

Towards a Chemistry, Molecular & Materials Science and Technology Virtual Research Community

Antonio LAGANA¹, Alessandro COSTANTINI² et al.

¹ University of Perugia, (IT)

² INFN and IT_NGI (IT)

alessandro.costantini@pg.infn.it

- Towards a Chemistry, Molecular and Materials Science and Technologies (CMMST) VRC
 - Motivations and collaborations
- The CMMST-EGI Virtual Team
 - Activities and projects
- Conclusions

- CC EGI Virtual Organizations (VO)s
 - COMPCHEM , GAUSSIAN, CHEM.VO.IBERGRID.EU, TRGRIDB
 - Researchers out of the existing CC Vos
- MOTIVATIONS
 - Gather researchers from a fragmented domain
 - Need to represent the Chemistry, Molecular & Materials Science and Technology community in EGI
 - Implement a synergistic model to allocate resources and competences in a cooperative way

- EGI-VT finalized @ EGI-CF aimed at assemble a VRC out of the existing Chemistry, Molecular & Materials Science and Technology oriented EGI Vos
- Collaborations
 - EGI existing VOs
 - COMPCHEM, GAUSSIAN, CHEM.VO.IBERGRID.EU
 - EU projects (MoSGrid and ScalaLife CC)
 - US Universities and Research centers
 - Collaborations and support:
 - several NGIs within EGI.EU (in particular NGI_IT)
 - MTA-SZTAKI (WS-PGRADE as WF engine)
 - XSEDE (Preparation of two proposals to access the XSEDE resources)

N	Topic	Task
1	How to exploit the capabilities of the existing EGI tools in building distributed workflows and “workflows of workflows” from various software packages	Task 1
2	How to exploit the capabilities of the existing EGI tools for distributing runs of CMMST applications on EGI and PRACE platforms	Task 2
3	How to attract more CMMST users into a common endeavour offering the possibility of assembling higher level of complexity applications and services	Task 3
4	How to utilize a credit system to encourage CMMST users to cooperate in developing higher level of complexity applications	Task 4
5	How to define a coordinated management body for such endeavours and configure a Virtual Research Community (VRC).	Task 5
6	How to operate the EGI VRC in a sustainable way	Task 6

- Services and tools offered by EGI to the CMMST VRC
 - EGI platforms
 - Operational services
 - Software tools and human services
- Technologies and services offered by the CMMSR-VRC through EGI
 - Computational Chemistry applications and expertise
 - the adoption of high level ICT instruments
 - Tools and services providing dedicated user support activities

- Definition of a Credit system model
 - costs to be paid for the Services utilized and Credits earned in return for the efforts spent
 - evaluation of Quality of Services (QoS) and Quality of Users (QoU)
 - adoption of user-layers within the community
- Bridging HPC/HTC resources
 - CMMST is developing a set of activities aimed at equipping its applications with a set of tools facilitating interoperability between HPC and HTC platforms with a unique point of access to the different infrastructures (portals, GUIs, etc)

- Implement a synergistic model to allocate resources and competences in a cooperative way
 - Cooperative endeavour based on
 - the combined expertise in the field of the molecular science
 - the adoption of high level ICT instruments
 - integration of GRIF Resource Selection System in WS-PGRADE
 - Bridging of HPC/HTC resources
 - Tools and services
 - application-related, providing dedicated user support and training activities
 - Under developmet (as DCC)
 - articulate a **Grid Economy Model** as Costs to be paid for the Services utilized and Credits earned in return for the efforts spent

- Virtual Research Communities offer a solid ground for collaborative computing (metrics, quality evaluation) and tools development
- Chemistry and Molecular and Materials Science and Technology (CMMST)-VT
 - Identify tools and services
 - Projects
 - Sustainability
 - HPC/HTC bridging
 - EU-US collaborations established
- Intention for the CMMST to become a DCC
 - Implement a synergistic model to allocate resources and competences in a cooperative way