ELCHEM EXPRESSION OF INTEREST FOR THE EGI, EUDAT AND INDIGO-DATACLOUD H2020 PROJECT PROPOSAL EINFRA12 (A)

Antonio Laganà, Master-up s.r.l.,Perugia, Italy
Noelia Faginas Lago, Università degli studi di Perugia, Italy
Osvaldo Gervasi, Università degli studi di Perugia, Italy
Sergio Tasso, Università degli studi di Perugia, Perugia, Italy

Abstract: *In this paper we present a proposal to empower the Molecular sciences educational community with a networked and standardized at European level e-learning environment leveraging on the already ongoing activities of the European Chemistry Thematic Network Association with the support of the test centers of some Higher Education Institutions. The proposal articulated into three subservices: management of EChemTest® Questions-and-answers libraries, the management of the Self-evaluation sessions, the collaborative building, revising, accessing of Learning Objects. The proposal is designed as part of the activities to be committed by the Chemistry, Molecular, Materials Sciences and Technologies (CMMST) Virtual Research Community (VRC) within the joint EGI, EUDAT and INDIGO-DataCloud H2020 project for the EINFRA12 (a) call.*

Service and activity descriptions

Describe the services that will be concerned by technical integration, consolidation and operations. Please provide a service description with a user point of view and make a distinction between final services and services components (enhancing parts of a service).
Thematic Service
Please provide as many service entries as necessary. Service is defined as: "the way to provide value to customers through bringing about results that they want to achieve".

SERVICE EL-CHEM (e-learning for Chemistry): *a proposal to empower the Molecular sciences educational community by a networked and standardized at European level e-learning environment leveraging on the already ongoing activities of the European Chemistry Thematic Network Association* (that already operates with more than 100 participating Higher Education Institutions (HEI)s, over 10 accredited test sites and 5 coordinated SMEs). The proposal aims to the creation of seamless services dedicated to e-learning and related analytics including hardware and software components, to the cross fertilization of activities for Self Evaluation of chemistry knowledge at various level of schooling and among different HEIs and different countries, to the adoption of pan-European interoperability of learning and evaluation procedures, to the development of Libraries of Questions and answers, learning objects, online courses, webinars (and stores them on a distributed repository) of Chemistry knowledge.

PROSUMERS: producers and users of Q&A of Chemistry knowledge, Self Evaluation Sessions, Learning Objects, MOOC (ECTN, Master-up, National test centers of HEI, Accredited Test sites of HEI).

SUBSERVICE n.1: *management of EChemTest® Libraries of the ECTN Association* *that is a service offered to the ECTN members through a network of 10 text centers and related to Chemistry Learning objects, Self Evaluation tests and proficiency certificates at School, University access, Eurobachelor and Euromaster levels*

a. Contact, report: < *Noelia Faginas Lago, Università degli studi di Perugia, Perugia, Italy* >
b. Link to the online: <in restructuring at present>
c. TLR8
d. http://www.expe.ectn-assoc.org/ <in restructuring at present>
e. Management of self-evaluation sessions for universities (members of ECTN over 100 HEIs)
f. Service already provided through Amazon
g. Bring the service into the EGI cloud for different use
h. Possibility of generalizing this framework to other science domains

SUBSERVICE n. 2: *cloud management of SES* *(Self Evaluations Sessions)* *of the EChemTest® service offered in Europe and outside Europe*

a. Contact, report: < *Dr Osvaldo Gervasi, Università degli studi di Perugia, Perugia, Italy* >
b. Link to the online: <in restructuring at present>
c. TLR8
d. http://www.eol.unipg.it/
e. Management of self-evaluation sessions at over 10 HEIs Test centers in Europe and outside EU (Vienna (A), Thessaloniki (GR), Budapest (HU), Krakow (PL), Helsinki (FI), Madrid (ES), Perugia (IT), Milan (IT), Genoa (IT), Naples (IT), Kazan (RU), Amsterdam (NL))
f. Service already provided through Amazon cloud
g. Bring the service into the EGI cloud for different use
h. Possibility of generalizing this framework for other science domains

SUBSERVICE n. 3: *management of GLOREP* *(Grid Learning Objects Repositories) the service offered to collaboratively build, revise, access Learning Objects with (at present) particular emphasis to Chemistry in connection with EChemTest® and Chemistry Eurolabels*

a. Contact, report: < *Dr Sergio Tasso, Università degli studi di Perugia, Perugia, Italy*>
b. Link to the online: <in restructuring at present>
c. TLR8
d. http://www.glorep.unipg.it/
e. Management the Learning object repository for 3 EU HEI (Perugia (IT), Thessaloniki (GR), Genoa (IT)
f. Waiting for link to Amazon
g. Bring the service into the EGI cloud for different use
h. Possibility of generalizing this framework for other science domains

Service overview	
Thematic Service name	*EL-CHEM*
Service description	(1) High-level description of what the service does in terms of functionalities it provides to the end users *Offers the use of the **European standards** developed by the ECTN (European Chemistry Thematic Network) Association for the definition of different levels of chemistry knowledge, implements seamless services dedicated to:* *-**e-learning analytics** (through Self Evaluation Sessions),* *-**cross fertilization** of activities supporting e-learning in chemistry at various level of schooling,* *-enhancing **the interaction among ways of teaching** in HEIs and countries,* *-the adoption of **pan-European interoperability of learning and evaluation** procedures,* *-the **development of Libraries of Questions and answers, learning objects, online courses, webinars** (and stores them on a distributed repository)* (2) Resources it enables access to *Necessary compute capabilities are expected to be provided by the project EGI, EUDAT and INDIGO-DataCloud e-infrastructures* (3) Relevant documentation *Examples of the service capabilities from a user point of view are given in* A. Laganà, A. Riganelli, O. Gervasi, P. Yates, K. Wahala, R. Salzer, E. Varella, J. Froehlich, ELCHEM: a metalaboratory to develop Grid e-learning technologies and services for chemistry, Lecture Notes in Computer Science 3480, 938-946 (2005). O. Gervasi, A. Riganelli, A. Lagana', A learning management system based on virtual reality and semantic web techniques in Chemistry studies in the European higher education area, R. Salzer, T. Mitchell, H. Muller-Solger Eds, Gesellschaft Deutscher Chemiker (2005) p. 105. Antonio Laganà, [EChemTest: The Assessment of Chemistry Knowledge](#), Nachrichten aus der Chemie, 54, 12, 1272-1272 (2006), Wiley VCH Verlag GmbH & Co. KGaA O. Gervasi, S. Tasso, A. Laganà, Immersive Molecular Virtual Reality based on X3D and Web services, Lecture Notes in Computer Science 3980, 212-221 (2006). A. Laganà, S. Crocchianti, N. Faginas Lago, A. Riganelli, C. Manuali, S. Schanze, From Computer Assisted to Grid Empowered Teaching and Learning Activities in Higher Chemistry Education in Innovative Methods in Teaching and Learning Chemistry in Higher Education, I. Eilks and B. Byers Eds, RSC Publishing (2009) p. 153-190 ; ISBN 978-1-84755-958-6 A. Laganà, O. Gervasi, A Priori Molecular Virtual Reality on EGEE Grid, International Journal of Quantum Chemistry,110, 446-453 (2009) S. Tasso, S. Pallottelli, R. Bastianini, A. Lagana', Federation of distributed and collaborative Repositories and its application on Science Learning objects, Lecture Notes Computer Science 6784, 466-478 (2011) S. Tasso, S. Pallottelli, M. Ferroni, R. Bastianini, A. Lagana', Taxonomy management

	in a Federation of Distributed Repositories: a chemistry use case, Lecture Notes Computer Science 7333, 358-370 (2012) S. Tasso, S. Pallottelli, M. Rui, A. Laganà, Learning Objects Efficient Handling in a Federation of Science Distributed Repositories, Lecture Notes in Computer Science 8579, 615-626 (2014)
Service provider	*Master-up srl (IT), University of Perugia (IT), ECTN Association (B), University of Amsterdam (NL), Krakow Jagiellonian University (PL), Thessaloniki Aristotle University (GR), University Complutense Madrid (ES), University of Milan (IT), University of Genoa (IT), University of Naples (IT), Technology University of Vienna (A), Eötvös University of Budapest (HU), University of Helsinki (FI)*
Service catalogue	*The service is planned to be transferred for Academic use to the EGI.eu catalogue by linking the different subservices.*
Value	*Provide either intermediate or final level proficiency level self-assessment tools for the evaluation of the competence on chemical knowledge. Collaborative development of Libraries, the assembling of support materials (learning objects and MOOCs) for basic concepts and integrated series of lectures provide further added value to the community collaborative European Educational activities. These activities and the expertise made available by the members of the community are rewarded through a credit making the service self-sustainable.*
Current TLR level1, acceptance criteria and validation/verification results	(1) service status in terms of completeness and maturity (including link to relevant documentation) *The various subservices are implemented in a coordinated way and local developments are then transferred also to the central manager or, in distributed repositories, they are transferred from the producer to the user infrastructure on demand. During (and after) the life of the project it is planned to exploit the EGI infrastructure at least for academic usage.* (2) service acceptance criteria defined by customers and/or users (including e.g. aspects related to interoperability, availability, installability, performance, portability, recoverability, safety, scalability, usability) *EGI rules for the VRCs (and in particular those of the CMMST VRC) will be adopted* (3) results of validation and verification activities involving service providers and user communities. *EGI rules for the virtual communities will be adopted by leveraging on the tools referenced in* C. Manuali, A. Laganà, A new collaborative Grid framework for SSCs Cracow 09 Grid Workshop, 188-195 (2010) ISBN978-83-61433-01-09

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[1] Technology Readiness Level:
https://ec.europa.eu/research/participants/data/ref/h2020/wp/2014_2015/annexes/h2020-wp1415-annex-g-trl_en.pdf

Access policy	*Policy-based: users are granted access to the service based on policies defined by the service provider(s) see* C. Manuali, A. Laganà, A new collaborative Grid framework for SSCs Cracow 09 Grid Workshop, 188-195 (2010) ISBN978-83-61433-01-09
Terms of use	Please provide a reference to the service terms of use, i.e. the rules which one must agree to abide by in order to use the service *EGI rules for the VRCs and ECTN Association specific rules will be adopted*
User groups and scientific disciplines served	*The service is intended mainly for members of the ECTN Association for which the VRCS policy will be adopted. The service is also open to non members and companies by making reference to pay per use EGI rules. (see https://mailman.egi.eu/mailman/listinfo/egi-pay-for-use)*
Service business model	*Costs of the service subservices will be regulated accordingly to the ECTN Association rules once approved by the community management board. Sharing of the incomes will occur through the credit mechanism implemented as described in* C. Manuali, A. Laganà, A new collaborative Grid framework for SSCs Cracow 09 Grid Workshop, 188-195 (2010) ISBN978-83-61433-01-09

Service architecture
Define the service by describing its components. A service is usually composed of different service components that enable or enhance the service. A service component is a logical part of a service that provides a function enabling or enhancing a service. Although a service component underlies one or more services, it usually does not create value for a customer alone and is therefore not a service by itself. Examples of service component are software, and services that are provided or could be provided by e-Infrastructures. For example:
- EGI https://www.egi.eu/services/
- EUDAT https://eudat.eu/services-support
- INDIGO https://www.indigo-datacloud.eu/service-component

Service components	Name of component	Functional description, applicable standards and needed resource capacity (if applicable) e.g. CPU Time, storage capacity etc.	Provider If already appointed
	EOL	Operated in Amazon (intended implementation on EGI.eu for Academic purposes)	
	Amazon	Storage capacity for libraries and session outcomes	

Service integration with generic e-Infrastructures
If applicable. Define the proposed technical integration/service enhancement activities for this service that are proposed to be funded in the project. For example software integration activities that concern general e-Infrastructure capabilities, like those provided by EGI, EUDAT, INDIGO-DataCloud and other software.

Integration activity and concerned service components	Integration activities are needed for: - data repository for shared knowledge - distributed compute power both for HPC and HTC
Overall necessary effort (Person Months) and timeline	30 PMs distributed over 3 years.
List of requested service components	Services are needed for the adaptation of the present cloud implementation with Amazon to the EGI one.

Infrastructure integration
This activity addresses challenge 2 of EINFRA-12 (A): "seamless operation of highly scalable and agile data and computing platforms and services dedicated to analytics including hardware and software components, database, compilers, analytics software, supported to easy user entry points for the community of users". By filling this section the applicant commits to make the service discoverable in a central service catalogue and available for access by international user communities.

Description of infrastructure integration activities relevant to the proposed thematic service (to be planned in the project)	*Infrastructure integration activities will be needed to integrate compute, storage, etc. to the end of supporting GLOREP and MOOCS subservices. Work will be provided partly (50%) as in-kind contribution to support wider usage and exploitation.*

Training
to develop human capital and generate innovation by fostering adoption by new user communities. Training activities requested in this project must be specific to this call and to the thematic services in scope in your expression of interest. They must not duplicate training activities already funded by other initiatives and projects.

Description of training activities relevant to the proposed thematic service (to be planned in the project)	*Training activities for the Test sites managers and users related to the running and exploitation of EChemTest®, GLOREP and MOOCS are planned as part of the project. Work will be provided partly (50%) as in-kind contribution to support wider usage and exploitation.*

Relevance to EINFRA-12 (A) challenges

EINFRA-12 (A) challenge (**remove those that are not addressed by your activity**)	*Specify your contribution to the challenges highlighted by the e-INFRA-12 (a) call, providing whenever possible concrete examples and key performance indicators.*
1. The operation of a federated European data and distributed computing infrastructure for research and education communities will optimise the access to IT equipment and services	*Users can specialize their contributions to the field of their competences while exploiting the competences of the other members for the areas in which they are least competent*
2. All European researchers and educators are in equal footing to access essential resources	*Access is on equal footing for users while producers can have preferential use thanks to the credits accumulated for the activities provided on behalf of the community*
3. Partnerships with industrial and private partners	*Partnership is encouraged not only from researchers but also from industrial and private partners*
4. Train people in research and academic organisations	*Training is included in the services ad subservices offered and are rewarded with credits*
5.	
6. More scientific communities will use storage and computing infrastructures with state-of-the-art services	*The service is tailored in a way that extension to other scientific communities is possible. This aspect is considered in more detail in section 3.*
7. The open nature of the infrastructure will allow scientists, educators and students to improve the service quality	*This policy is encouraged by a credit reward policy of the community*
8. Increase the incentives for scientific discovery and collaboration across disciplinary and geographical boundaries. It will further develop the European economic innovation capacity and provide stability to the e-infrastructure.	*The service will further develop the European common ground for education in molecular sciences and related economic innovation capacity and use of the e-infrastructure.*