THE "OPEN MOLECULAR SCIENCE CLOUD" WORKSHOP REPORT

Antonio Laganà, CNR ISTM - UOS Perugia, 06100 Perugia, Italy

1. BACKGROUND

On Agust 29, 2018, the Board of the CTC (Computational and Theoretical Chemistry) Division of EuChemS during its meeting in Liverpool deliberated to hold the CTC 2019 European Conference (EUCO 2019) in Perugia (IT) from Sept 1 to Sept 5 (to be chaired by A. Laganà (AL)) and have a special focus on Open Molecular Science Cloud (OMSC)). On the same day, at the Symposium "*Methods of computational chemistry: challenges and new developments"* held in the same place, D. Crawford (DC) presented the activities of the US Molecular Sciences Software Institute (MolSSI) having also a strong OMSC connotation. During the discussion that followed, AL proposed to organize a joint OMSC workshop by side to the CTC EUCO 2019.

On Apr 8, 2019 the MolSSI Board of Directors approved the application submitted by AL and deliberated to financially support the joint OMSC workshop and the participation of up to 7 Early Stage Researchers (ESR)s from US.

2. THE GENERAL SCHEME

The general timetable of the Perugia CTC EUCO 2019 is given in Figure 1 below (see the

	Monday September 2nd		Tuesday September 3rd			Wednesday September 4th		Thursday September 5th	
8:20 - 09:00 9:00 - 9:40 9:40 -10:00 10:00 -10:20 10:20 -10:40 10:40 -11:00	Registration **K1: General theory issues (P. Szalay)** (chair: A. Fernandes) O1: F. Keshavarz O2: F. Sessa O3: M. Springborg O22: L. Turi	9:00 - 9:40 9:40-10:00 10:00-10:20 10:20-10:40 10:40-11:00	**K4: Electronic structure and strong correlation (W. Klopper)** (chair: P. Reinhardt) O12: M Yañez O9: G. Aucar O10: N. Bandeira O27: F. Palazzetti	**TCCM Workshop** (chair: M. Alcami) 9:40-10:00 Introduction: M. Alcami 10:00-10:15 TCCM1: P. Rosales 10:15-10:30 TCCM2: J. Lubani 10:30-10:45 TCCM3: E. Vos 10:45-11:00 TCCM4: D. Barreiro	9:00 - 9:40 9:40 -10:00 10:00 -10:20 10:20 -10:30 10:30 -10:50	**K7: HPC for Photochem. and MD (D. Smith)** (chair: H. Lüthi) O19: J. Alba O20: S. Caputo RT1: I. Conti O21: D. Escudero	8:20 - 09:00 9:00 - 9:20 9:20 - 9:40 9:40 - 10:00 10:00 - 10:20	**K10: Biochemistry (P. Fernandes)** (chair: Z. Courna) O28: P. Sánchez Murcia O29. I. Shamovsky O30: R. Silaghi Concluding Remarks 09:00 - 09:40 The VHERLA Cloud Platform: G. Villiaro 09:40 - 10:20 Photovoltaic Calculations on VHERLA: E Mosconi
11:00-11:20	**Coffe Break**							10:20	Dispersal. Bus to Accademia delle Scienze and Tiburtina Station in Rome
11:20-12:00 12:00-12:20 12:20-12:40 12:40-12:50 12:50-13:00	**K2: Solid state and Materials (S. Evangelisti)** (chair: M. Yañez) O4: L. Adamska O5: E. Ronca RT4: A. Solé-Daura RT5: A. Solom-Català	11:20-12:00 12:00-12:20 12:20-12:40 12:40-13:00 13:00 -13:10	**K5: Machine learning, Cheminformatics QSAR (G. Cruciani)** (chair: T. van Mourik) O32: K. Nikolic O8: F. Abdelmounaim O11: M. Coden RT2: J. Jasper	11:20-11:35 TCCM5: E. de Aragao 11:35-11:50 TCCM6: J. Cerda 11:50-12:05 TCCM7: E. Remesal 12:05-12:20 TCCM8 J. Delgado 12:20-12:35 TCCM9 L. Vázquez 12:35-13:00 Final discussion	11:20 - 12:00 12:00 - 12:20 12:20 - 12:40 12:40 - 13:00	**K8: Force Fields (J. P. Piquemal)** (chair: R. Sayós) O23: S Ruiz-Barragan O24: T. Beu O25: J. Brandão		
13:00-14:30	**LUNCH**								**OMSC Project Accademia delle Scienze (Rome)**
14:30-15:10 15:10 - 15:30 15:30 - 15:40 15:40 - 16:00 16:00 - 16:20	**K3: Catalysis (R. Sayós)** (chair: K. Nikolic) O6: B. Klumpers RT3: I. Man O7: T. Marforio O31: R. Góra	14:30-15:10 15:10 - 15:30 15:30 - 15:50 15:50 - 16:10	**K6: Spectroscopy (C. Cappelli)** (chair: P. Szalay) O13: P. Beaujean O14: S. Jähnigen O15: M. Mendolicchio	**Training Event on Learning Objects Repository: S. Tasso **Training Event on Echemtest: O. Gervasi	14:30-15:10 15:10 - 15:30 15:30 - 15:45 15:45 - 16:00 16:00 - 16:15 16:15 - 16:30	**K9: The EU Open Science Cloud Pilar Project (F. Ruggieri)** (chair: S. Kast) O26: S. Rampino RT6- MolSSI: S. Seritan RT7- MolSSI: V. Cruzeiro RT8- MolSSI: G. Jones RT9- MolSSI: S. J. Maat	14:00-14:10 14:10 - 14:50 14:50 - 15:30 15:30 - 16:10	Welcome by the President of the Accademia delle Scienze F. Ruggieri A. Laganà D. Smith
16:20-18:30	Coffee break and Poster Sessions: 1(odd) and 2 (even)	16:10 - 16:30 16:30-16:50 16:50-17:10 17:10-17:30	Coffee break O16: A. Puglisi O17: M. Swart O18: A. Fouda	Coffee break **Dissemination event of Echemtest: S. Tortorella	16:10 - 16:30 16:30 17:00-19:00	Coffee break Walk to the "Galleria nazionale dell'Umbria" Tour at the "Galleria nazionale dell'Umbria"	16:10 - 16:50 16:50 - 17:30 17:30 - 18:10 18:10- 19:10	J. Piquemal E. Blurock C. Bo General Discussion (to be continued on Friday 6th, 09:00-11:00)
19:00 - 20:30	Welcome Party (University Main Quadrangle)	17:30-	CTC board meeting	GEM-TCCM project meeting	20:00-23:00	Conference Dinner	19:10	Buffet Dinner and informal work group discussion

* These events will be held at the Dipartimento di Matematica e Informatica, Via Vanvitelli 1, Room C3
† This event will be held at the Dipartimento di Chimica, Biologia e Biotecnologie, Via Elce di Sotto 8, Room H

Fig. 1 – SCHEME OF THE OMSC WORKSHOP ACTIVITIES

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http://www.dcbb.unipg.it/euco2019 web site for details and abstracts).
The scheme of Fig. 1 provides the following information:
♦ **Time schedule** (in the light blue columns)**,**
♦ **Keynote and contributed shared lectures delivered in Perugia** (in the first next rhs white column from Monday to Thursday morning),
♦ **Parallel training activities run in Perugia (**in the second next rhs white column of Tuesday and of the morning of Thursday),
♦ **MOSEX (Molecular Open Science Enabled Cloud Services) project development sessions of the OMSC workshop held at the Accademia delle Scienze in Rome** (on Thursday afternoon and Friday morning).

3. KEYNOTE AND CONTRIBUTED CTC ORAL PRESENTATIONS

♦ The **keynote lectures delivered on Monday September 2** were:
•*P. Szalay* "General Theory Issues",
•*S. Evangelisti* "Clifford Boundary Conditions for Periodic Systems",
•*R. Sayos* "First Principles-based Kinetic Monte Carlo Simulations in Heterogenous Catalysis: Applications to Water-gas Shift Reaction with Several Catalysts".
These keynote and the related contributed oral presentations illustrated the main theoretical and computational subjects of the conference. The oral presentations were followed in the evening by two poster sessions and by the welcome party held at the University main quadrangle. While walking to the party, a visit was paid to the Mosaic of Orpheus playing the Lyra to attract a series of animals known to Romans (the floor of the Roman bath located on the basement of the Department of Chemistry, Biology and Biotechnology of the University) and to the Etruscan arch marking the access to the ancient town centre.

♦ The **keynote lectures delivered on Tuesday September 3** were:
•*W. Klopper* "Bethe –Salpeter Correlation Energies of Atoms and Molecules",
•*G. Cruciani* "Computational Chemistry and Artificial Intelligence",
•*C. Cappelli* "Full Atomistic Embedding Approaches for the Computational Spectroscopy of Complex Systems: Status and Perspectives".
These keynote and the related contributed oral presentations switched the emphasis of the communications towards more OMSC oriented subjects.

♦ The **keynote lectures delivered on Wednesday September 4** were:
•*D.G.A. Smith* (from MollSSI) "Advancing the Computational Molecular Sciences through Better Theory and Better Software",
•*J.-P. Piquemal* "Scalar Polarizable Molecular Dynamics using Tinker-HP",
•*F. Ruggieri* "European Open Science Cloud and the EOSC-Pillar Project".
These keynote and the related contributed (the latter mainly from MollSSI grant holders) oral presentations were centred on OMSC technologies.

♦ The **keynote lecture delivered on Thursday September 5 morning** was:
•*P.A. Fernandes* "Dynamic and Chemical Disorder in Enzymatic Reaction Mechanisms".
The keynote and the related contributed oral presentations dealt with computational applications to biological complex systems.

4. PARALLEL OMSC TRAINING EVENTS

♦ The **first OMSC parallel training event was run on Tuesday September 3 morning** by *M. Alcamì,* (the coordinator of the Theoretical Chemistry and Computational Modelling (TCCM) Erasmus mundus Master). During the training event the TCCM Master students discussed their research work and singled out the knowledge relevant to the forming of the common European contents of the Master useful to assemble Questions & Answers (Q&A)s of the corresponding Echemtest® level 4 library of the de facto standard of the European Chemistry Thematic Network (ECTN).

♦ The **second OMSC parallel training event was run on Tuesday September 3 afternoon** by *S. Tasso* (the author of the used OMSC distributed repository management software G-Lorep) at the Department of Mathematics and Computer Science of the University of Perugia with the participation of *A. Laganà* (the author of the Learning Objects (LO)s relevant to Chemical Reactions used for that purpose) and *M. Alcamì*. During the training event the participants were trained on searching, downloading, modifying and re-using the G-Lorep LOs of the Molecular Science (MS) community.

♦ The **third OMSC parallel training event was run on Tuesday September 3 afternoon** (to follow the second one) by *O. Gervasi* (the author of the used OMSC e-test manager LibreEOL) at the Department of Mathematics and Computer Science of the University of Perugia with the participation of *A. Laganà* and *M. Alcamì*). During the training event the participants were taught how to manage the Echemtest® Self Evaluation Sessions (SES)s on a given Test Centre (TC) by defining the e-test takers, choosing the desired library, working out the e-test outcomes, etc.

♦ The **fourth OMSC parallel training event was run on Tuesday September 3 evening** by *S. Tortorella* (the coordinator of the Italian Chemical Society committee for Chemistry dissemination) at the Department of Mathematics and Computer Science of the University of Perugia on how to disseminate Chemistry knowledge using Echemtest® sessions on "Chemistry for everyday life" a library developed by *A. Michalack* and *K. Szczeponek* at the University of Krakow.

♦ The **fifth OMSC parallel training event was run on Thursday September 5 morning** by *G. Vitillaro* (the designer and implementer of VHERLA, the cloud image of the University of Perugia infrastructure as a virtual data centre on the GARR national cloud) and *E. Mosconi* (the author of the VHERLA cloud application to Photovoltaics) at the GIO Hotel using the University-CNR ISTM VHERLA cloud infrastructure for MS calculations".

5. THE MOSEX PROJECT DEVELOPMENT AT ACCADEMIA DELLE SCIENZE

♦ The **first MOSEX project development session was run on Thursday September 5 afternoon** (starting from 14:00 after a bus transfer from Perugia) at the Accademia delle Scienze in Rome according to the following programme:
- *V. Aquilanti* "Welcome from the President of the Accademia",

- *F. Ruggieri* "The European Open Science Cloud Pillar Project",
- *A. Laganà* "MOSEX (Molecular Open Science Enabled Cloud Services)",
-*D.G.A. Smith* "The MolSSI Quantum Chemistry Archive Project",
-*J.-P. Piquemal* "Cloud Molecular Science Services on Tinkertools Infrastructure",
-*E. Blurock* "Cloud Services for Reaction Modelling",
-*C. Bo* "IOCHEM-BD: Tools for Open Access Publishing and much more"

At the end of the presentations, a general discussion chaired by *A. Laganà* was held. In addition to the above listed speakers, *A. Lombardi, N. Faginas Lago* (University of Perugia), *Z. Cournia* (Academy of Athens), *A.M. Paci* (CNR Rome), *S. Rampino* (Scuola Normale Pisa), *P. Szalay* (Eovtos University Budapest) took part to the discussion.

The outcomes of the discussion were then summarized by AL as follows:
The presentation "The European Open Science Cloud Pillar Project" (EOSC-Pillar) delivered by F. Ruggieri singled out the fact that the EOSC-Pillar is a project concerned with central Europe (Italy, France, Germany and Austria) and that, by the end of the year 2020, a call for subprojects will be opened to user communities of those countries wishing to produce and offer cloud services. Accordingly, there will be enough time to design the fine articulation of MOSEX (Molecular Open Science Enabled Cloud Services) and of the cloud services to offer by leveraging different levels of participation to the subproject (internal to the Pillar, among other EU areas and outside EU). As a result, it was decided to continue the discussion on Friday morning by allocating further time for short presentations by the US ESRs still as part of the joint general discussion without having separate work group activities.

♦ The **second MOSEX project development session was run on Friday September 6 morning** (starting from 9:00)

Activities were started with the presentations of:
-*V.W.D. Cruzeiro* (Supercomputer Center San Diego) on massive use of networked supercomputers for accurate estimates of molecular properties,
-*G. Jones* (University of Tennessee Knoxville) on the development of recyclable wavefunctions for accurate evaluation of different molecular properties,
-*J. Maat* (University of California Irvine) on the evaluation of quality evaluation of services and validation of software
-*S. Seritan* (Stanford University) on providing massive cloud computing of electronic structure, artificial intelligence techniques and basic computational Chemistry know how

At the end of the presentations the general discussion was started again on the issues raised with the participation of *D.G.A. Smith*, *J.-P. Piquemal*, *E. Blurock*, *C. Bo*, *Z. Cournia* and *A.M. Paci*.

The discussion was at the end summarized by AL as follows:
In order to get ready for the next year EOSC-Pillar call for subprojects, the participants to the OMSC Workshop commit themselves to contribute to the offering, within the MOSEX project, of the following cloud services:
1. **electronic structure and equilibrium molecular configurations** with particular focus on the MolSSI Quantum Chemistry Archive supported by D. Smith,
2. **reactive and non reactive dynamics studies** with particular focus on molecular dynamics services on the Tinkertools infrastructure supported by J-P Piquemal**,**
3. **design of bioactive molecules** for pharmacological and biological systems with particular focus on cloud services supported by Z. Cournia and G. Cruciani,

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4. **management of distributed repositories** like the IOCHEM-BD (materials) under the coordination of C. Bo and the CHEMCONNECT (combustion) under the coordination of E. Blurock,
5. **dissemination, publication, evaluation and validation of molecular knowledge** through Glorep (LOs for supporting the learning of chemical competences), EChemtest® (e-tests for assessing chemical competences) and VIRT&L-COMM (e-magazine for editorial activities of the MS community) under the coordination of *A. Laganà*.
A tentative road map for the writing of the first draft of the subproject proposal was suggested and the participants were asked to send to AL the materials produced for the workshop before circulating it.

6. PARTICIPANTS' STATISTICS AND TECHNICAL SUPPORT

♦**The pdf file "conference_participants" lists** the names of the CTC EUCO 2019 participants together with their affiliations. Related fields of scientific activities are described in the already mentioned book of abstracts. Altogether, 74 scientists attended the above mentioned activities (plus 10 invited keynote lecturers and 5 local organizers) of which 20 females.

♦**Country per cent participations are**: Italy 25%, Spain 19%, Germany 12%, France 6%, USA 5%. Three people attended from Portugal and Romania. More scattered attendance (one or two participants) was from Bulgaria, Czech Republic, Hungary, Sweden, United Kingdom, Argentina, Algeria, Austria, Bulgaria, Croatia, Finland, Netherlands, Poland, Quatar, Serbia.

♦**Specialists' support** was given by 2 colleagues of the Department of Mathematics and Computer Science of the University of Perugia, 2 colleagues of the Department of Chemistry, Biology and Biotechnology of the University of Perugia (plus 2 students), 2 colleagues from ISTM CNR of Perugia, 1 expert from Molecular Horizon srl, 2 experts from Master-UP srl. For the activities held in Perugia classrooms and facilities of the University of Perugia were used in addition to those of the Hotel GIO.

♦**The Department of Mathematics and Computer science infrastructural support** consisted in the use of the e-test computer room (and related technical support) registered as Test Center of EChemTest®, equipped with 35 computers and the cloud enabled version of LibreEol

♦**The CNR-ISTM unit and the Department of Chemistry, Biology and Biotechnologies of the University of Perugia infrastructural support** consisted in the use of VHERLA. Figure 2 shows the GARR Network hosting VHERLA as a virtual data centre.

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Fig. 2 – SCHEME OF THE GARR NETWORK HOSTING VHERLA

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