THE MOLECULAR SCIENCE COMMUNITY FOR **OPEN SCIENCE**

Antonio Laganà, MASTER-UP srl, Perugia (IT)

In January 2016 during the Annual Joint Programming Conference of the DG Research & Innovation of the European Commission Commissioner Moedas quoted from a speech of June 2015 the sentence

"There is a revolution happening in the way science works. Every part of the scientific method is nowadays becoming an open, collaborative and participative process" Speech at "A new start for Europe" Conference, 22 of June, 2015, Brussels

Open Science is, in fact, part of an **Open approach** to the process

Investigating-> Discovery-> Analysis-> Writing-> Publishing-> Outreach-> Assessment

that is an important pillar of the modern European approach to societal problems.

The resulting **European Open Science Agenda** http://ec.europa.eu/research/openscience/ is articulated in 5 broad policy action lines:

Fostering and creating incentives for Open Science (establish an Open Science policy platform, promote best practices and citizen science),

Removing barriers for Open Science (propose EU code of conduct, develop proper metrics, address open data availability and skills, enhance data professional reuse)

Mainstreaming and further promoting Open Access policies (extend the H2020 Open access pilot, develop EU guidelines for IPR and related data management),

Developing an Open Science cloud (develop common interfaces, data standards, maintenance, interoperability and sustainability)

Embedding Open Science in society to make science more responsive to societal and economic expectations (establish an Open Science Cloud for data, protocols and methdologies)

The strategic role of the above mentioned **European Open Science Cloud** relies on:

-the creation of cost effective, privacy and IPR conscious virtual environments allowing EU researchers to store, manage, analyse and reuse data

-the federation of existing and emerging data infrastructures

-the driving interdisciplinary data to knowledge and innovation for societal needs

Among other activities of the H2020 programme "Science with and for Society" (2016-17) like proposals for establishing Expert groups on European Open Science cloud, implementing the Open Science Monitor, training on Open Science the following ones:

•Call for proposals: 'Joint open science initiatives'- SWAFS WP 2017, EUR 3 million

•Call for proposals: 'Piloting the European Open Science Cloud'- INFRA WP 2016, EUR 10 million

•Establishing expert groups on 'rewards for Open Science' and 'changing business models for publishing'

can be interesting opportunities for the Chemistry, Molecular, Materials Science and Technologies (CMMST) Virtual Research Community (VRC) and the COMPCHEM Virtual Organization (VO). For this reason we submitted the following MOSEX expression of interest:

ISSN: 2279-8773

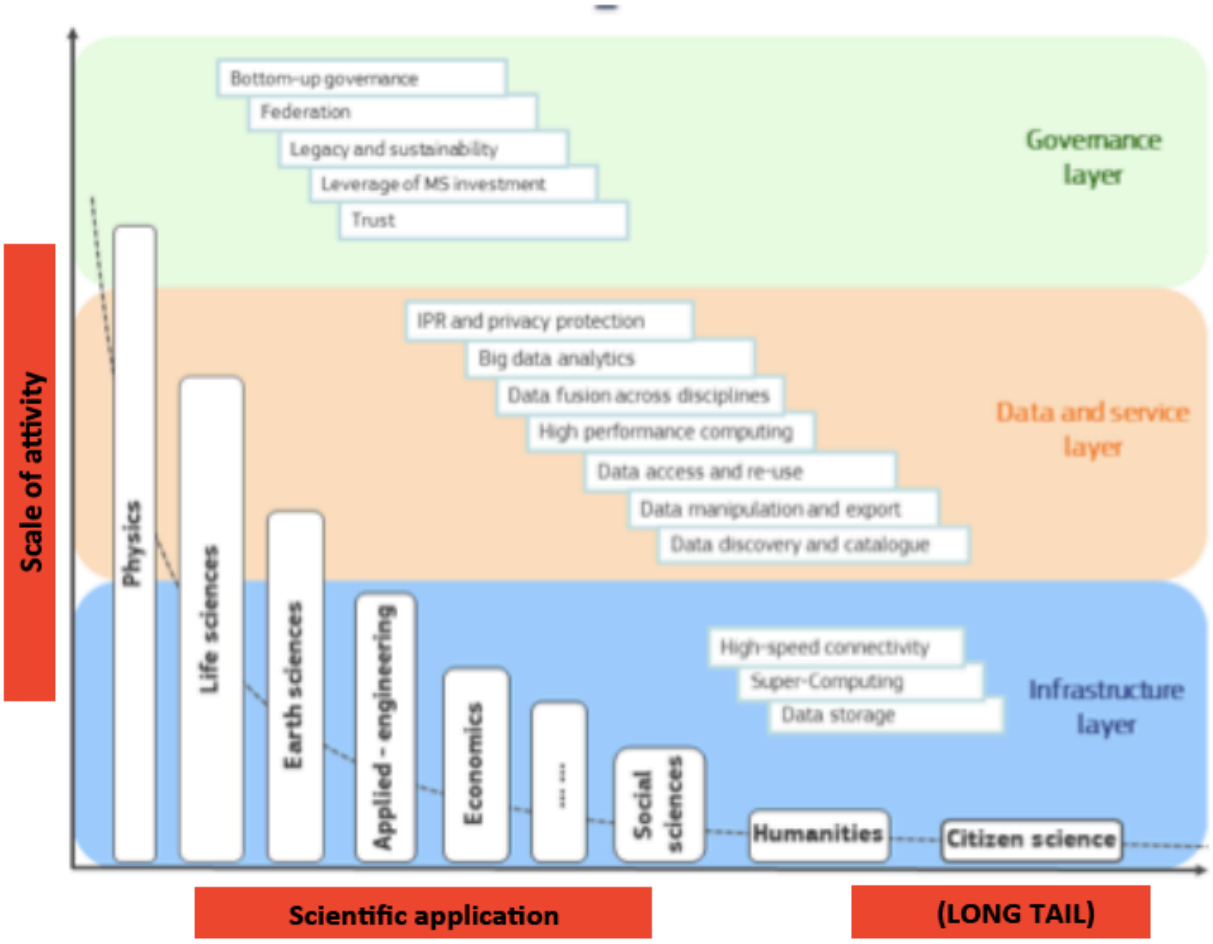
Science Demonstrator Title	MOSEX (Molecular Simulators Enabling Cloud Services)
Contact Name(s) and Organisation(s)	Antonio Laganà, Master-UP srl, Perugia (IT) Sonja Herres Pawlis, Technische Hochschule, Aachen (D) Ernesto Garcia, Universidad del Pais Vasco, Vitoria (E) Edward Blurock, Blurock Consulting, AB (SW) Osvaldo Gervasi, University of Perugia (IT) Antony K Smith, European Chemistry Thematic Network (B)
Demonstrator Description	- MoSgrid (HPC supercomputing user Network for Molecular science electronic structure Ab initio calculations) - GeMS Grid Empowered Molecular Simulator (Distributed calculations of the efficiency of chemical processes for aerothermodynamics, plasmas, energy storage, etc.) - GLOREP (Distributed repository for Molecular sciences Learning objects) - ECHEMTEST^{+} (Cloud based evaluator of chemical knowledge)
Science Area	Computational Chemistry
Relationship to European/national research organisations, Research Infrastructures, & equivalent Initiatives	CMMST Virtual Research Community EGI (NL) Computational Chemistry Division of EUCHEMS (B) European Chemistry Thematic Network (B) Connection is also made with CINECA for computing time and data storage as well as with the Oklahoma Supercomputer Center in Norman for computing, networking resources and societal applications (climate and energy in particular)
Broader Impact	MOSEX has the following unique characteristics: - Produces both structural data for existing (and, possibly, new) chemical compounds and efficiency parameters for elementary (and composite) chemical processes in the field materials, energy, health, technological processes, etc. - Reuses produced chemical data to perform simulations generating innovation at higher level of complexity in the above mentioned fields

ISSN: 2279-8773

	- Leverages on resulting chemical knowledge to teach, train and evaluate people in education and professions
Data Class & Description	The present use of MOSEX is entirely open although with access regulated by the different sub-communities
Data Challenges	The different levels of networked production, reuse and educational exploitation of data are coordinated with the support of the three European entities mentioned above (EGI, EUCHEMS, ECTN) at the different levels of - EGI: resource provision, integration, findability and accessibility, - EUCHEMS: chemistry societal and innovation finalization and reusability - ECTN: educational, training and dissemination The participation of some SMEs is important for providing sustainability to the reuse of the data and knowledge produced. Among the tools produced and used for that purpose are the networking media of EGI, the e-magazine VIRT&L COM of Master-UP as well as the Newsletters of EUCHEMS and ECTN.
Current Analysis Status	The science demonstrators already working are those of MosGrid and the components of GEMS operating on grid. Some of them are being adapted for cloud operations. In addition under way is the implementation on cloud of GLOREP and ECHEMTEST+
Compute & Data Resources	Compute resources are provided by the project partners through EGI Federated infrastructures, MosGrid, CINECA and the Oklahoma Supercomputer center which will be cooperating in the EOSC pilot. The same infrastructures will provide data storage eventually also through EUDAT
Use of Open Science services	The outcomes of the project will be the production of datasets for combustion, aerothermodynamics and other computational chemistry sectors. Regular publications will be made on the VIRT&L-COMM e-magazine that belongs to the open journal system as well as on the most outstanding journal of chemical sciences and technologies. Workflows and Meta-workflows produced will also be freely used and circulated among the members of the community. Also Data produced will be to a large extent of free usage by the members of the related communities as part of an Open Science model by the demonstrator.

ISSN: 2279-8773

for the inclusion of Molecular Science simulators Enabling Cloud Services within the being assembled H2020 proposals as illustrated in the figure below.



ISSN: 2279-8773