BRIDGING GRID, CLOUD, SUPERCOMPUTING AND STORAGE RESOURCES AT A GLOBAL SCALE

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The European Grid Infrastructure (EGI) is a federation of over 340 resource centres, set up to provide computing services and resources to European researchers and their international collaborators [1]. EGI is coordinated by EGI.eu, a not-for-profit foundation created to manage the infrastructure on behalf of its participants: National Grid Initiatives (NGIs) and European Intergovernmental Research Organisations. EGI supports research collaborations of all sizes: from the large teams behind the Large Hadron Collider at CERN and Research Infrastructures in the ESFRI roadmap, to the individuals and small research groups that equally contribute to innovation in Europe.

Multinational research consortiums involving dozens of labs and universities are now part of the computational chemistry landscape. Multi-national scientific communities can draw many benefits from having a partnership with EGI. For example, they can have uniform access to the massive computation resources and support services of the National Grid Initiatives, they can benefit from the workshops and forums organised by EGI members, they can receive support on resolving specific technical issues, and they become involved in the user-focussed evolution of EGI's production infrastructure.

This presentation will provide an overview of the EGI infrastructure platforms, focussing on recent achivements in integrating and federating new types of resources into it [2][3]. As a result of these activities, cloud systems, voluntarily and dedicated desktop grids, supercomputers of the PRACE and XSEDE infrastructures, storage resources of the EUDAT infrastructure bacame available for scientific communities who wish to use these for distributed and parallel applications. These various types of resources can serve a large variety of scientific data processing and data mining algorithms, high-performance computing simulations, data transfer and repository applications. The presentation will provide examples of such use cases.

The Chemistry, Molecular & Materials Science and Technology (CMMST) community recognised the advantages of having a dedicated partnership with EGI, and – under the coordination of the representative from the computational chemistry division of EUCHEMS – began to work with EGI.eu in February 2013 on the setup of an 'EGI Virtual Research Community' (VRC) [4]. The VRC aims to be the voice of the Chemistry, Molecular & Materials Science and Technology community within EGI, driving for production quality and sustainable applications, tools, services and resources for scientific users based on on the solutions that exist in EGI. The presentation will also provide an overview of the plans for the CMMST VRC.

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References:

[1] European Grid Infrastructure: http://www.egi.eu
[2] EGI Federated Cloud: http://go.egi.eu/cloud
[3] EGI-EUDAT-PRACE integration pilots: https://wiki.egi.eu/wiki/EGI_EUDAT_PRACE_collaboration
[4] Desktop Grids integration in EGI: https://wiki.egi.eu/wiki/Desktop_Grids_integration
[5] 'Towards a Chemistry, Molecular & Materials Science and Technology Virtual Research Community' EGI-InSPIRE Virtual Team project: https://wiki.egi.eu/wiki/Towards_a_CMMST_VRC