THE CLOUD FOR A FEDERATION OF REPOSITORIES OF MOLECULAR SCIENCE LEARNING OBJECTS

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1. INTRODUCTION

G-Lorep is a technology aimed at facilitating the sharing of Learning Objects (LOs) among a federation of repositories distributed among the members of a scientific community wishing to offer them to other community members and to get them further developed by their contributions. The G-Lorep network structure allows each website to work stand-alone and to use at the same time a central database to share LO information on the network. Accordingly, each federate contacts the central node when it needs to update the information of its own database. At present the central node is placed on a server physically located inside the University of Perugia in order to guarantee a direct control of the system and is specialized in Molecular Science (MS) applications [1, 2, 3, 4, 5, 6]. The specific set of LOs considered here is related to the MS theoretical and computational foundations of the teaching course on Mechanisms and Dynamics of Chemical Reactions (MDCR).

2. THE DEMAND FOR COOPERATIVE LEARNING OBJECTS: THE PROSUMER MODEL

The design of LOs supporting Chemistry e-learning was a central task of the European Chemistry Thematic Network (ECTN) and its Association. The ECTN project (later named ECTN-1) begun its activities in1996 by gathering together over 130 Chemistry departments. Its first commitment was the definition of the so called European Core Chemistry for which ECTN designed and developed a solid de facto standard for Organic Chemistry (OC), Physical Chemistry (PC), Inorganic Chemistry (IC), Analytical Chemistry (AC). During the next ECTN-2 project appropriate e-test Libraries of Questions and Answers (Q&A)s for General Chemistry 1 and 2 (GC1 for Schools and GC2 for Universities), Biological Chemistry (BC3), AC3, IC3, OC3 and PC3 at Bachelor level were assembled and implemented with the technical support of the Perugia and Vienna Universities.
The next funded ECTN-3 and ECTN-4 projects led to the establishing in the years 2003/2009 of the Virtual Education Community (VEC) committee that developed a higher level view of LOs based on multimedia and networked ICT technologies [7]. Next (during the 2009/2015 period of the EC2E2N-1 and EC2E2N-2 projects) work on LO support material of the MDCR course considered in the present paper was performed leveraging the collaborative user/producer model (that is often referred to as Prosumer) in MS education [5, 6].
The main features of the Prosumer collaborative scheme are: self-consistency, modularity, availability, reusability, interoperability with no locality and no (or extremely limited) ownership constraints of the knowledge as is typical of cloud services. These features are highly desirable as they give utmost thoroughness to information by prompting knowledge provision be flexibly aggregated and readily used (and re-used) thanks also to the association with metadata which allow to verify the existence and the properties of the information.

3. THE PATHWAY TO MDCR LOS

The design and development of MDCR LOs has leveraged the last twenty years of European projects. The first step was moved within the COST (www.cost.eu/) Action D23 (METACHEM, www.cost.eu/COST_Actions/cmst/D23 launched by the University of Perugia in the year 2000). D23 initiated the development of tools connecting the activities of different Molecular Science research laboratories (called Metalaboratories) operating on networked computers [8]. D23 was followed in the year 2006 by another COST Action (D37 | Grid Computing in Chemistry:

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GRIDCHEM) to the end of developing collaborative distributed grid solutions and paradigms for molecular science research [9]. This evolution line was then continued by the initiatives CMMST (a Virtual Research Environment), COMPCHEM (a Virtual Organization), GEMS (the Grid empowered molecular simulator) developed within the EGEE (Enabling Grids for E-sciencE) and the EGI (European Grid Infrastructure) European projects through specific MS computational applications [10, 11, 12]. In particular for our purpose they allow:

- the use of specialized web portals and workflows facilitating the production of data and know how as well as the re-use of the produced data and knowledge for education, training and further research

- the production and provision of computational means designed for dealing with molecular and materials disciplines when carrying out multi-scale treatments necessary to reproduce the observables of realistic systems in the area of energy, environment, materials, pharmacology, chemistry, biology, biotechnologies, medicine, etc.

For the specific purpose of the MDCR course a significant impulse was given by the Theoretical Chemistry and Computational Modeling (TCCM) European Master and by the homonymous ITN European Doctorate (https://tccm.qui.uam.es/) coordinated by the Universidad Autonoma of Madrid. In particular related teaching activities prompted the writing of the book "Chemical Reactions: basic theory and computing" [13] and made extended use of the related LOs in the School of Open Science Cloud, (SOSC) (see https://indico.cern.ch/event/605204/overview and http://services.chm.unipg.it/ojs/index.php/virtlcomm/issue/view/25) held in Perugia on June 2017 and the one month long Intensive Course (IC) of the last edition of the already mentioned TCCM Erasmus Mundus Master (Perugia September 2018).

4. THE PROPOSED MDCR LOS

The proposed MDCR LOs are articulated in four sections according the following scheme:

Section 1
The course begins by considering the modelling of the experimental outcomes (the thermal rate coefficients) using the Transition State (TS) approach within a thermodynamics formulation of the problem. From the analysis of the inconsistencies of the TS model (useful for a phenomenological systematization of experimental data yet useless for predictions) the efficiency of chemical processes is rationalized in terms of collisions of two structure-less bodies using classical mechanics (in which atoms are considered as mass points) and simple model interactions (like pure Coulomb attraction and/or repulsion, hard sphere, mixed attraction at long range plus repulsion at short range (Sutherland, Morse and Lennard-Jones)).

The classical mechanics conceptual machinery, relying on analytical procedures tackling the problem of solving related Newton and Hamilton equations for simple model interactions, is analysed in this section by associating an estimate of the final properties (like the angle of deflection, cross sections and rate coefficients, all quantities of experimental relevance) for different initial conditions.

Pseudo-codes designed for computational classical mechanics procedures based on basic numerical procedures devoted to the integration of the mentioned Newton or Hamilton equations, are provided in this section by associating a set of trajectories starting from different initial conditions to the angle of deflection, cross sections and rate coefficients.

Section 2
The observed failure of the classical mechanics treatment to reproduce some key features of measured data (like the elastic differential cross section in two body collisions) is traced back to the quantum nature of molecular processes and to the related uncertainty principle. This drives the reader to the use of quantum techniques for evaluating the properties of both bound and elastically

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scattered atom-atom systems by integrating the Schrödinger equation both in its time dependent and time dependent form. Related quantum treatments are then discussed and analytical solutions are first worked out for some prototype cases to the end of guiding the reader to use of special functions.

Then some of the most popular techniques and related pseudo-codes useful for integrating numerically the already mentioned corresponding Schrödinger equation for generic atom-atom interactions are illustrated and applied in order to compare related results with corresponding classical ones.

Section 3

At this point the assumption that atoms are structure-less can be abandoned and theoretical treatments more properly handling the electronic structure can be adopted. To move along this direction we discuss here some techniques commonly used for evaluating *ab initio* electronic energies and discuss the adoption of both one-electron functions and variational principle. Along this line, the electronic structure of polyatomic molecules, molecular orbitals, Hartree-Fock and Self Consistent Field (SCF) Molecular Orbital (MO) treatments are discussed in some detail and post Hartree-Fock Configuration Interaction, Multi configuration self-consistent fields and Perturbation methods for the calculation of electronic energies and other molecular properties are illustrated.

To better deal with reactive processes the general nuclei + electrons systems are considered and the various components of the Hamiltonian are described in both the time dependent and the time independent schemes by decoupling electrons and nuclei dynamics and making specific reference to atom diatom systems.

Section 4

In this section concepts and techniques to be used for carrying out dynamical calculations of reactive systems starting from atom-diatom elementary collisions are considered. To this end the motion of nuclei is disentangled from the electronic one by introducing the Born-Oppenheimer approximation. Then the different sets of coordinates (Jacobi, internuclear distances, natural, etc.) for atom-diatom systems and their bias towards specific uses are discussed. The aim of this is the singling out of the coordinates better suited for formulating the different terms of the many body expansion of the interaction potential including the Bond Order (BO) variables, the Rotating BO (ROBO) models, the Many Process Expansion (MPE) of the interaction, the mobile least square fitting of the potential. Different formulations of dynamics equations are discussed for classical and quantum treatments of molecular dynamics including time dependent and time independent approaches. By integrating dynamics equations the typical features of the microscopic phenomenology of elementary processes (such as the effect of a different allocation of energy to the various degrees of freedom in promoting reactivity, the importance of providing an accurate representation of the potential energy surface, the merits and demerits of adopting reduced dimensionality approaches or treating quantally some degrees of freedom while handling classically the others, the usefulness of singling out the periodic orbits of dynamical systems for rationalizing the key features of their reactive properties (including the categorization of transition state effects). Then some extensions of the dynamical studies to large systems both in terms of adopting Force Field techniques to build related potential energy surfaces and in terms of using classical mechanics treatments of atoms (or group of atoms) are considered and truly complex computational applications dealing with systems concerned with some technological innovations (e.g. particle flux through nanopores or catalytic conversion of CO_2 in methane) and the crediting of community computational services provision are presented.

The basis of modern concurrent computing paradigms and technologies (from micro level to grids and cloud) and their applications (including some popular computing packages) to some prototype reactions are discussed in order to single out the role played by the energy allocation to different

degrees of freedom. Mention to virtual organizations, grid computing and Open Molecular Science Cloud is also made.

Some examples of the MDCR LOs produced in collaboration with the Multimedia Centre of the University of Perugia [14] are accessible at the G_Lorep address https://glorep.unipg.it. Work is in progress to further improve the cloud distribution of the G_Lorep by adopting a Platform as a service (PaaS) strategy.

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