Towards a Material and Molecular Science Research Community

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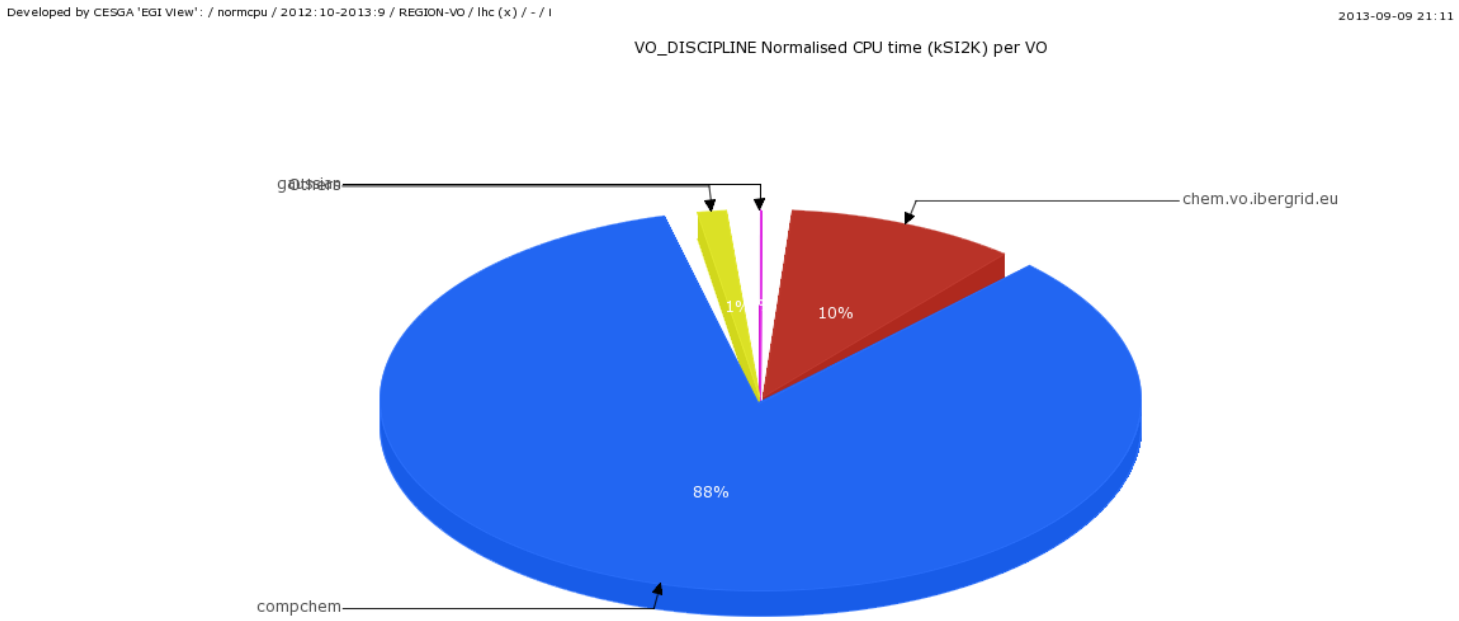
Summary

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

The CC domain in EGI

- CC EGI Virtual Organizations (VO)s
  - COMPCHEM , GAUSSIAN, CHEM.VO.IBERGRID.EU
  - Researchers out of the existing CC VOs

Normalised CPU time
K.SI2K.Hours
1/2013 - 1/2014



COMPCHEM
18,311,531

GAUSSIAN
278,244

CHEM.VO.IBERGRID.EU
2,137,536

TRGRIDB
222

Towards a CMMST VRC

- 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 project aimed at
  - assemble a VRC out of the existing Chemistry, Molecular & Materials Science and Technology oriented EGI VOs
  - Identify, develop and/or import tools, services and resources needed by the VRC
  - develop a proposal to establish a new CMMST VRC in EGI

Towards a CMMST VRC

- 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)

The CMMST Virtual Team

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

Services and tools offered by EGI to the CMMST VRC

- EGI platforms
  - EGI High Throughput Computing
  - Federated Cloud Platforms
- Operational services
  - through which the VRC could federate its own resources
- Software tools and human services
  - to coordinate the community,
  - to facilitate communication inside the VRC,
  - to assure continuous exchange of relevant information between the VRC and the rest of EGI,
  - To attract new members

Services and tools

Technologies and services offered by the CMMSR-VRC trough EGI

- Cooperative endeavour based on
  - the combined expertise in the field of the molecular science
  - the adoption of high level ICT instruments
- Computational Chemistry applications
  - ab initio calculation of the electronic structure of molecular systems and the assemblage of ab initio based potential energy surfaces
  - integration of quantum and/or classical equations of motion
  - handling of the statistical and higher scale treatments
- Tools and services
  - application-related, providing dedicated user support activities

Encourage cooperation

- The members of the VRC are requested to be proactive for the development of the VRC
  - development of tools and services
  - attracting financial resources
    - elaborate joint applications for funding and research projects
    - develop within the VRC commercial services

- All the activities and services offered to the community are to be identified, recognised and rewarded
  - Key aspect of the synergistic nature of the proposed CMMST VRC
  - evaluation of the Quality of Services (QoS)
  - evaluation of the Quality of Users (QoU)
  - adoption of user-layers within the community

User levels

Membership level	Description
End-user	*Passive*: Run a program implemented by other members *Active*: Implement at least one program for personal use
SW provider	*Passive*: Implement at least one program for use by other members *Active*: Provide interactive management of the implemented programs for cooperative usage
Resource provider	*Passive*: Confer to the VRC additional hardware *Active*: Provide basic services, tools and related support
Stakeholder	Take part to the development and the management of the VRC

Structure of the VRC

- Mangement body
  - Board of Stakeholder (BoS)
    - representatives of the stakeholder VOs
    - representatives of main stakeholder resource providers
    - representatives of the most contributing (in terms of nationality of the members) stakeholder National Grid Infrastructures.

- Members elected by the BoS
  - VRC leader: is the person representing the VRC and is the MoU contact point
  - VRC deputy leader: is the person elected by the BoS acting on the behalf of the VRC leader
  - VRC activity coordinators

Structure of the VRC

VRC activity coordinators: persons appointed by the BoS coordinating the VRC activities

- Ensuring a strong coordination with EGI and the participant VOs
- acting as experts in the assigned roles (as from the VRC-EGI MoU)
  - User support and training activities (A1) Coordinator
  - Operations activities (A2) Coordinator
  - Technical activities (A3) Coordinator
  - Communication and Dissemination activities (A4)Coordinator

Projects

- 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)

Activity as VRC

- 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

Conclusion

- 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 became a DCC
  - Implement a synergistic model to allocate resources and competences in a cooperative way