VIRT&L-COMM.23.2022.5

THE ECTN VEC: FROM EChemTest® TO MOLECULAR OPEN SCIENCE and EDUCATION CLOUD SERVICES

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ABSTRACT *– In this paper the cloud evolution of EChemTest® services is illustrated. Both the offsetting of debits through credits for the ECTN member institutions and the charging to third parties within the ad hoc implemented Prosumer model are illustrated to the end of documenting the development of the collaborative features of EChemTest®. The most recent proposal of transforming it into a European Open Science Cloud activity is also mentioned.*

1) THE COMPUTER BASED EVALUATION OF CORE CHEMISTRY COMPETENCES – The European Chemistry Thematic Network (ECTN) [1] developed by the year 2000 the so called "Core Chemistry": a *de facto* European standard for University teaching contents of the three year first degree (Bachelor) and of the two year specialization second degree (Master) by defining an optimal mix of Organic, Physical, Inorganic and Analytical Chemistry subjects. On this ground ECTN developed a framework for the cycles of qualification in chemistry (the Chemistry Eurobachelor®, the Chemistry Euromaster®, the Chemical Technology Euromaster® and the Chemistry Doctorate Eurolabel®) obtainable either in a specific accreditation (and its renewal) process or as an add-on to the national accreditation. On the same ground the ECTN Work Group "Evaluation of Core Chemistry" (WG10) chaired by P. Mimero (Lyon, FR) designed several libraries of Questions and Answers (Q&A)s for use when assessing through e-tests the chemistry skills possessed by the students. The relevant established libraries (named EChemTest®) were: General Chemistry 1 **(GC1)** for the upper secondary school, General Chemistry 2 **(GC2)** for Bachelor studies access, Analytical Chemistry 3 **(AC3)**, Biological Chemistry 3 **(BC3)**, Inorganic Chemistry 3 **(IC3)**, Organic Chemistry 3 **(OC3)** and Physical Chemistry 3 **(PC3)** for Master studies access. Assessments were carried out by running on a PC one hour long Self Evaluation Sessions (SES)s using the commercial software Question Mark (QM) at the computer rooms of a subset of ECTN member Universities centrally coordinated by the WG10 chair with the support of H. Krebs (to produce new ICT tools), C. Manuali (to maintain the central server) and A. Laganà (to take care of the evolution towards a distributed service).

2) THE INCUBATION OF DISTANCE ASSESSMENT CHEMISTRY COST METALABORATORIES – As anticipated in ref. [2] and discussed in more detail in ref. [3], the rapid evolution of the distributed computing infrastructures in Europe (built and nurtured by the projects Enabling Grids for E-sciencE (EGEE) [4] and further consolidated by the European Grid Infrastructure (EGI) [5] ones) succesfully coordinated National Grid Initiatives in forming the country-wide building blocks of the pan-European Grid aimed at delivering advanced computing services to scientists and educators engaged in carrying out multinational projects. At the same time the European COST (COoperation in Science and Technology) [6] (a funding organisation for research and innovation networks) supported the building of connections across Europe among the institutions willing "*to build the so called European Metalaboratories (clusters of geographically distributed Laboratories working in a co-ordinated way on a common project by sharing manpower, hardware and software), fostering innovative solutions for chemical applications and a new paradigm for collaborative research.* In the case of ECTN this occurred first with the **D23** COST action **METACHEM** [7] (17/10/2000-18/07/2005) whose main objective was "*the exploitation of the potentialities of meta and grid computing for developing computational applications, connecting the know how distributed among several research*

ISSN: 2279-8773

laboratories … As an additional benefit the emphasis given to e-learning has to be mentioned." In particular, educational aspects were taken care by the ELCHEM d23/0005/01 project thanks to the active participation of more than 10 members of ECTN and stimulated the establishing of the Virtual Education Community (VEC) committee. The most decisive step towards the use of interoperable technologies based on advanced networking and semantic web approaches was then made by the workgroup **ELAMS** (E-science and learning approaches in molecular sciences) coordinated by O. Gervasi of the Department of Mathematics and Computer Science (DMI) of the University of Perugia within the **GRIDCHEM** [8] (06/07/2006-05/07/2010) **D37** COST Action. Within such collaboration, aimed at extending EChemTest® to virtually all the member Universities of ECTN, use was made of the on-line assessment system EOL [9] (developed on a Linux environment by making an extensive use of open source software components) and of the learning management system SELE [10] (integrating learning and assessment using the semantic web). This led to the establishing in some countries of a National Test Centre (NTC or, shortly, TC) coordinating, where feasible, Accredited Test Sites (ATS)s for managing, local activities. In EOL, in fact, the user interface interacts with no significant bottle-necks with the content manager and with the on line assessment system allowing the student registered at a given session to run the relevant SESs (30 randomly selected questions matching the chosen level of difficulty) in the chosen subject and language and get, as well, the relevant evaluation.

3) AIMING AT SUSTAINABILITY: THE LAUNCH OF THE ECHEMTEST+ SPECIAL PROJECT – After the above mentioned successful implementation of a fully shareable and supportive EChemTest® EOL environment accompanied by the launch in 2012 of Virt&l Comm (the present international online electronic scientific magazine offering a forum for presenting the work carried out by Virtual Innovation, Research, Teaching & Learning Communities), the next step (due to the coming to an end of the EU financial support to thematic network projects (like those of ECTN)) was the effort to open it to the largest possible number of users (including third parties). As a matter of fact, after some unsuccessful attempts to establish a joint venture to fund EChemTest® (either through the partnership with an international publisher or a joint venture with some international Chemical Societies) it was possible to arrange a joint COST, EUREKA and ECTN meeting [11] held in Brussels and assemble a EUREKA cluster. The cluster was made of five academic spinoffs [12] members of the "Sustainable entrepreneurship" work-package (WG3) of the EC2T2N2 project and was coordinated by Master-up srl (a spinoff of the University of Perugia acting as an EChemTest® Agency) with the support of CEFIC [13] whose innovation manager (WS) regularly attended the WG3 meetings. Then, in the period 2014-16, the previous QM contract was terminated and the special project ECHEMTEST+ was launched after the approval of the relevant Business Plan (BP). On that ground the cost of a single SES (the EChemTest® key product) was set at 120€ based on the assumption of 1000 fully paid SESs. Then, until June 15, 2016 the available EChemTest® Q&As were checked and ported on EOL. The first training event based on the ported official version of the EOL Libraries was run on October 15. During the whole 2017 the SESs were further checked, a calendar of the annual training events was set for the next years to be held for the TC/ATS coordinators during the ECTN GA and a total of about 2500 SESs were run by the 10 most active TC/ATSs (Budapest, Milan, Krakow, Vienna, Genoa, Kazan, Amsterdam, Thessaloniki, Perugia, Ljubljana) confirming the figures of the BP.

4) A PROOF OF SUSTAINABILITY FOR THE PROSUMER EChemTest® (2016-2017) – The above mentioned results, led to the adoption of the so called Prosumer [14, 15] model for the management the EChemTest® service. In fact, not only the above given number of yearly run SESs are one order of magnitude larger than those run when using QM, but while before the activation of the ECHEMTEST+ project there were only two leading EChemTest® users (Lyon and Helsinki) running a few dozens of SESs per year, during the year 2017 the top TC/ATSs were four (Milan, Budapest, Krakow and Vienna) all running more than 300 SESs each. At the same time new activities were run for assembling the level 4 Q&A libraries of "Cultural Heritage" and

"Computational Chemistry" respectively by Thessaloniki and Perugia, for translating the most popular libraries in other European languages (like Vienna for the German version of the GC1 and GC2 Libraries) and for creating a new one (like Krakow for the "Chemistry for everyday life" one to be used for running students' international contests). In the meantime, though, some sites, like Cologne, Leuven, Reading and Ioannina, ceased their activities mainly because of the retirement (without replacement) of the local ECTN representative, new TCs were activated like the Kazan (Russia) and La Paz (Bolivia) ones shown in Table 1. The key feature of the adopted Prosumer model is the fact that the same subject may act both as producer and as consumer (or user) of the EChemTest® services. An ECTN member may, in fact, use its TC/ATS in order to assess the chemistry competences of either its own students or other students or third parties using also the on line SESs. This allows the offsetting of the Prosumers' debits (due to services used) through credits (associated with services provided) and can be taken care either by a TC/ATS or by an ECTN Agency. Services provided to non ECTN members (as is the case of individuals and third parties) are paid activities handled through the Chem Learn portal [https://chem-learn.com].

5) ECHEMTEST+ MISSION ACCOMPLISHED (2018-2020) – As shown in Table 1 taken from ref. [11], the full operability of the project ECHEMTEST+ proved the validity of the Prosumer model. The table confirms also the intensive use of EChemTest® services made by the Krakow, Milan, Vienna and Budapest TC/ATSs all running each over 300 SESs a year. The Table also confirms the importance of the GC1 and GC2 Q&A Libraries (whose run SESs account for about half of the total) for access to the Bachelor studies in Chemistry. The other half is almost evenly distributed among the AC3, IC3, OC3 and PC3 Q&A Libraries the ones mostly used to access to Master Studies.

TC\LIB	GC1	GC2	AC3	BC3	IC3	OC3	PC3	CH4	Total
AMSTERDAM		56							56
BUDAPEST			79	41	88	84	92		384
GENOVA		40	39		27	41	39		186
KAZAN		98							98
KRAKOW	**360**	174	52		58	60	36		740
LA PAZ	1								1
MILANO	63	2	**128**		**126**	**126**	**126**		571
PERUGIA			2		9	39	4		54
SIENA		12				13			25
THESSALONIKI	17	15						28	60
VIENNA		**447**							447
Total	441	844	300	41	308	363	297	28	2622

TABLE 1: Number of SESs declared as run by the TCs/ATSs in the year 2018 divided by type.

Further information was obtained from the detailed analysis of the credits and debits accumulated by the TC/ATSs while carrying out EChemTest® activities which are shown in Table 2. In green and red respectively In Table 2 Q1 are the SESs run by a TC/ATS for its own University (generating debits) while Q2, Q3 and Q4 are those run by that TC/ATS for another ECTN member, ECTN and a third party, respectively (generating credits). Other SESs generating debits are the Q5 ones (those run by a different TC/ATS that gets the relevant credits). An Institution gets credits for the Q&As created (Q6) or the Q&As revised (Q7) and for the hours spent in dissemination activities (Q8). Overall resulting credits and debits (excluded the first 100 SESs given for free) are shown in the rightmost column. Table 2 singles out in the blue boxes

also the credits declared for services provided either to ECTN or to its members and fully confirms that the credits generated in this way by the Prosumer scheme may largely compensate the debits. accumulated (as is the case of Krakow (NTC.PL)).

Reports for the year: 2018 (closed)	Q1. Number of own sessions run (with no errors)	Q2. Number of sessions run on behalf of other ECTN Members	Q3. Number of sessions run on behalf of ECTN	Q4. Number of sessions run on behalf of an external Institution	Q5. Number of sessions run by any other ECTN Member on my behalf	Q6. Number of hours spent for creating a new library's question	Q7. Number of hours spent for correcting an existing library's question	Q8. Number of hours spent for dissemination activities	CREDITS / DEBITS
NTC.HU	503	0	96	0	0	0	0	0	-1298.50
NTC.AT	546	0	0	0	0	0	0	0	-1561.00
NTC.NL	49	0	0	0	0	0	0	2	0
NTC.RU	123	0	0	0	0	0	20	0	-160.00
NTC.PL	181	411	0	0	0	0	0	0	74.5
NTC.SI	10	0	0	0	0	0	5	0	0
NTC.GR	48	0	0	0	0	0	0	2	0
NTC.SP	0	0	0	0	0	0	25	0	0
ATS.PERUGIA.IT	85	0	0	0	0	0	0	0	0
ATS.MILANO.IT	549	0	0	0	0	0	0	20	-1501.50
ATS.GENOVA.IT	39	0	0	0	0	0	0	0	0
ATS.NAPOLI.IT	0	0	0	0	0	0	0	0	0

TABLE 2: The offsetting of debits and credits for the different TCs/ATSs in the year 2018.

6) THE FINAL IMPLEMENTATION OF THE PROSUMER MODEL – The high level of operability achieved by EChemTest® at the end of the ECHEMTEST+ special project not only fully proved the validity of the Prosumer model but also stimulated a discussion on the use of Open Molecular Science Cloud (OMSC) in computational chemistry research and education. As a matter of fact during the first week of September 2019 (three months before reporting on the ECHEMTEST+ project at the ECTN Administrative Council (AC) in Rome) the 12th European Conference (EUCO) of the Computational and Theoretical Chemistry (CTC) division of EuChemS held in Perugia focused on cloud research and education activities by launching the Molecular Open Science Enabled Cloud Services (MOSEX) project (explicitly related to EChemTest® as debated during the OMSC workshop jointly managed with the US Molecular Sciences Software Institute (MolSSI) at the Accademia Nazionale delle Scienze dei XL in Rome) [16]. Yet, a few weeks after the announcement before the ECTN AC in Rome of the completion of the ECHEMTEST+ project, the unforeseen explosion of the COVID 19 pandemic displaced the ECTN General Assembly (GA), in which such matter was planned for discussion, to September 2020. Yet, at the GA the scene was taken by a debate on the formulation of the Annex to the Budapest EChemTest® MoU. There it became apparent that the differences in the text of such Annex was responsible for a different evaluation of generated debits and credits. Upon a proposal of the ECTN Secretary, the EChemTest® balance was zeroed and a simpler Annex was written (and approved later by the GA and by the TC/ATS coordinators) to come into effect starting fron January 1st, 2021.

7) THE 2021 RESULTS, CONCLUSIONS AND A LOOK FORWARD – The resulting 2021 balance generated by the automatic procedures of the above mentioned Chem Learn portal [17]) is planned for approval by the next ECTN GA on April 2122. Its key data are shown in Table 3. A total of 455 credits were produced by La Paz and Ljubljana for activities on behalf of the Q&A Libraries. No use was made of such credits, though, because the COVID 19 prevented any student activities and the creation of the associated debits. A significant amount of debits was instead generated by Budapest (ntc.hu) for more than 400 SESs. The heaviest user of the EChemTest® SESs was, as in the previous years, Milan that accumulated a debit of 2985.50€. Milan did also gain a credit of 146.67€ thanks to the issuing of IPCs reducing, so far, its debit to 2838.83. In terms of credits use the most positive cases are Genoa and Perugia. For both the overall debit is

either negligible or null (depending on whether they did or not exceeded the quota of free one hundred SESs) while their share of the sum paid by the test takers for getting the IPCs exceeds it. On the contrary, while the IPC incomes of Milan are the largest ones (actually half of the total) they are still largely insufficient to offset the debit that would require that at least 25% of the test takers apply for the IPC.

TC\ATS	PROSUMER CREDIT	PROSUMER DEBIT	IPC INCOME	THIRD PARTY INCOME	INCOMES - DEBIT
BUDAPEST	0	1200.50	0	0	-1200.50
GENOA	0	42	80	0	38
KRAKOW	0	73.50	0	0	-73.50
LA PAZ	437.50	0	0	0	0
LJUBLJANA	17.50	0	0	0	0
MADRID	0	224	0	0	-224
MILAN	0	2985.50	146.67	0	-2838.83
PERUGIA	0	0	66.67	160	226.67
VIENNA	0	997.50	0	0	-997.50
Total	455	5523	293.34	160	

Table 3: Year 2021 credits/debits balance of EChemTest® TC/ATS. Please notice that the debit of Budapest (ntc.hu) for more than 400 SESs has been paid in advance.

As is apparent from the fifth column of Table 3 (third party incomes) an alternative to the increase of the request of IPCs is the promotion of the offer of EChemTest® SESs to third parties. Examples of third party SESs provided to individuals (i.e. not requested through a TC/ATS as discussed in ref. [11]) are **a)** the case of the two EU students having applied individually for a SES to the VEC and **b)** the case of a group of students of the USS G. Donegani of Crotone [18].

YEAR: **2021**

AGENCY	NTC/ATS Referral	SESSIONS	INCOMES (euro)
VEC	ats.perugia.it	2	40
I.T.I. 'G. Donegani' of Crotone (IT)	ats.perugia.it	6	120

Table 4: Year 2021 sessions and incomes from third party activities.

In particular, as shown by the first line of Table 4, in the case of the two students having applied directly to the VEC, the 1/3 fraction of competence of the Agency goes to the VEC. On the contrary, as shown by the second line of Fig. 4, in the case of the Donegani USS, in which the school acted as an Agency by establishing a LEA, the 1/3 fraction of competence of the Agency is

handled by him/her. A final comment on the incomes generated by third party activities is that the VEC may use them either to reward the most active TC/ATS or to promote further activities.

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ISSN: 2279-8773