applied for a PRACE project: unfortunately not succeeded.

**AC**: Italian Grid Infrastructure representative

Support in services and resources usage. Contribution to tasks 1 and 2

Covering the technical support to the VT

**MC**: University of Milano

Expert in reaction dynamics and theoretical chemistry; links with the HPC Center and Dept. of Chemistry and Biochemistry of the Texas Tech University at Lubbock (US)

**AL** took the floor to the end of presenting possible interactions with the following communities (which are aware of the VT activities and could be involved in dissemination):

* Division of Computational Chemistry (DCC) of the European Chemical Society (EUCHEMS)
* European Chemistry Thematic Network (ECTN) Association
* Future input expected by **PO** (UK) out of his e-Science project
* Possible non EU collaboration from Alan Sill and Williams Hase (HPC Center and Dept. of Chemistry and Biochemistry of the Texas Tech University at Lubbock (US))
* Expected contacts from Brasil before the end of the VT project

**Item 4.** Discussion

After an active discussion on possible interactions **SF** proposed to give two weeks to the participants in order to better understand the aim of the VT and the role of each participant on it.

**Item 5.** Emerging issues and actions

The participants committed themselves to send, within the next two weeks, comments to the other members using the mailing list. The comments will be integrated in the minutes and will be used as starting point to address Task 1.

**CMMST members:** accepted on the proposal made by **SF**

**Item 6.** AOB

None

**Item 7.** Details of the next meeting and presentations

The following calendar for the next meetings is proposed

March 19, April 23, May 21, June 18, July 23, August 2

Scheduled time 11:00 – 13:00 CET

Teleconferencing tool WebEx

**Meeting closes at 10:56**

Some participants experienced HW/SW problems. RM offered to give them proper support in order to solve such problems before the next WebEx teleconference.

ITEMS PROVIDED IN POST TELECONFERENCE

**GS**

1. The Virtual Research Communities (VRCs) that already exist in EGI from various scientific fields are listed here: <http://www.egi.eu/community/vrcs/>   
   There is a 'Memorandum of Understanding' document for each of theM. While an MoU does not tell what a scientific VRC does, it describes the activities and services that the particular scientific community does together with EGI.   
   So these MoUs could help us define the type of services and activities that the CMMST VRC could do in the EGI context.   
     
   2. Workflows came up as a topic of investigation work within the VT. Since September 2012 EGI.eu is involved in a FP7 workflow project, titled 'Building a European Research Community through Interoperable Workflows and Data' (ER-flow in short).   
   - You can find a short introductory leaflet about ER-flow, its services and workflow platform: <http://www.erflow.eu/documents/388575/526049/ER-flow+flyer>   
   - ER-flow organise a "Workflow Application Porting Workshop" in London between 19-22 of March: <http://www.erflow.eu/19-22-march-2013-application-porting-workshop> The Workshop will bring together the representatives of scientific communities, scientific projects with workflow experts from ER-flow and SHIWA to experiment with services of the SHIWA Simulation Platform, and to actually port workflow applications to European e-infrastructures with the platform during the event. The event is free and open to anyone. I recommend VT members to attend the event because it could help you built up an understanding of workflows, available workflow tools in grid context.   
   Let us know if you attend - we would appreciate a report from you after the event on the VT list.   
     
   3. Some of the VT members are unfamiliar with grids, with EGI. We could organise an online Webinar presentation about EGI to the VT. The webinar could introduce various services that EGI can offer to a CMMST VRC. These services can be roughly categorised as   
   - Tools to integrate scientific applications and models with grids and clouds (Portals, workflow frameworks, APIs,...)   
   - Tools to facilitate collaboration inside the CMMST research community (Applications Database, Training Marketplace, Document server, Wiki pages, Email lists, ...)   
   - Tools to operate software services for CMMST researchers (Monitoring tools, accounting tools, helpdesk,...)   
   Would you find such a Webinar helpful?   
   Maybe similar webinar presentations could be given by other members of the VT about thier tools and contributions to the CMMST VRC? (e.g. Antonio about GEMS?)

**SF**

Taking into account that there is a large CMMST group among European scientists, with some of them worldwide renowned, acting on methodological and application problems, **SF** propose in the next meeting to discuss how the CMMST VT can attract their interest in EGI. Item 3 of **GS** suggestions goes in this direction.

Some other thoughts are:

-Concentrate in a few popular open software like DL\_POLY, NAMD, GROMACS, GAMESS.

-Concentrate in specific applications – material, biological, environmental.

-Prompt the development of new software tools for bridging EGI and PRACE

applications.

-Prompt the development of Molecular Dynamics (classical-semiclassical-quantum)

algorithms for distributed and high performance computing.