THE MOLECULAR SIMULATOR ENABLED CLOUD SERVICES: MOSEX

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Leveraging the progress made by D23 METACHEM [1] and D37 GRIDCHEM [2] Actions within COST [3] and by the COMPCHEM VO [4] and the CMMST VRC [5] within the EGEE III [6] and EGI Inspire [7] EU initiatives, the Molecular Science (MS) community wishes to candidate itself for a collaborative project within the European Open Science Cloud (EOSC) [8] Pillar Initiative in order to overcome the current fragmentation of MS knowledge by sharing the outcomes of publicly funded research with minimal (or no) restriction. To this end a cloud platform was activated at the Dipartimento di Chimica, Biologia e Biotecnologia (DCBB) of the University of Perugia, and later extended to the CMS^2 Consortium [9] and its OpenStack cloud image (VHERLA) was implemented at the GARR Cloud [10] node of Palermo as a Virtual Data Center.

VHerla services are aimed to produce/discover data set(s) metadata querying, access/download data set(s), run/check/terminate experiment/computations using downloaded data, intermediate data, incorrect/useless runs, preserve**:** correct results for further use, support reproducibility of extremely large and streaming data when input data set(s) cannot be stored, annotate, curate, preserve produced data by cycling from raw measured data, to annotated experimental data and metadata for a better re-use, to simulation based formulation of mechanism and observables for consistency checks. The cycle is repeated to a satisfactory convergence for validated availability in cloud.

MOSEX, the Molecular Simulator Enabled Cloud Services being implemented on VHerla focuses in particular on:

1. electronic structure and equilibrium molecular configuration properties for spectroscopy, synthesis, photovoltaic and photochemical processes studies;
2. classical and quantal reactive and non reactive efficiency studies for elementary and complex detailed kinetics;
3. structure-property relationships studies for pharmacological and biological systems;
4. management of distributed repositories and databases for chemical systems: e.g. IOCHEM-BD and CHEMCONNECT;
5. dissemination, publication and assessment of molecular knowledge: e.g. EChemtest® e-tests, VIRT&L-COMM e-magazine, G_LOREP Learning objects.

References

1] https://www.cost.eu/actions/D23/#tabs|Name:overview/
2] https://www.cost.eu/actions/D37/#tabs|Name:overview/
3] https://www.cost.eu/
4] https://www3.compchem.unipg.it/compchem/
5] https://wiki.egi.eu/wiki/Towards_a_CMMST_VRC),
6] https://cordis.europa.eu/project/rcn/87264/factsheet/en
7] https://www.egi.eu/about/egi-inspire/
8] https://ec.europa.eu/research/openscience/index.cfm?pg=open-science-cloud
9] http://www.cms-2.org/index.php
10] https://www.eosc-portal.eu/

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