**5th CMMST VT teleconference - 18/07/2013**

Scheduled time 15:00 – 17:00 CET

The teleconference was hosted by the EGI Webex system

Agenda:  
 1. Welcome  
 \* acknowledge all participants (including new ones)  
 \* apologies received  
 \* note any absent members  
 2. Acceptance of previous Minutes  
 \* <https://indico.egi.eu/indico/conferenceDisplay.py?confId=1647>  
 3. Introduction by Chair with outline of aims of this meeting  
 4. Discussion of the activities status  
 \* Report on status of CMMST workshop @ICCSA conference, Ho Chi Min City (Vietnam) June 24-27 (papers, meeting, ...)  
 \* online Webinar presentation about application and tools offered by EGI to the CMMST VRC. [Indico link](https://indico.egi.eu/indico/conferenceDisplay.py?confId=1647)  
 \* activities at the European Computational Chemistry division, Sopron (HU) 1-5 September (contributions deadline, papers, TCCM PhD workshop, ...) <http://www.euco-cc9.mke.org.hu/>  
 5. VRC proposal document (M2, M3, M4)  
 \* M1 and M2: items achieved (Sec 2)  
 \* Discussion over the CMMST VRC (Sec. 3)  
 \* Discussion over services and technologies (Sec. 4 and 5)  
 6. Horizon 2020 as CMMST VRC?  
 7. Emerging issues  
 8. AOB  
 9. Details of next meeting date, time, purpose.

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 You can do that at: https://egi.webex.com/docs/T28L/mc0806l/en\_US/support/xplatform.htm

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MINUTES

**Meeting starts at 15:07**

**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, Ernesto Garcia (**EG**) ES, Stavros Farantos (**SF**) GR, Jelena Tamuliene (**JT**) EGI.eu

*Apologies*: Carlo Manuali (**CM**) IT, Michele Ceotto (**MC**) IT, Klemens Noga (**KN**) **CZ**,

Peter Annousek (**PH**) CZ, Peter Oliver (**PO**) UK, Marco Verdicchio (**MV**) FR, Gyorgy Lendvay (**GL**) HU, Fermin Huarte (**FH**) ES, Daniele Cesini (**DC**) IGI, Remco Havenit (**RH**) NL, Akos Benksura (**AB**) HU, Evangelia Varella (**EV**) GR, Alan Sill (**AS**) USA, Wu Heng (**WH**) USA, Sergio Maffioletti (**SM**) CH

**Item 2.** Acceptance of previous minutes

Minutes of the previous teleconference have been approved by the attenders.

**Item 3.** Introduction

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

<https://indico.egi.eu/indico/conferenceDisplay.py?confId=1752>

whose articulation is sketched below:

* Discussion of the activities status
  + CMMST workshop @ ICCSA 2013
  + online Webinar about application and tools offered by EGI to the CMMST VRC
  + European Computational Chemistry division
* VRC proposal document (M2, M3, M4)
  + M1 and M2: items achieved (Sec 2)
  + Discussion over the CMMST VRC (Sec. 3)
  + Discussion over services and technologies (Sec. 4 and 5)
* Horizon 2020 as CMMST VRC?
* WebEx conferences
* Administrative aspects (if any, by Richard McLennan)

**Item 4.** Discussion of the activities status

*- ICCSA 2013, Ho Chi Min City (Vietnam) June 24-27*

Workshop devoted to the CMMST community – The contributions here listed were presented as CMST contributions to dissemination

* Jeff Crawford, Zachary Eldredge, and Gregory Parker: Using Vectorization and Parallelization to Improve the Application of the APH Hamiltonian in Reactive Scattering;
* Sergio Tasso, Simonetta Pallottelli, Giovanni Ciavi, Riccardo Bastianini, and Antonio Laganà: An Efficient Taxonomy Assistant for a Federation of Science Distributed Repositories: a Chemistry Use Case
* Marzio Rosi, Stefano Falcinelli, Nadia Balucani, Piergiorgio Casavecchia, and Dimitrios Skouteris: A theoretical study of formation routes and dimerization of methanimine and implications for the aerosols formation in the upper atmosphere of Titan
* Leonardo Pacifici, Marco Verdicchio, and Antonio Lagana: Multi Reference versus Coupled Cluster ab initio calculations for the N2 + N2 reaction channels
* Alessandro Costantini, Diego Michelotto, Marco Bencivenni, Daniele Cesini, Paolo Veronesi, and Emidio Giorgio: Implementation of the ANSYS commercial suite on the EGI Grid Platform

*- EGI Service offerings to CMMST community – Webinar*

Webinar presentation held by GS from EGI.eu providing an overview of the services that the European Grid Infrastructure Collaboration offers to the 'Chemistry, Molecular & Materials Science and Technology' community (CMMST). The presentation has been delivered for the members and partners of the 'Towards a CMMST VRC' Virtual Team project of EGI. <https://indico.egi.eu/indico/conferenceDisplay.py?confId=1647>

For further information about this project please refer to https://wiki.egi.eu/wiki/Towards\_a\_CMMST\_VRC.  
   
 The following topics are covered in the Webinar:  
 \* The EGI collaboration (stakeholders, members, users, projects, etc)  
 \* EGI User support structure +++  
 \* EGI Services for scientific communities:  
 \* Virtual Organisations  
 \* Grid services ++  
 \* Cloud infrastructure +++++  
 \* Services for community management and collaboration +++  
 \* Ready-to-use scientific applications that are integrated

with the EGI ++++  
 \* Workflow development and execution tools in EGI

(incl. workflow of workflows) ++++  
 \* Scientific gateway portals in EGI +++++  
 \* Connecting (federating and sharing) high performance

computing and storage resources ++  
 \* Links to other e-infrastructure initiatives +  
 - Infrastructure integration activities with EUDAT and PRACE  
 - Comparison of portals, mention the CHAIN portal

*- Computational Chemistry division of EUCHEMS, Sopron in September 1-5*

* Full section on distribute computing (GRID, PRACE)
* **GS** has been invited and he confirmed that will attend the conference of the Computational Chemistry division of EUCHEMS

**Item 5.** VRC proposal document (M2, M3, M4)

Discussion

Before starting the telecom **GS** and **RM** provided the following list of 11 comments related to the circulated VRC proposal:

1. The document deals already with the 3rd milestone of the VT (M3) as said in the Wiki. (The VRC proposal that is shared with the VT members is M3). The final deliverable of the VT, the “proposal for the setup of a CMMST VRC in EGI” (M5) will be the refined version of this document. Accordingly it is suggested not to mention in the document to what milestone it is referred. It is therefore appropriate to present the document as the “Proposal for the setup of the CMMST VRC in EGI that has been prepared in an EGI-InSPIRE VT project'. This requires small changes on the title page, in the abstract, introduction, and a few other places.   
  
2. The VRC plan emerged as an outcome of the technical and non-technical investigations that the VT covered. (See the definition of M2 in the Wiki). So this document should include the listing of these investigation areas, the results of the investigations and some description of how the outputs are used within the VRC plan. (I think there is a placeholder for this on page 5 in section 2.1). M1 includes the investigation areas, you can get them from there.   
  
3. It is suggested to add a section about the tools that EGI.eu provides for scientific communities to help them coordinate/structure themselves. We can provide you the description of these tools, so you can then decide which tool you think the VRC should use. You can include the descriptions of the envisaged use of these tools in the VRC proposal.   
  
4. Section 3.2 mentions that “the COMPCHEM VO is to join forces with VOs like GAUSSIAN, WeNMR, etc.) - be more specific, how do you want to join forces? (E.g. monthly teleconference, face-to-face meeting at EGI forums, etc)

5. In section 3.3.1 change 'task' to 'activity' everywhere. (That's why these are shortened as A1, A2, ... in the VRC MoU template). The same section should include your initial thoughts on who (individuals, institutes, other?) are going to participate in each activity, and how the activity coordinators will be connected to and communicate with these members. There were a number of chemistry research institutes and teams who provided support letter for the VT. How are these come into the VRC? How can others join the VRC? Consider adding a 'value proposition' to the document that would describe why CMMST institutes/groups should join the VRC.

6. The role of the credit, QoS, QoU systems in the VRC is unclear. What are these systems and what are they used for? For decision making by the VRC management body?

7. Section 3.3.2  Activity A2: Services and operations - it is unclear what services and sites (if any) the CMMST community wants to federate into EGI, and what is the status of this federation activities. (e.g. linking to EGI operation tools, middleware installation, VO setup, etc)

8. Section 3.3.6 Sustainability - what exactly does the VRC need to sustain? People, software, anything other? How will you do that? From institutional funds? From setting up new projects? Give some ideas here please.

9. Section 4.1 - are the listed applications registered in the EGI AppDB? Are they integrated with EGI grid or cloud? Is there any application that is not integrated with EGI yet, but should be for the CMMST VRC to function properly?

10. 4.2 Provided EGI tools and services - what do you want to do with these? The list is too long. You cannot use and support all of these tools. What are the relevant tools for the VRC? How will the VRC management body make these relevant tools available for the members? What support do you expect from the providers of the tools and services? And from EGI.eu?

11. 5 New project: HPC-HTC INTEGRATION - the CMMST community is not involved in the EGI-EUDAT-PRACE pilots, so we suggest to move this section into an appendix. (It's related work.) We also suggest to add a sentence or two to the end of this section that describes why these pilots are relevant for the CMMST VRC. (I assume because the pilots are expected to result a set of tools and recommendations that the CMMST community can use to run integrated workflows on EGI-EUDAT-PRACE)

**AL** took the floor by emphasizing that the opportunistic model offered by the Grid to the communities is the one matching important requirements of the users which are often overlooked as are workflows and credit system mechanisms. **AL** asked for comments related to the VRC proposal document.

**SF** asked to **GS**, accordingly to **GS**-**RM** comments, if the proposed document is appropriate as a proposal.

**GS** answered that the purposed of the document are twofold: collect critical mass for the CMMST community and prepare a MoU for EGI. On this basis the document is a “point to start” and the provided comments can help in making the VRC document stronger.

**RM** proposed to focalize the efforts to those tools and applications really important for the community.

**AL** and **SF** agreed on that, yet a huge effort is needed in order to gather together the community and build the VRC.

**AL** continued by saying that as a community CMMST has users but also not enough effort to be really effective. Moreover, build-up the VRC requires effort and as the community is growing-up the structure of the VRC (and related interactions among members) will consolidate.

On such process, continued **AL**, an important role is played by the credit economy planned to be integrated in the CMMST community.

**GS** said that the credit system is a key element and for this reason has to be better described in the VRC proposal, in particular how to distribute efforts and benefits.

**GS** continued asking to **AL** if the document is directed to the CMMST community or to EGI.

**AL** answered that in Section 1 and 2 there is a first tentative to prepare the MoU and to figure out the steps needed to growing-up the community; in Section 3 actions to implement the VRC have been proposed but have to be consolidated: in Section 4 and 5 the focus has been concentrated to the applications and tools offered to the community and have to be refined.

**SF** took the floor saying that the community has a core of applications in EGI and this has to be reported and focused in the proposal.

**JT** agreed making as an example WLCG and WENMR VRCs representing people which activity is focused on well defined items.

**RM** said that the aim of the document should be a proposal to form a VRC to promote some products, now is only a list of tools.

**AL** said that the document will be revised by reducing the number of tools and adding motivations for applications and tools used.

**GS** offered to provide material for Section 4.

**GS** and **RM** proposed also to prepare a separate document in the form of a MoU to be presented to EGI.eu and attached to the VRC proposal document where to define the commitments between the CMMST community and EGI.eu.

**Item 6.** Horizon 2020 as CMMST VRC?

**AL** asked if this is the right time to discuss of this point.

**GS** proposed to drop from the agenda this point and concentrate the effort to the document and the MoU.

Participants agreed to drop Item 6 from the agenda.

Actions

* **AL**-**AC**-**GS** improve the document and the MoU
* **AC** set a doodle for the next telecon for the second week of September 2013

**Item 7.** Emerging issues and actions

None emerged by the participants

**Item 8.** AOB

None emerged by the participants

**Item 9.** Details of the next meeting and presentations

Next meeting proposed to be scheduled in the second week of September 2013.

A doodle to set the date and time of the next meeting will be opened by **AC**.

The teleconferencing/webinar tool WebEx will be used.

**Meeting closes at 16:25**