TOWARDS OPEN MOLECULAR SCIENCE CLOUD SERVICES

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BACKGROUND AND MOTIVATIONS

-Open science cloud - Following the launch of the European Open Science Cloud (EOSC) project on November 2018, Open Science Pillar and OpenAIRE Advance lines of activity have been started to the end of reshaping the scholar system of communication towards openness and transparency for scientists.

-Open Molecular Science Cloud (OMSC) - In order to enable the Molecular Science Community to provide cloud services to its members, the VHERLA infrastructure (the cloud image of the Perugia OpenStack platform devoted to the activities of the CMS^2 Molecular Sciences consortium (http://www.cms-2.org/index.php)) was implemented as a Virtual Data Center within the **GARR** (http://www.garr.it/b/eng) **Cloud** [1].

-Joint MolSSI-EuChemS workshop – A satellite initiative of the EuChemS Computational and Theoretical Chemistry (CTC) Division European Conference CTC EUCO2019 (Sept 1-5, 2019 - http://www.dcbb.unipg.it/euco2019) is the joint OMSC MolSSI-EuChemS workshop devoted to *software-related challenges relevant to computational molecular sciences*. The first section of the workshop will be held in Perugia (Sept 3-5) aimed to show with the following programme:

SECTION 1 (voluntary basis) -September 3 afternoon (Perugia)

14:30 - 14:45 A. Laganà: Opening

14:45 - 18:30 O. Gervasi, S. Tasso: *Training event on dissemination, assessment and certification of Molecular Science Knowledge on cloud*

-September 4 (Perugia)

9:00 – 11:00 D. Crawford (and contributed papers): *HPC for Photochemistry and Molecular Dynamics*

11:20 – 13:20 J.P. Piquemal (and contributed papers): *Force fields*

14:30 – 16:10 F. Ruggieri (and contributed papers): *Open Molecular Science Cloud and Distributed Computing*

16:30 – 18:30 *Informal discussion*

20:00 Banquet

-September 5 morning (Perugia)

9:00 – 11:00 G. Vitillaro (*VHerla cloud)*, E. Mosconi (*Photovoltaic application)*,

11:30 Bus Transfer to Rome of people involved in the second section "Writing the OMSC project"

-Writing an OMSC project for the Open Science Pillar – The second section of the joint OMSC MolSSI-EuChemS workshop will be held in Rome (Accademia delle Scienze -Sept 5-6) to write an OMSC implementation project for the Open Science Pillar.

SECTION 2 (max 25 people) -September 5 afternoon (Rome)

14:15 Welcome by the President of Accademia delle Scienze

14:30 – 15:20 F. Ruggieri: *The EU Open Science Cloud Pillar Project*

15:20 – 16:10 A. Laganà: *MOSEX (MOlecular Simulator Enabled Cloud Services)*

16:10 – 17:00 D. Crawford: *OpenFF (Open Force Field Consortium) Services*

17:00 break

17:30 – 18:20 R. Sayos: *First-principles based kinetic simulations Services*

18:20 – 19:10 C. Bo: *IOCHEM (organization, publication and storage of molecular information)*

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19:10 - 20:30 Buffet DINNER
20:30 Transfer to the Hotel for the night

-September 6 morning (Rome)

9:00 – 10:00 *General Discussion and wok groups forming*
10:00 – 12:00 *Work Groups activities to design tasks of the OMSC PROJECT*
12:00 A. Laganà: *Closing remarks and Dispersal*

MOSEX: MOLECULAR SIMULATOR ENABLING GRID SERVICES

MOSEX is a project aimed to improve the services offered on the cloud from/to the Molecular Science members and is meant to rely on some extensions and enhancements of the present VHERLA infrastructure (assembled in Perugia for the activities of the CMS^2 consortium generated in June 2017 for an Open Science Cloud School and running on the OpenStack platform).

a) The proposed infrastructure targets are:

1. Extension of the project "cnr-istm" on GARR-CLOUD to the end of the year 2019 (or replacement with a new project) with associated re-definition of hardware (mainly storage and flavors)
2. Availability of Infiniband (or at least Ethernet 40/100 Gbe) for "cnr-istm" in order to exploit parallelism in production runs
3. Availability of GPUs on the platform
4. Support by GARR-CLOUD to implement on DCBB/ISTM/PG a local OpenStack/CEPH for federation with GARR-CLOUD and extension to DFG and DMI
5. Transfer of VHERLA from GARR-CLOUD to the DCBB/ISTM/PG cluster with the termination of "cnr-istm" or definition of continuation condition for the "cnr-istm" project.

b) The proposed service targets are:

1.Molecular science competence dissemination
The main initiatives are the **EChemTest®** and GLOREP cloud services leveraging an ECTN international network of both National Test Centres (NTC)s (and Accredited Test Sites (ATS)s) adopting the Prosumer model [2,3].
2. electronic structure and dynamical properties computing programs
GEMS (small molecules chemical processes (including ab initio determination of analytical Potentials), their Quantum/Classical dynamics efficiency and properties obtainable from the analysis of the wavefunction) and possibly other packages
3. Drug design programs and cloud services
(QSPR and 3D QSPR models)
4. Distributed repository of molecular science data
CHEMCONNECT (organization, publication and storage of molecular information on combustion), IOCHEM (organization, publication and storage of molecular information on materials)
5. Publishing and dissemination of molecular knowledge
VIRT&L-COMM (e-magazine for virtual community activities dissemination).

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REFERENCES

1] G. Vitillaro and A. Laganà – vherla: a virtual molecular science data center allocated on the garr cloud, Virt&L-COMM 2018-12-11

2] A. Laganà, O. Gervasi, S. Tasso, D. Perri, F. Franciosa, The ECTN Virtual Education Community prosumer model for promoting and assessing chemical knowledge, Lecture notes comput science 10964, 533-548 (2018).

3] I. Nonaka, H. Takeuchi, The Knowledge-Creating Company, Oxford University Press (1995).