

TOPIC GRANULARITY FOR MOLECULAR SCIENCE LEARNING OBJECTS

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1. INTRODUCTION

Some of us have submitted to the conference GARR 2020 "Sostenibile/Digitale - Dati e tecnologie per il futuro" to be held at the University of Palermo (IT) on May 20-22, 2020 a contribution illustrating the efforts spent to implement the Molecular Open Science Enabled Cloud (MOSEX) project within the European Open Science Cloud (EOSC) Pillar (<https://www.eosc-pillar.eu/>) initiative. MOSEX is aimed at establishing a cloud service for the validation of the value of the rate coefficient parameters of elementary chemical processes via an iterative synergistic use of theory and experiments. It is articulated in the following actions:

- 1) electronic structure and equilibrium molecular configuration properties for spectroscopy, synthesis, photovoltaic and photochemical processes studies;
- 2) classical and quantum 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;
- 5) dissemination, publication and assessment of molecular knowledge;

the last of which (action 5) includes, among other objectives, the development of e-learning and e-assessing tools and dissemination mechanisms for the Open Molecular Science Cloud (OMSC) as decided at the OMSC workshop sessions held in Sept. 2019 at the Accademia delle Scienze in Rome [1]. This effort is part of the activities of the Virtual Education Community (VEC) Committee of the European Chemistry Thematic Network (ECTN) Association which aims at supporting chemists in jointly designing, implementing, integrating and re-using on the cloud Molecular Science (MS) Learning Objects (LOs) of the appropriate size and structure [2].

In the present contribution we focus on an application dealing with the subject "Molecular Dynamics and Chemical Reactivity" (MDCR) of the Theoretical Chemistry and Computational Modelling (TCCM) Erasmus+ Master [3] study programme with particular concern with the LOs associated with the book "Chemical reactions: basic theory and computing" [4] implemented on the Glorep platform [5].

In particular, here we consider first in Section 2 the level of granularity adopted for the design of modular reusable LOs. Then we describe the level of technological implementation of the LOs adopted at various stages of development in Section 3. Finally we discuss the actual "state of the art" of the development of our case study in Section 4 calling for collaboration and proposing a ranking criterion for evaluating possible contributions in Section 5.

2. COLLABORATIVE STRATEGY FOR RE-USABILITY

The first phase of the approach adopted to develop re-usable LOs follows the **scope of the objective** collaborative strategy aimed at maximizing the virtuous evolution of their contents through an appropriate use of the granularity and a maximum enhancement of the virtuosity of their sharing at the four levels of the "holistic granularity" [6]. As to the granularity, we opted for adopting the highest microlevel one and for leaving with the user the decision on how to

recombine the grains into a final full LO. Such a choice, ensures an evolution in time and complexity of the LO content while simplifying its classification and facilitating the search of the learning units within complex DataBases. On top of that such approach enhances the virtuosity of the knowledge sharing by facilitating an extended and continuous updating of the contents through the pro-active collaboration of the whole community of teachers belonging to the involved scientific areas. In particular, we focused our efforts on the design, implementation and development of a re-usable MODular Learning Objects Composer (called RE MOLOC) a technology allowing an easy production, revision and refining of Open Molecular Science Knowledge.

RE MOLOC is meant to be a VIRTUOUS tool enabling scientific communities to progressively increase the number and enrich the quality of the related LOs through the composition of elementary educational objects (called here microunits). This occurs through the direct autonomous production of the mentioned microunits (or a set of them) by single (or groups of) teachers and the subsequent insertion into a shared on-line platform. The members of the community can then freely and repeatedly draw, withdraw, edit and publish subsequent versions of a LO and direct students to their use.

The second phase of the approach adopted to develop re-usable LOs aims at composing, out of the stored LOs an extended database of audio- and/or video-lectures. The basic features of the database will be:

- 1) EVOLUTIONARY EDUCATIONAL CONTENTS (which are the basis for assembling a high quality LO) thanks to the progressive review associated with the continuously shared revision;
- 2) SUFFICIENT DIGITAL QUALITY (audio/video quality, adequate file weight, etc.) thanks to the use of sufficiently high quality standard tools for personal production;
- 3) TAGGING (and portability of elementary information) thanks to an appropriate definition of the microunits;
- 4) EFFICIENT CHAINING (of the various LO components) thanks to the use of an ad hoc designed software providing "intelligent" coordination and supply activities;

A fundamental parameter of the proposed solution is the type of granularity used for the elementary LOs on the parcelling of the educational contents aimed at optimizing their reuse. This implies the adoption of:

- a) a versatile tool allowing the assembling of the designed elementary LOs by selecting them to the end of fulfilling a particular educational need of the "targeted" courses. This implies the possibility of selecting and organizing the material produced by other teachers and integrating it with one's own;
- b) a fast and simple verification procedure for the validity of the components of the elementary LOs and of the resulting (after modification) assemblies through the action of well recognized Auditors and Editors using an effective electronic publishing methodology;
- c) a mechanism of constant control, updating, comparison and usage evaluation not only limiting material's obsolescence or erroneous delivery but also ranking the LOs by quality;
- d) a definition of the type and level of granularity of the elementary LOs suited to make them portable building blocks among different courses of a community of teachers and learners.

3. LEVELS OF TECHNOLOGICAL IMPLEMENTATION

In order to start the process of collaborative development it is usual to adopt easy to use low technical quality tools (lack or inadequate lighting, acoustic insulation, bandwidth and/or data compression) as typical of "user friendly" technologies associated with the teacher's self use of popular free (or nearly free) instrumentation for audio/video recording like webcams, microphones, notebooks, tablets, smartphones with some attention to the number of pixels (for image definition) and the size of the produced files. Typical is the use, in this case, of open source (or extremely cheap proprietary) software enabling basic editing and, possibly, of a directional microphone for a recording free of environmental noise. This is usually the case of the:

SLIDES + AUDIO MICROUNIT SOLUTION

Hardware: PC

Software: Open Broadcasting Software (OBS)

Operations:

a – (if not yet installed) download and install OBS from <https://obsproject.com/download>

a1 export slides as jpg images

b1 – start OBS

c1 – in section *Source* click icon +

c2 – *Image*

c3 - *Create New* (type name of the microunit e.g. “LO-microunit-xyz”)

c4 – click OK

d1 – in section *Controls* click *Settings*

d2.1– *Output*

d2.2 – on item *Recording Path* click *Browse* and select the folder for saving the file

d2.3 – on item *Recording Format* select *mp4*

d3.1 – *Audio*

d3.2 – on item *Mix/Auxiliary Audio Device* select microphone and press OK

e – when ready click *Start Recording* (section *Controls*)

f – in the lower *Application* bar click the *Presentation* icon

g1 – when the microunit is completed click the OBS icon in the lower *Application* bar

g2 – press *Stop Recording* (section *Controls*)

Next step of the process is the adoption of an:

INTEGRATED WEBCAM VIDEO + AUDIO MICROUNIT

Hardware: PC with integrated webcam (**e.g. Notebook**)

Software: Open Broadcasting Software (OBS)

Operations:

a – (if not yet installed) download and install OBS from <https://obsproject.com/download>

b1 – start OBS

c1 – in section *Source* click icon +

c2 – *Video Capture Device*

c3 - *Create New* (type name of the microunit e.g. “LO-microunit-xyz”)

c4 – on item *Device* select the webcam and click OK

d1 – in section *Controls* click *Settings*

d2.1– *Output*

d2.2 – on item *Recording Path* click *Browse* and select the folder for saving the file

d2.3 – on item *Recording Format* select *mp4*

d3.1 – *Audio*

d3.2 – on item *Mix/Auxiliary Audio Device* select microphone and press OK

e – when ready click *Start Recording* (section *Controls*)

f – when the microunit is completed click *Stop Recording* (section *Controls*)

A further step forward of the process is the adoption of an:

EXTERNAL WEBCAM VIDEO + AUDIO MICROUNIT

Hardware: PC with external Webcam (USB-Plug&Play e.g. Logitech HD Pro Webcam C920)

Software: Open Broadcasting Software (OBS)

Operations:

a – connect the webcam Usb to the Computer (no hardware needs to be installed for the Plug&play camera) and (if not yet installed) download and install OBS from <https://obsproject.com/download>

b1 – start OBS

c1 – in section *Source* click icon +

c2 – *Video Capture Device*

c3 - *Create New* (type name of the microunit e.g. “LO-microunit-xyz”)

c4 – on item *Device* select the webcam and click OK

d1 – in section *Controls* click *Settings*

d2.1– Output

d2.2 – on item *Recording Path* click *Browse* and select the folder for saving the file

d2.3 – on item *Recording Format* select *mp4*

d3.1 – Audio

d3.2 – on item *Mix/Auxiliary Audio Device* select microphone and press OK

e – when ready click *Start Recording* (section *Controls*)

f – when the microunit is completed click *Stop Recording* (section *Controls*)

This is usually also the final step of the process that leads to sufficiently advanced products (both in terms of contents and in terms of aesthetic) which deserve to be permanently stored and archived for further use.

4. THE MOLECULAR DYNAMICS AND CHEMICAL REACTIVITY CASE STUDY

The first set of LOs designed and implemented for the book “Chemical reactions: basic theory and computing” [4] can be accessed by all users (even if not authenticated) to search within the Glorep repository (see ref. [5] in the downloadable Glorep User Guide). To this end the user should:

-Type the address of a glorep server on a browser e.g. <https://glorep.unipg.it/>

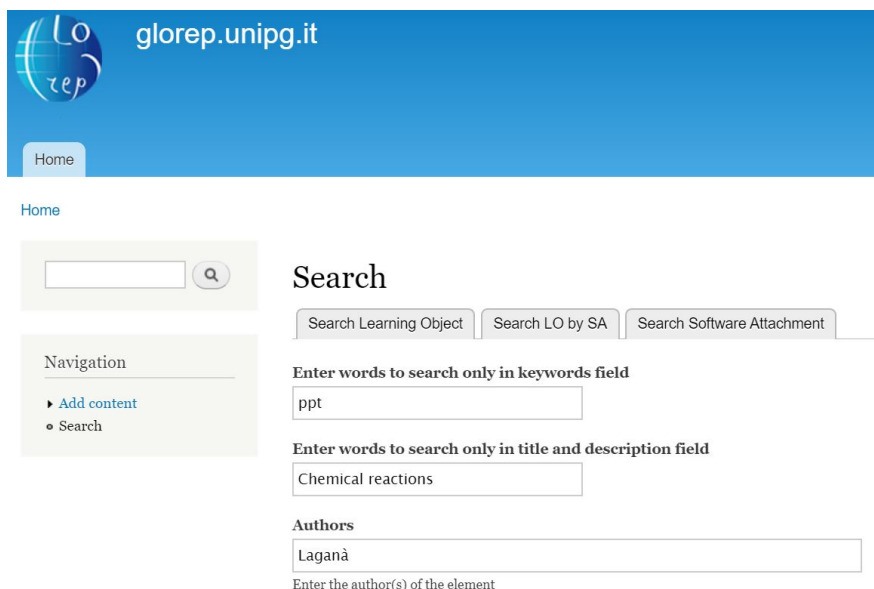
-Click on “**Search**” on the Navigation panel on the left side of the page. This will open the [Search page](#) where advanced searches can be carried out by filtering some LO metadata as shown in the example shown below.:

a. Type the “**ppt**” word to search in *keywords* field

b. Type the “**Chemical reactions**” words in *title and description* field

c. Type the “**Laganà**” words in *Authors* field (see fig.1)

d. By clicking out of the field the results of your search will show up at the bottom of the page (see fig.2)



The screenshot shows the search interface of the Glorep repository. At the top left is the logo and the URL 'glorep.unipg.it'. Below it is a 'Home' button. The main search area is titled 'Search' and contains three tabs: 'Search Learning Object', 'Search LO by SA', and 'Search Software Attachment'. There are three search input fields: 'Enter words to search only in keywords field' with the text 'ppt', 'Enter words to search only in title and description field' with the text 'Chemical reactions', and 'Authors' with the text 'Laganà'. Below the 'Authors' field is a small text label 'Enter the author(s) of the element'.

Figure1 - Screenshot of the LO search page of Glorep

Title	Description	Category	Keyword	Author	Associated Software
Chemical Reactions: basic theory and computing	The course we discuss here, Chemical Reactions: basic theory and computing written by Gregory .A. Parker and myself, has been designed to help the students of the European Erasmus Mundus Master in "Theoretical Chemistry and Computational Modelling" (TCCM) to familiarize with both theoretical methods and computational techniques useful to handle the treatment of chemical reactive processes at microscopic level. The general scheme of the book is illustrated by the Learning Object (LO) LO00. In it the reader is driven to disentangle elementary events out of the kinetics of complex systems in which reactive and non-reactive processes combine and compete in different ways depending on the interactions and momenta of the involved species. Then theoretical and computational techniques for dealing with two-, three-, four- and many-body collisions are discussed (by leveraging preferentially elementary gas phase processes) and out of the obtained detailed microscopic information complexity is regained in order to extend the treatment to very large systems by introducing the necessary approximations, using the appropriate experimental and computational apparatuses with specific reference to Open Science approaches	541.39 - Chemical reactions	ppt	Antonio Laganà	

Figure 2 – Screenshot of the descriptor of the LO

The LO page (see fig.3) can be opened by [clicking on its title](#). On that page the LO description and other information can be read. As can be seen from the figure, the considered LO, is divided into chapters. By clicking the [Download](#) button an authenticated user can start the download of the single chapter containing in this case the ppt file of the present version (under revision) for corrections and improvements.

The screenshot shows the descriptor page for the Learning Object (LO) titled "Chemical Reactions: basic theory and computing". The page includes a search bar, a navigation menu with "Add content" and "Search", and a main content area with the following details:

- Title:** Chemical Reactions: basic theory and computing
- Description:** The course we discuss here, Chemical Reactions: basic theory and computing written by Gregory .A. Parker and myself, has been designed to help the students of the European Erasmus Mundus Master in "Theoretical Chemistry and Computational Modelling" (TCCM) to familiarize with both theoretical methods and computational techniques useful to handle the treatment of chemical reactive processes at microscopic level. The general scheme of the book is illustrated by the Learning Object (LO) LO00. In it the reader is driven to disentangle elementary events out of the kinetics of complex systems in which reactive and non-reactive processes combine and compete in different ways depending on the interactions and momenta of the involved species. Then theoretical and computational techniques for dealing with two-, three-, four- and many-body collisions are discussed (by leveraging preferentially elementary gas phase processes) and out of the obtained detailed microscopic information complexity is regained in order to extend the treatment to very large systems by introducing the necessary approximations, using the appropriate experimental and computational apparatuses with specific reference to Open Science approaches
- Author(s):** Antonio Laganà
- Language:** en
- Keyword:** ppt
- Structure:** linear
- LifeCycle:** Status : final
- Educational:**
 - Interactivity Type : expositive
 - Learning Resource Type : slide
 - Interactivity Level : very low
 - Semantic Density : high
 - Intended End User Role : learner
 - Context : higher education
 - Language : en
- Rights:**
 - Cost : no
 - Copyright : yes
 - rights_Description : For academic use only
- References to the Learning Object:**
 - Chemical Reactions: basic theory and computing - Introduction
 - Submitted by Laganà on Tue, 04/17/2018 - 21:41
 - attachment: A-LO00-introduction.ppt (1496kB)

A "Download!" button is visible at the bottom of the page.

Figure 3 – Screenshot of the Download of the LO description

An example taken from the second set of LOs, obtained by dressing a previous version of the slides with the recording of an external webcam and an audio unit, can be accessed in the same way, but typing the “**video**” word to search in the *keywords* field (see fig.4)

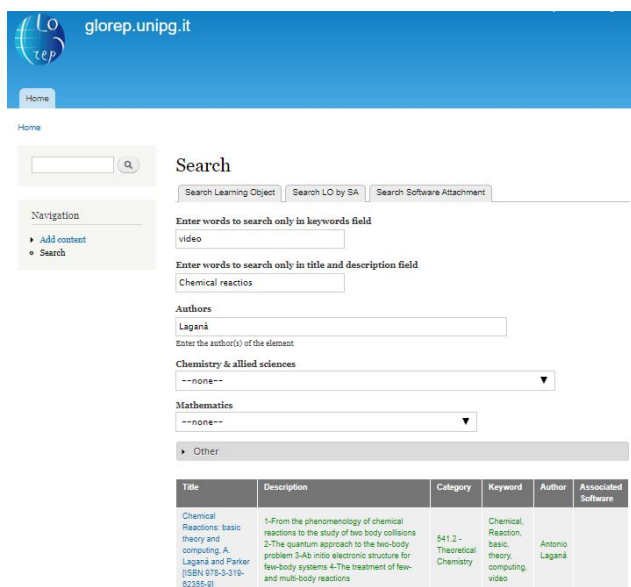


Figure 4 - Screenshot of the access to the Video LO

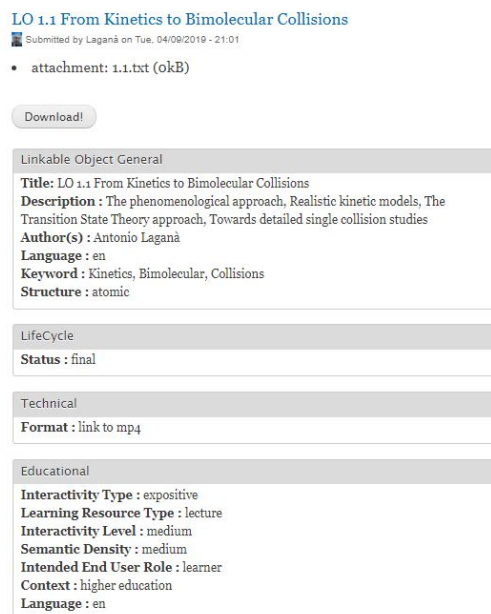


Figure 5 - Screenshot of the access to the youtube Video

And then by clicking the **download** button in a specific chapter (see fig.5) the user can access the related youtube video by the **link** inserted into the downloaded file (see fig. 6).

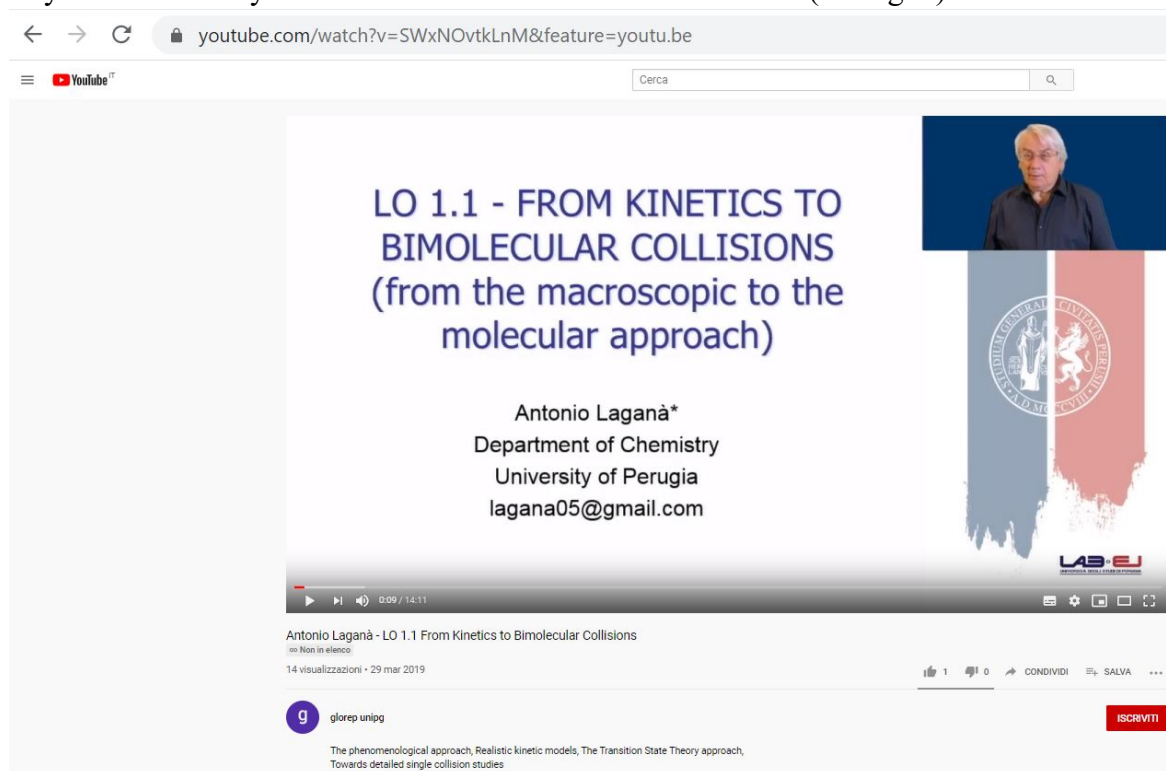


Figure 6 – Screenshot of the above mentioned youtube file (<https://youtu.be/SwxNOvtkLnM>)

5. RANKING MECHANISMS AND FINAL OMSC CONSIDERATIONS

In order to introduce a ranking mechanism for the different versions of a LO produced through collaboration and subsequent improvements, use will be made of Collaborative Filtering (CF) [7, 8]. CF ranks and promotes services to the user by leveraging the history of past services. The CF algorithms being implemented in Glorep are based on the estimate by the user of the Quality of Service (QoS) provided by the LO and are scaled by the Quality of the User (QoU) having contributed to the formulation of the QoS. Such algorithm is shared with other activities of the MOSEX project when dealing with the production of services for other activities like the production of scientific data, its validation and its re-use within the more general EOSC-Pillar economy.

REFERENCES

- 1] A. Laganà, The Open Molecular Science Cloud, VIRT&L-COMM <http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/220>
- 2] A. Moriconi, S. Pasqua, A. Laganà, E-learning granularity for a chemical reactivity learning objects, 2019; <http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/215>; ISSN: 2279-8773
- 3] <https://www.emtccm.org/the-erasmus-mundus-master/>
- 4] A. Laganà, G.A. Parker, Chemical Reactions Basic Theory and Computing, Springer International Publishing 2018; ISBN 978-3-319-62355-9
- 5] S. Tasso, Glorep User Guide, <https://glorep.unipg.it/>
- 6] J. Strobel, Gretchen Lowerison, R. Côté, P. C. Abrami and E. C. Bethel - "Handbook of Research on Learning Design and Learning Objects: Issues, Applications, and Technologies" - 2009 - DOI: 10.4018/978-1-59904-861-1.ch017
- 7] C. Manuali, A. Laganà, Trial User, Resources and Services Quality Evaluation for Grid Communities Sustainability, Computational Science and Its Applications--ICCSA 9156, 324-338 (2015)
- 8] A. Puri and M. Bhonsle, A Survey of Web Service Recommendation Techniques based on QoS values, International Journal of Advanced Research in Computer and Communication Engineering, Vol. 4, Issue 12, December 2015