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MOLECULAR OPEN SCIENCE ENABLED CLOUD SERVICES (MOSEX) FOR CHEMICAL EDUCATION

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ABSTRACT
In this paper the Molecular Open Science Enabled Cloud Service (MOSEX) project developed in our laboratory in collaboration with other European academic and research institutions is presented. The particular application considered here is the determination and validation of the reaction parameters of elementary chemical processes through an iterative synergistic use of theory, computations and experiments for use in education. The cloud image (VHERLA) of the computational infrastructure of MOSEX implemented at the GARR Cloud node of Palermo as a Virtual Data Centre is also illustrated in order point out the type of support used for the Learning Objects and the On Line Courses of the European Chemistry Thematic Network (ECTN).

1) PREAMBLE – The high level of operability achieved by the European Chemistry Thematic Network (ECTN) [1] EChemTest® [2] activities has increasingly required the support of high level educational materials to help students in developing a rigorous approach to basic computational chemistry concepts. To this end, in September 2019 (a couple of months before presenting the conclusions of ECHEMTEST+ (the project aimed at proving the sustainability of the EChemTest® activities) before the ECTN AC in Rome, the 12th European Conference (EUCO) of the Computational and Theoretical Chemistry (CTC) division of EuChemS [3] was held in Perugia by gathering together (see Table 1)
a) (Monday-Tuesday) 40 Parallel short presentations of the research work (**TCCM 1-40**) carried out by the students of the Theoretical Chemistry and Computational Modelling (TCCM) European Joint Doctorate (EJD) [4],
b) (Monday-Thursday) 10 Keynote presentations (**K1-K10**) from invited speakers followed by 20 contributed selected oral presentations (**O1-20**), 40 selected students' research telegrams (**RT1-RT40**) and 2 afternoon joint coffee break-poster sessions,
c) 2 Parallel training sessions on Learning Object repositories and on EChemTest® (Tuesday afternoon) and 1 on Cloud computing (Thursday morning).
d) 1 OMSC workshop held at the Accademia Nazionale delle Scienze dei XL [5] in Rome (Thursday afternoon after a chartered bus transfer to Rome with packed lunch on board and Friday) jointly organized with the Molecular Sciences Software Institute (MolSSI) [6].

2] THE IMPLEMENTATION OF MOSEX ON THE CLOUD - The focal point of the workshop was, indeed, the discussion of the proposal of launching the Molecular Open Science Enabled Cloud (MOSEX) project aimed at establishing a cloud service for science and education services based on high level evaluations of the efficiency parameters of chemical processes (e.g. cross sections and rate coefficients). As mentioned above, in order to implement MOSEX an international team of molecular scientists was by activating links with several research centres and consortia of research data infrastructures for molecular science (MS). At the same time an OpenStack platform (Herla) we established at our CNR Institute including the Department of Chemistry, Biology and Biotechnology (DCBB) of the University of Perugia. Later its cloud image (VHERLA) was implemented at the GARR Cloud node of Palermo [7] as a Virtual Data Centre to the end of establishing a cloud service for the validation of the value of the efficiency parameters of elementary chemical processes via an iterative synergistic use of theory and experiments.

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	Monday 02		Tuesday 03		Wednesday 04	Thursday 05
08:20-09:00	REGISTRATION & OPENINGS					K10: Biochemistry (P. Fernandes)
09:00- 09:40	K1: General theory issues (P. Szalay)		K4: Electronic structure and strong correlation (W. Klopper)		K7: HPC for Photochem. and MD (D. Crawford)	O19-O20
09:40-10:00	O1	TCCM1-2	O7	TCCM 25-26	O13	RT37-RT38
10:00-10:20	O2	TCCM 3-4	O8	TCCM 27-28	O14	RT39-RT40
10:20-11:00	RT1-RT4	TCCM 5-8	RT13-RT16	TCCM 29-32	RT25-RT28	GEN. CTC ASSEMBLY
11:00-11:20	coffee break					
11:20-12:00	K2: Solid state and Materials (S. Evangelisti)		K5: Machine learning, Cheminformtics QSAR (G. Cruciani)		K8: Force Fields (J. P. Piquemal)	Dispersal Rented bus to ACCADEMIA XL and Tiburtina train station (Rome) with train connection (maximum 25 seats) (to book)
12:00- 12:20	O3	TCCM 9-10	O9	TCCM 33-34	O15	
12:20-12:40	O4	TCCM 11-12	O10	TCCM 35-36	O16	
12:40-13:20	RT5-RT8	TCCM 13-16	RT17-RT20	TCCM 37-40	RT29-RT32	
13:20- 14:30	LUNCH					---------- FROM 2 PM ON PROJECT MEETING OPEN MOLECUL. SCIENCE CLOUD at ACCADEMIA XL (ROME)
14:30- 15:10	K3: Catalysis (R. Sayós)		K6: Spectroscopy (C. Cappelli)	E-tests, Learning Objects	K9: Open Molecular science, cloud, Distr. computing (F. Ruggieri)	* Link to programme
15:10-15:30	O5	TCCM 17-18	O11	training event ON LO REPOSITORY	O17	
15:30-15:50	O6	TCCM 19-20	O12		O18	
15:50-16:10	RT9-RT12	TCCM 21-24	RT21-RT24		RT33-RT36	
16:30- 18:30	coffee break + poster session 1		coffee break + poster session 2 + CTC Board meeting	Training on Echemtest	coffee break + poster session 3 CTC Board (meeting contin.)	
18:30-20:30	Welcome Party		TOURS: National gallery (to book)		CONF. DINNER (to book)	

TABLE 1: Timetable of the 12th European Conference (EUCO) of the Computational and Theoretical Chemistry (CTC) division of EuChemS.

3] THE MOSEX VHERLA SERVICES - VHerla MOSEX services are specialized on:

a) producing/discovering/access/download,
b) run/check/terminate improper results/validate,
c) annotate/curate/preserve,

data inherent to elementary molecular processes when satisfactorily converged.
Initial activities in this respect trace back to D23 METACHEM [8] and D37 GRIDCHEM [9] Actions of COST [10] and within COMPCHEM VO [11] and CMMST VRC [12] activities of the EGEE III [13] and EGI Inspire [14] EU initiatives. In VHerla the services have been evolved towards an insertion into the European Open Science Cloud (EOSC) [15] Pillar Initiative. This is aimed at providing OMSC with the ideal cloud breath necessary to overcome the current limits and fragmentation of molecular science research and technologies in the field.
More precisely, MOSEX is aimed at gathering together the competences of its members in:
1. electronic structure and equilibrium molecular configuration properties methods and computational techniques for spectroscopy, synthesis, photovoltaic and photochemical processes;
2. quantum, quantum-classical and classical methods and computational techniques for reactive and non reactive efficiency studies for elementary and complex detailed kinetics;
3. structure-property relationships approaches to the determination of the properties of more complex (combustion, materials, energy conversion, etc.) systems;
4. management of distributed repositories and databases for chemical systems [16-18];
5. dissemination, publication and assessment of molecular knowledge: e.g. EChemtest® e-tests, VIRT&L-COMM e-magazine, G_LOREP Learning objects (LO) repository [19].

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3] THE MOLECULAR DYNAMICS AND CHEMICAJ REACTIVITY LEARNING OBJECTS – Among the dissemination, publication and assessment of molecular knowledge services mentioned above, we focus in this section on the description of some educational materials developed for the TCCM EJD and implemented as LOs aimed at helping the EChemTest® test takers of the Computational Chemistry level 4 Library of Questions and Answers (Q&As). More specifically the LOs have been designed according to the guidelines of the book "Chemical reactions: basic theory and computing" [20] based on the concept of micro-granularity adopted for the LOs accessible by the users at the Glorep repository [21] at https://general.glorep.org. The sequence of the implemented LOs (not yet completed) is:
LO1.1) From kinetics to bi-molecular collisions
LO1.2) Classical mechanics of two particle collisions (positions and momenta).
LO1.3) Classical mechanics computational methods: merits and limits.
LO2.1) Quantum two body systems: analytical methods.
LO2.2) Quantum two body systems: numerical methods.
LO3.1) The quantum treatment of few body systems.
LO4.1) Advanced concurrent computing technologies for modelling molecular processes.
LO5.1) Few body systems: a case study of the grid empowered molecular simulator.
LO5.2) Many body systems: back to classical methods.
LO5.3) Modern technologies and new applications.

4] INTERNUCLEAR DISTANCE VERSUS BOND ORDER REPRESENTATIONS – A key problem of the treatment of reactive processes described in the above mentioned LO6 is the formulation of a proper "process coordinate" suited to describe the evolution of the molecular system from the reactant geometry to the desired product one. Commonly used representations of molecular processes are those given in terms of internuclear distances (r_{AB} for the pair of the A and B atoms). However, while such representation is satisfactory in the case of non reactive systems (i.e. when the initial and the final arrangements coincide) the use of internuclear distances (or even worse of the corresponding Jacobi coordinates) makes it difficult to provide a continuous analytical formulation of a realistic Potential Energy Surface (PES) and of the associated Minimum Energy Paths (MEP)s even for the most elementary reactive systems like the atom diatom ones. As a matter of fact, the use of the Bond Order (BO) variable n ($n=exp[-\beta(r-r_0)]$) to represent diatomic interactions (see the rhs panel of Fig. 1) is not only more compact than that of the internuclear distance r but is also ideally suited for polynomial expansions of relevant PESs and MEPs. Furthermore, as shown in Fig. 2, the use of the polar formulation of the Rotating BO (RBO) variables ($\rho^2=n_1^2+n_2^2$ and $\alpha=atan(n2/n1)$) allows the use of α as a uniquely and analytically defined **process coordinate** connecting two subsets of atoms of a three (generalizable to more atoms) molecular system that is extremely useful for dissemination, publication and assessment of molecular knowledge in EOSC services.

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A3] CTC di EuCHEMS
A4] Theoretical Chemistry and Computational Modelling European Joint Doctorate (https://cordis.europa.eu/project/id/642294)
5] https://www.accademiaxl.it/
6] https://molssi.org/

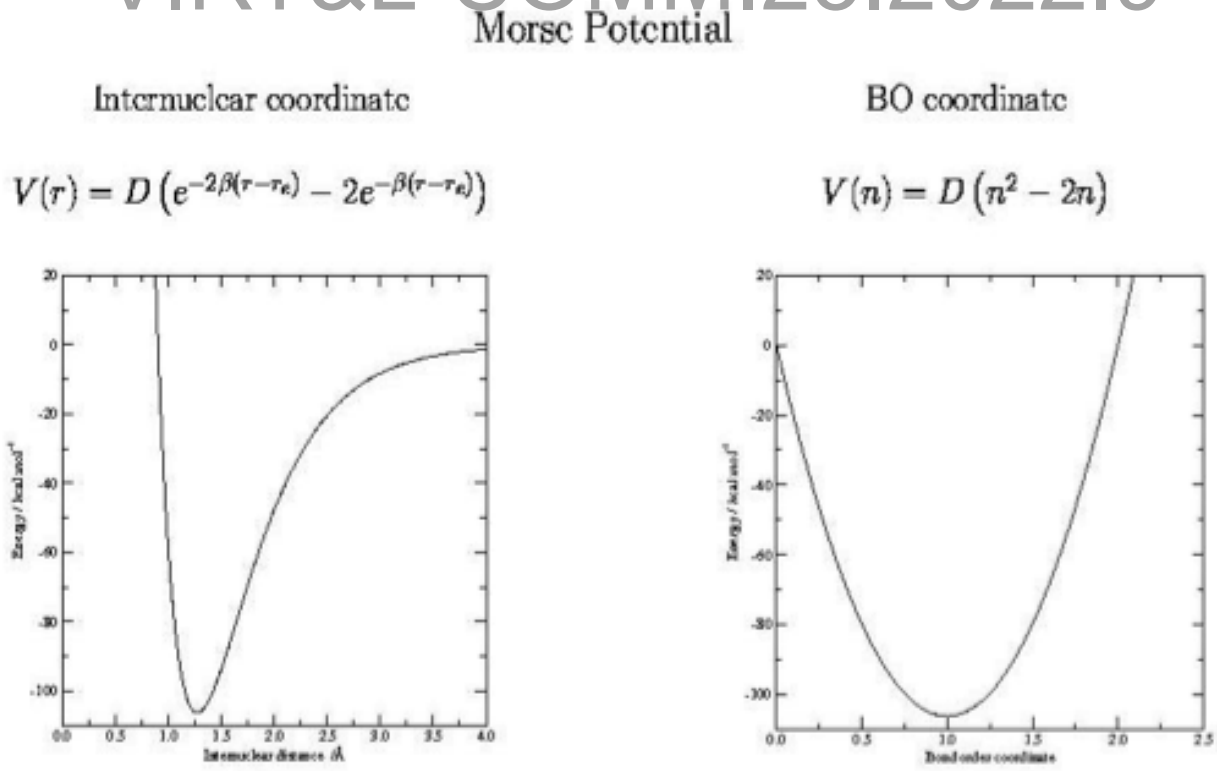

FIGURE 1: Sketch of a generic Morse potential plotted as a function of the internuclear distance r (lhs panel) and as a function of the corresponding BO variable n (rhs panel)

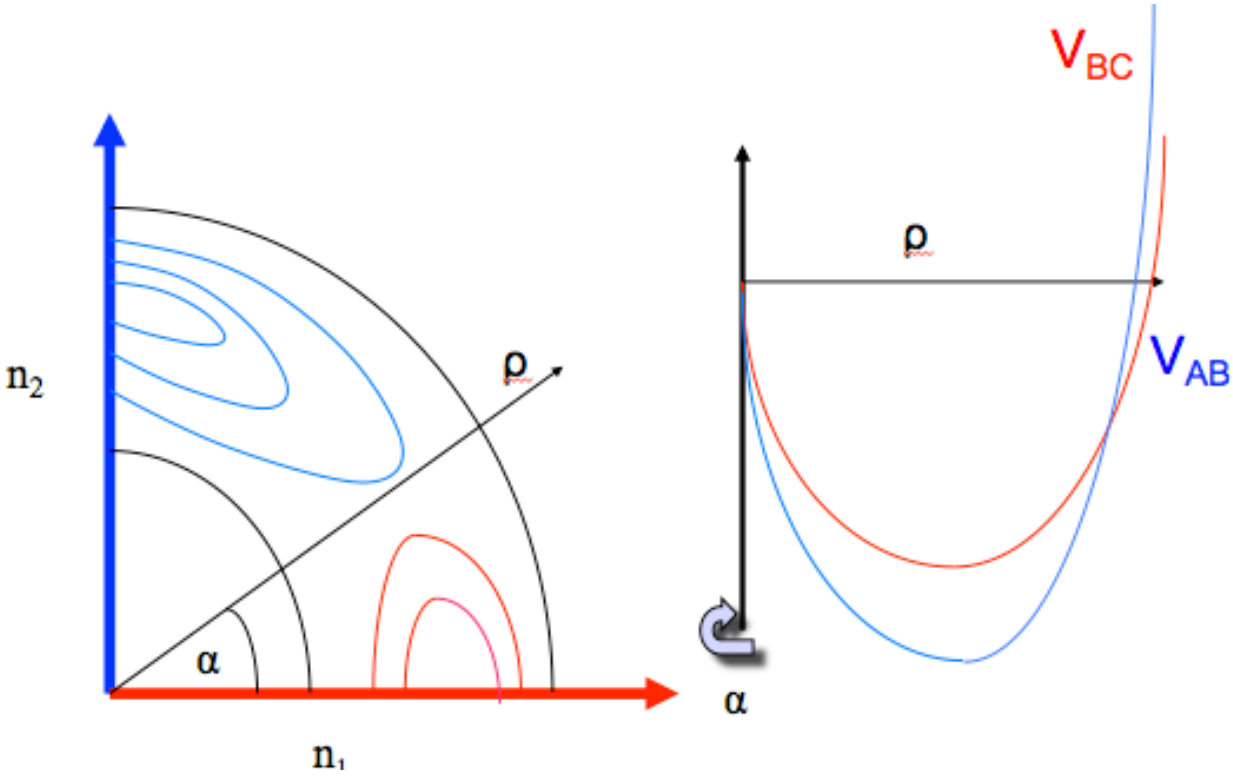

FIGURE 2: The RBO fixed collision angle representation of the isoenergetic contours (lhs panel) of a three different atoms PES for a generic atom-diatom A + BC → AB + C process (contours in red for the reactant side, in blue for the product one). The corresponding overlapped representation of the two asymptotic cuts of the PES is given in the rhs panel.

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