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# From molecular beam technologies to virtual experiments and communities

**Antonio Laganà**[1]

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**Abstract**
In the last 50 years, the impressive results on chemical kinetics from crossed molecular beam experiments have been assisted by theoretical and particularly computational progress, among which are: (1) the design and implementation of the SIMBEX (SImulation of Molecular Beam EXperiments) procedure on parallel and distributed computers aimed at rationalizing the dynamical behavior of the investigated systems on the ab initio computed molecular interactions; (2) the establishing of theoretical and computational research and educational networks (like the Quantum Reactive Scattering and European Chemistry Thematic Network), the assembling of virtual research communities (like the meta- and the grid-chemistry ones within the Collaboration in Science and Technology (COST) initiatives to enhance synergic and cooperative work levering on highly productive platforms; (3) the participation in the management of both the Italian and the European grid infrastructures initiatives; (4) the development of molecular open science-enabled cloud services within the European Open Science Cloud (EOSC). Levering on the mentioned collaborative efforts, important open science initiatives have been implemented. The present paper illustrates a prototype model apparatus for the production of methane out of $CO_2$ using renewable energy sources and a prosumer (producer–consumer) model for delivering online chemistry competence tests. Finally, a suggestion is made to establish networked local services of the academy for high school education.

**Keywords** Elementary chemical processes · Reactive scattering · Virtual communities · Open science cloud

## 1 From high performance to metachem and gridchem computing

After the establishment in Perugia (Italy) of the pioneering laboratory operating in Europe dedicated to investigating the kinetics of chemical processes by the technique of molecular beams (Boato and Volpi 1999; Aquilanti 2009), an accompanying activity providing theoretical and computational assistance was started (Aquilanti and Laganà 1975; Aquilanti et al. 1980; Laganà 2016).

The importance of exploiting high-performance computing (HPC) came in 1975 under the auspices of CECAM (Centre Européen de Calcul Atomique et Moléculaire), then located in Orsay (Paris) and directed by Carl Moser. A CECAM workshop "Collisions on potential energy surfaces of excited states" was coordinated by William Lester (IBM) and attended by the main experts of the field. Innovative three-dimensional quantum treatments of chemical reactions based on the use of hyperspherical coordinates were discussed together with remote access and distributed computing as a step toward high-throughput computing (HTC).

About 10 years later, most of the participants of the Orsay workshop convened in Cambridge to establish a Quantum Reactive Scattering (QRS) community (Laganà 2014) supporting collaborative efforts in that field based on networked computing. As emphasized in the reports before the latest QRS meeting (Laganà and Manuali 2023), a subset of its laboratories have developed in the years concurrent computing applications and established a QRS-related virtual organization (VO) within the European COST (Collaboration in Science and Technologies)

This paper belongs to the Topical Collection originated from contributions to the conference held in Rome, March 27–28, 2023, on Chemical Kinetics at Micro-, Meso-, Bioscales, dedicated to Giangualberto Volpi (1928–2017, Linceo from 1994) promoted by Accademia Nazionale dei Lincei and Fondazione Guido Donegani.

✉ Antonio Laganà
lagana05@gmail.com

[1] Department of Chemistry, Biology and Biotechnologies, University of Perugia, Perugia, Italy

Action D23 (https://www.cost.eu/actions/D23/) named METACHEM. METACHEM has provided distributed computing resources and effective distributed solutions for chemical applications developed by its member research laboratories to provide new powerful a priori realistic simulations for several scientific, technological and environmental chemical applications. In particular, METACHEM led to the implementation of shared software packages supporting the management of collaborative crossed beam experiments by means of a chain of separate computing steps called SIMBEX (Gervasi and Laganà 2004a, b) based on a data model (and a corresponding software library) called Q5cost aimed at simplifying quantum chemistry (QC) code interoperability by defining both a standard specifically designed for the interchange of data and a converter for implementing it by making it possible to manage huge complex data collections.

Next step was the establishing of D37 (https://www.cost.eu/actions/D37/) GRIDCHEM COST Action adopting the "new information technology tools of Grid computing". The Action was articulated into the following workgroups: (1) PHOTODYN (Computational Photochemistry and Photobiology), (2) QDYN (Quantum Dynamics Engine for Grid Enabled Molecular Simulators), (3) ELAMS (E-science and Learning Approaches in Molecular Science), (4) DECIQ (Code Interoperability in Computational Quantum Chemistry), and (5) CCWF (Computational Chemistry Workflows and Data Management).

As pointed out in its web page, D37 had a strong impact on the Grid implementation of the computational tools dealing with the exact calculations of the dynamical evolution of chemical systems. As a matter of fact, the QDYN project developed out of SIMBEX the more general grid empowered molecular simulator (GEMS) that allows the linking of the grid empowered computational machinery to a large variety of CMB experiments. Actually, as discussed in Casavecchia (2000), in which the detailed articulation of a CMB apparatus is illustrated and the activities of GEMS are ideally tailored to suit the detailed implementation of GRIDCHEM applications. This was confirmed in detail for the OH + CO gas phase reaction thanks to the development of the single stream procedure calculating the measured crossed molecular beam intensity $N_{LAB}(\Theta',t')$ depending on the crossing angle $\Theta'$ and the velocity distribution t' of the reactants (Balucani et al. 2012).

As shown in the top layer of Fig. 1, the first step of the GEMS procedure (INTERACTION) carries out a set of ab initio calculations so as to determine, at various levels of accuracy within the Born–Oppenheimer approximation, the electronic structure of the molecular system and a pointwise representation of the potential energy surface (PES) including the geometries relevant to the evolution of the reactive process.

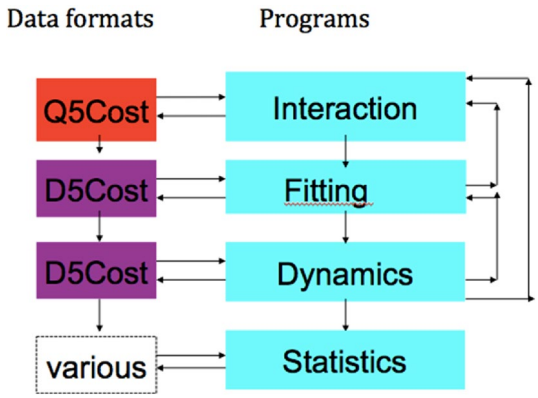


**Fig. 1** The data formats (lhs column) and the computational procedures (rhs column) initially developed within the D37 (GRIDCHEM) COST Action and then adopted by GEMS and, later, by a prototype carbon-neutral fuel production apparatus discussed in Sect. 3

Then, as a second step, the FITTING procedure shown in the second layer of Fig. 1 interpolates the computed ab initio values (after properly complementing them using information available from the literature) to ensure smoothness and physical consistency to the resulting fitted PES as it was the GEMS key target within the European Grid Infrastructure (EGI) activities (https://www.egi.eu).

## 2 The European Grid Infrastructure and the open science cloud

To assemble an integrated (theory, computation and experiment) collaborative distributed infrastructure devoted to the study of molecular processes, the complete GEMS workflow for gas phase processes has to be adopted by adding both the DYNAMICS and the STATISTICS procedures of GEMS to the already mentioned INTERACTION and FITTING ones (see the rhs column of Fig. 1). GEMS, in fact, collects in a single flowchart all that is needed by a detailed accurate description of a gas phase atomic–molecular process starting from the ab initio calculations carried out in the INTERACTION block and then fitting them using a suitable functional form to produce an accurate PES in the FITTING block. Then, the detailed evolution in time of the elementary processes undergone by the considered system on that PES (under the statistically relevant set of initial dynamical conditions) is computed in the DYNAMICS section. After collecting the outcomes of the DYNAMICS section for a statistically significant number of events, an averaging of the dynamical outcomes is performed in the final section STATISTICS to estimate the target measurable properties of the investigated system. As a result of the in-principle unlimited extension of the Grid, GEMS can be considered as the reference workflow for rationalizing gas phase processes

(Balucani et al. 2012). This allows the generalization of GEMS into a meta-workflow suited not only for describing rarified gas phase processes, but also those performed in realistic conditions [including those performed in the condensed phase (Kruger et al. 2017)].

When moving toward open molecular science projects, GEMS has become part the European Open Science Cloud (EOSC) applications within the recently formed HERLA platform (Laganà and Vitillaro 2018) jointly established among the members of the cluster formed by the Perugia sections of CNR and INFN, and the Departments of Physics (PHYS) and of Chemistry, Biology and Biotechnology (CHM) of the University of Perugia, whose scheme is illustrated in Fig. 2.

To better offer its services worldwide and extend them to a higher level, Herla was allocated as a virtual data center on the GARR Palermo node and the relevant images (VHERLA) were transferred on the OpenStack GARR Cloud platform. In 2019 VHERLA started supporting MOSEX (Molecular Open Science Enabled Cloud Services) (Laganà and Vitillaro 2020) https://www.researchgate.net/publication/269398521_A_Grid_Knowledge_Management_System_aimed_at_Virtual_Research_Communities_Sustainability_based_on_Quality_Evaluation. MOSEX is an EOSC pilot (designed as a follow-up of the EGI COMPCHEM VO activities) tailored to offer a global cloud environment for the Chemistry, Molecular & Materials Science and Technology (CMMST) Virtual Research Community (VRC) at large (including, in perspective, the Virtual Research Environment of the already mentioned QRS community (Laganà 2014). The CMMST VRC (https://wiki.egi.eu/wiki/VT_Towards_a_CMMST_VRC) is, in fact, a group of like-minded individuals organized by disciplinary and computational models which play a key role in chemistry. Multi-national scientific communities, after all, can benefit from having VRC EGI partners. For example, they can use the resources and the support provided by the National Grid Initiatives (in terms of workshops, forums and tools) for solving specific technical issues using shared services, the user-focused evolution of production infrastructures, etc.

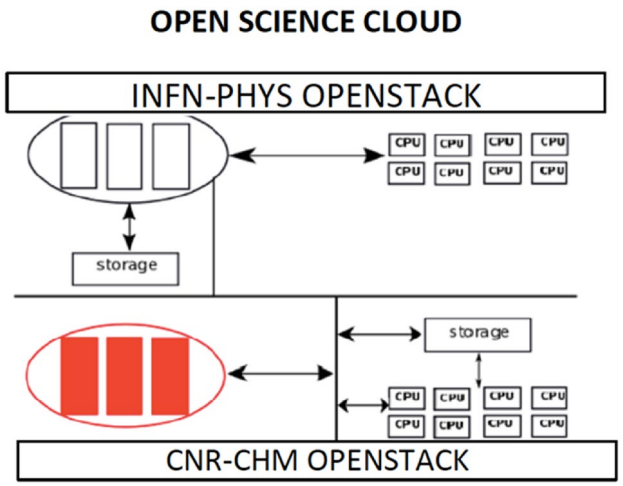


**Fig. 2** The scheme of the Herla cloud platform

As a matter of fact, MOSEX is designed for gathering together and offering services on the cloud in the case of subjects such as molecular electronic structure and dynamics (including the ab initio determination of the relevant analytical potentials), astrochemical processes, drug design tools, distributed repositories of molecular science data, dissemination and evaluation of molecular knowledge, etc. In particular, the CNR–CHM open-stack section of VHERLA is specifically addressed to support the theoretical and computational inorganic chemistry and the computational dynamics and kinetics activities of the Chemistry Department of the University of Perugia as well as the HPC applications of the Department of Mathematics and Computer Science of the University of Perugia and of the Perugia branch of the Research National Centre (CNR) of the Italian Molecular Sciences and Technologies Institute. Accordingly, data handled by MOSEX are useful to convert the outcomes of the computing components of GEMS (associated with the three top lines of the Program (rhs side column of Fig. 1) into measurable properties via the appropriate statistical treatments performed by the statistic treatments associated with the bottom line of that column.

The data formats associated with the sequence of the computational tasks INTERACTION, FITTING, DYNAMICS and STATISTICS of GEMS given in the lhs column of Fig. 1 are Q5COST and D5COST (plus other minor ones) (Angeli et al. 2007). They are useful not only to meet the specific requests of the users of MOSEX when converting the outputs of their computational procedures into properties of the system of their interest, but also to single out the features relevant to organizational and business aspects the community and to the structuring of the relevant business model.

## 3 A prototype carbon-neutral fuel production apparatus

A typical computing activity developed within the MOSEX project is that of the PROGEO reactor producing $CH_4$ (represented in Fig. 3 by a small yellow cloud). The PROGEO reactor (https://en.wikipedia.org/wiki/Sabatier_reaction last seen on march 25, 2023) relies on a Paul Sabatier reactive scheme that produces methane out of $CO_2$ using hydrogen generated by water electrolysis powered by a renewable energy source.

The PROGEO reactor (https://materiali.sostenibilita.enea.it/structure/matpro last seen 26/3/2023) installed at

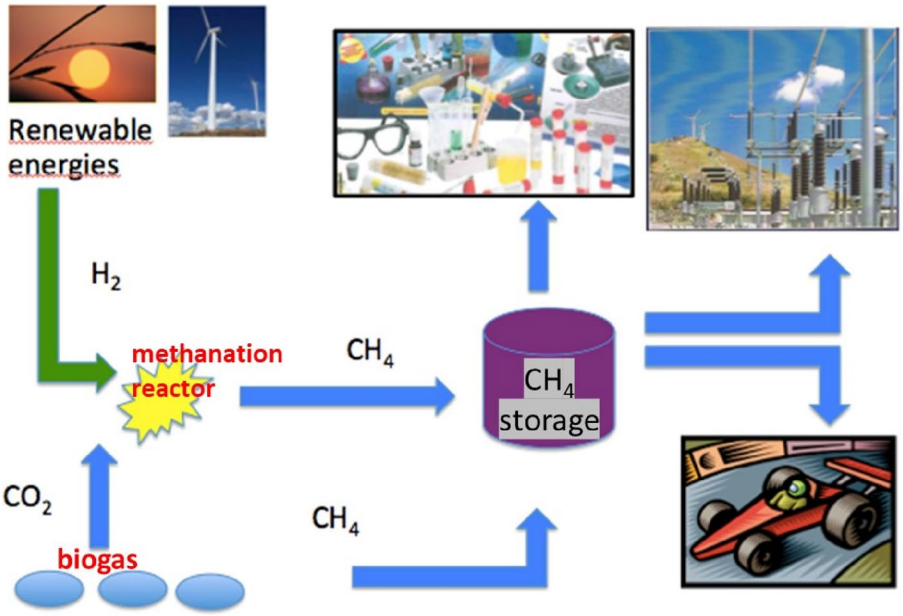


**Fig. 3** Scheme of the carbon-neutral production of $CH_4$ from waste $CO_2$ using $H_2$ generated from renewable energy sources

the Department of "Civil and Environmental Engineering" of the University of Perugia) is a scalable (from 20 kW to 1 MW) apparatus using the solid-state KATALCO$_{JM}$ 11-4MR catalyzer (an Ni-based metal alloy commercialized by Johnson Matthey and modeled by the list of equations given below) of the Paul Sabatier (https://en.wikipedia.org/wiki/Sabatier_reaction last seen on march 25, 2023) type. PROGEO generates methane out of $CO_2$ using the hydrogen generated by a water electrolyzer powered by renewable energy sources.

In the scheme shown in Table 1, the following initial conditions are adopted:

- the equilibrium $E_a$-forward for adsorption of the free $CO_2$ gas on the catalyst surface is set equal to zero,
- the equilibrium $E_a$-reverse for desorption of the $CO_2$ gas from the catalyst surface is set equal to 8.3 kJ/mol),
- the equilibrium $E_a$-forward for adsorption of the free $H_2$ gas on the catalyst surface is set equal to 4.0,
- the equilibrium $E_a$-reverse for desorption of the $H_2$ gas from the catalyst surface is set equal to 77.1 kJ/mol),
- the equilibrium $E_a$-forward for adsorption of the free CO gas on the catalyst surface is set equal to zero,
- the equilibrium $E_a$-reverse for desorption of the CO gas from the catalyst surface is set equal to 127.7 kJ/mol),
- the equilibrium $E_a$-forward for adsorption of the free $H_2O$ gas on the catalyst surface is set equal to zero,
- the equilibrium $E_a$-reverse for desorption of the $H_2O$ gas from the catalyst surface is set equal to 49.0 kJ/mol).

**Table 1** Elementary steps of the kinetic Monte Carlo (KMC) scheme adopted for the modeling to the PROGEO reactor

| Step | $E_a$-forward (kJ/mol) | $E_a$-reverse (kJ/mol) |
|---|---|---|
| $CO_2 + * <-> CO_2*$ | 0.0 | 8.3 |
| $H_2 + 2* <-> 2H*$ | 4.0 | 77.1 |
| $CO + * <-> CO*$ | 0.0 | 127.7 |
| $H_2O + * <-> H_2O*$ | 0.0 | 49.0 |
| $CO_2* + H* <-> COOH* + *$ | 113.1 | 155.6 |
| $CO_2* + 2H* <-> C(OH)_2* + 2*$ | 292.3 | 217.8 |
| $CO_2* + * <-> CO* + O*$ | 93.7 | 169.3 |
| $COOH* + * <-> CO* + OH*$ | 306.8 | 306.7 |
| $C(OH)_2* + H* <-> CH_2O* + OH*$ | 98.7 | 125.7 |
| $CH_2O* + H* <-> CH_2* + OH*$ | 163.7 | 154.1 |
| $CO* + * <-> C* + O*$ | 237.4 | 111.8 |
| $CO* + 2H* <-> CH* + OH* + *$ | 221.4 | 146.1 |
| $2CO* <-> CO_2* + C*$ | 339.6 | 109.0 |
| $C* + H* <-> CH* + *$ | 69.2 | 154.1 |
| $CH* + H* <-> CH_2* + *$ | 68.2 | 61.9 |
| $CH_2* + H* <-> CH_3* + *$ | 71.4 | 105.6 |
| $CH_3* + H* <-> CH_4* + 2*$ | 137.4 | 178.7 |
| $O* + H* <-> OH* + *$ | 137.9 | 116.0 |
| $OH* + H* <-> H_2O* + *$ | 137.9 | 99.9 |
| $H* + * <-> * + H*$ | 13.0 | 13.0 |
| $CO* + * <-> * + CO*$ | 10.0 | 10.0 |
| $O* + * <-> * + O*$ | 48.0 | 48.0 |
| $OH* + * <-> * + OH*$ | 21.0 | 21.0 |

To accelerate convergence of the calculations, the pre-exponential factors for the diffusive processes were multiplied by a scaling factor, enabling the extension of the simulations to longer times (while checking that no change in the final results occurs). Further care was taken to ensure that the used unit cell contains more than one site. As reported in Martì Aliod (2018) the prototype machine confirmed both the validity of the implemented technologies and the importance of modulating the pressure of the involved species by segmenting the reactor in different sectors and adopting, at the same time, a finite volume reactor to reach convergence between the initial and final total and partial pressures.

An interesting way of reducing the empiricism of this approach is to focus on using pure gas phase processes, managed by means of proper quantum treatments (as is the case of $CO_2/H_2$ plasma mixtures generated by microwave discharges in which cases one can convert $CO_2$ into a mixture of $CH_4$ and other interesting molecules). An approach of this type has been adopted when dealing with $OH + CO$ (Balucani et al. 2012) and with the $H_2 + CO_2$ case (Capriccioli et al. 2017). $CO_2$ can be, in fact, doubly ionized by UV rays to the $(CO_2)^{2+}$ metastable dication, whose short time life leads to a Coulomb explosion into the $CO^+$ and $O^+$ fragments bearing a high kinetic energy (ranging from 2 to 6 eV). More in general, the project not only implies the regulation of the conditions in which the $H_2 + CO_2$ reaction maximizes the desired product yield, but it deals also with the problem of using different biogas sources to unveil the discovery and the development of new pure gas phase technologies. It allows, in fact, the generation of high-resolution molecular beams coupled with electronic and mass spectroscopy to investigate the microscopic dynamics of chemi-ionization processes in single collision experimental conditions by resolving the different reaction channels in single quantum states and characterizing completely the structure and the properties of the relevant transition state of the process (Falcinelli et al. 2018).

## 4 Quality of users and quality of services

Figure 4 illustrates the information on which the procedures used to deliver cloud services are managed, monitored, and turned into account items using the GriF (Grid Framework) and the GCreS (Grid Credit System) tools.

As shown in Fig. 4, GRIF is made of two Java servers (YC, the Consumer, and YR, the Registry servers) and one Java client (YP, the Provider). The entry points to the computational platforms are the user interfaces (UI) which are able to capture, out of the data supplied by the monitoring sensors of the distributed computing infrastructure (DCI), the information relevant to a proper management of the used computational applications and articulate them into sequential, concurrent or alternative quality paths by adopting a service-oriented architecture (SOA) and Web services. This allows at the same time the guided search for the compute resources on the DCI and the evaluation of the quality of the user (QoU). The computational services provided by the DCI are necessary to regulate the submission of the tasks, the monitoring of the activities, and the collection of the results of the simulations. Credits are then assigned (relying on a community agreed metrics) to evaluate the QoU, the quality of service (QoS) and the resources ranking (RR)

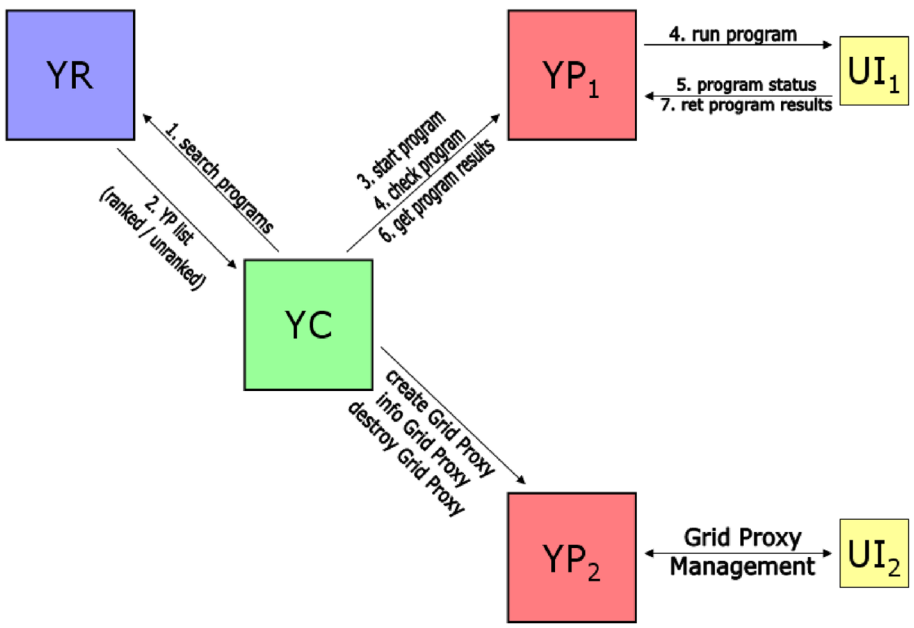


**Fig. 4** Sketch of the GriF flowchart and of its server and user interfaces

of the activities offered as a service using the GriF and the GCreS tools developed by the CMMST VRC and its VOs.

A scheme of this type was first implemented by the COMPCHEM VO and later adopted (after adaptation) by CMMST and the other VRCs. Relying on the past experience of the member VOs, the use of GCreS to reward both the QoU (for compute resources and applications) and the QoS (for provision of the service to the other members of the community) makes it possible to assign the users with a congruent amount of credits (according to the agreed mechanisms). A detailed general discussion of the definition and use of the QoU evaluation parameters is given in Martì Aliod (2018). These credits, redeemable in terms of a preferential utilization of the community resources (selection of compute systems, DCI services, low- and high-level capabilities, memory size, cpu/wall time, storage capacity plus financial resources) do not only foster collaboration among the members of a community, but also motivate related researchers to participate in the multi-competence teams committed to undertake even more ambitious and challenging bids. This has, obviously, resulted in an enhancement of the competition among different teams (competitive collaboration) to further promote the production of tools fostering the establishing of virtual communities and the dissemination of the knowledge produced.

## 5 The ECHEMTEST prosumer model

Among the activities of the European Chemistry Thematic Network Association (ECTN) (a non-profit making association registered in Belgium as an outcome of 6 years of activity (1996–2002) of the homonymous network) made of over 120 members coming from 30 different European countries and with associate members worldwide, a virtual education community (VEC) has been established. The VEC has developed a multi-lingual series of online tests (ECHEMTEST) that can be used for certification/validation of competence in chemistry at various levels (interested institutions can apply for membership and get involved in using/providing cloud services made sustainable by the adoption of appropriate QoU and QoS evaluation mechanisms. At the basic level, provision/usage of hardware and software and relevant credits/debits assignment are simple to define and measure as is the case of the online design and distribution of learning objects (LO) (Bastianini et al. 2011) in science an technologies (often referred to as STEMs).

The most advanced and innovative service is the management of exams online (EOL) tools like those designed to evaluate chemistry competences (Gervasi and Laganà 2004a, b) carried out by the federation of collaborative test centers (TC) established at some of the universities belonging to ECTN and having joined the relevant VEC activities (see Table 2). Going into more detail, the relevant ECHEMTEST libraries of questions and answers (Q&A) designed (and sometimes associated with relevant LOs) to support the acquisition and the assessment of chemistry competences are articulated as follows:

- -Level 1: upper secondary school, General Chemistry 1 (GC1),
- -Level 2: university access, General Chemistry 2 (GC2),
- -Level 3: end of bachelor studies (Analytical Chemistry 3 (AC3)**;** Biological Chemistry 3 (BC3)**;** Chemical Engineering (CE3)**;** Inorganic Chemistry 3 (IC3)**;** Organic Chemistry 3 (OC3)**;** Physical Chemistry 3 (PC3)).

The assessment of competence at the various levels and subjects is carried out by running for each of them a 1 h-long self-evaluation session (SES) articulated in a set of 30 questions/answers selected randomly among those of a proper level of difficulty. The activation of the various SESs at the different TCs is managed using the various GriF tools implemented in EOL.

**Table 2** The ECHEMTEST annual (2018) global report

| Test Center | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | BALANCE/€ |
|---|---|---|---|---|---|---|---|---|---|
| Amsterdam | 49 | - | - | - | - | - | - | 2 | 0 |
| Budapest | 503 | - | 96 | - | - | - | - | - | -1298.50 |
| Genoa | 39 | - | - | - | - | - | - | - | 0 |
| Kazan | 123 | - | - | - | - | - | 20 | - | -160.00 |
| Krakow | 181 | 411 | - | - | - | - | - | - | 74.50 |
| Liubljana | 10 | - | - | - | - | - | 5 | - | 0 |
| Madrid | - | - | - | - | - | - | 25 | - | 0 |
| Milan | 549 | - | - | - | - | - | - | 20 | -1501.50 |
| Perugia | 85 | - | - | - | - | - | - | - | 0 |
| Thessaloniki | 48 | - | - | - | - | - | - | 2 | 0 |
| Vienna | 546 | - | - | - | - | - | - | - | -1561.00 |

The report of the year 2018 given in Table 2 shows that the number of SESs activated at the various accredited test sites (ATS) or national test centers (NTC) during that year were as follows: Milano (786), Budapest (749), Krakow (618), Vienna (477), Madrid (149), Kazan (117), Genova (109), Ljubljana (68), Amsterdam (53), Siena (48), Perugia (47), Thessaloniki (42), and La Paz (1). The SESs were run mainly in the presence at an official ECTN TCs and partly remotely online at one of the properly equipped ECTN TC. A key advantage of EOL is, therefore, a full free sharing among the community members of the teaching and assessing materials with no limitations on the number of member institutions and users involved. Accordingly, in the Web-based scheme adopted by EOL, the user interface interacts with the content manager and with the online assessment system with no limits. This means that, in principle, from any of the local ECTN TCs, the student after registering can access the desired material and run any SESs for the chosen subject and language (among those available) and leave the session at the end (standard ECHEMTEST SESs are made of 30 randomly selected questions matching the chosen level of difficulty). To enhance the sustainability of ECHEMTEST, the GriF side of the accounting system adopts the innovative Prosumer (producer–consumer) scheme (Franciosa et al. 2018). This allows the institutions carrying out ECHEMTEST operations to lever on the following debit–credit compensation rules which are illustrated with the help of Table 2 quoting the outcomes of the year 2018:

- DEBIT—Q1 indicates the SESs run at a TC on behalf of its own university, and Q5 indicates the SESs run by a different subject on behalf of the one being considered;
- CREDIT—Q2 indicates the SESs run at a TC for another ECTN member university, Q3 indicates the SESs run for ECTN as such, Q4 indicates the SESs run for a third party, Q6 indicates the hours spent in creating questions for a new library, Q7 indicates the hours spent in correcting existing questions, and Q8 indicates the hours spent for dissemination activities;
- TC OVERALL CREDITS/DEBITS BALANCE—the rightmost column shows the resulting credit (green) or debit (red) after taking into account the bonus of the first 100 free SESs assuming that the relevant university is actively contributing.

It is, however, to be commented here that, in some cases, the data reported in the table provided by the involved universities differ (sometimes significantly) from those recorded by LibreEOL.

The global report of the sessions run in the year 2018 given in Table 2 for the different (Q1–Q8) services and the final annual balance (credits in green and debits in red) single out that (figures evidenced in blue are concerned with the SES provided by the corresponding TC on behalf of ECTN itself or another ECTN member) the cost of ECHEMTEST is not only quite low when adopting the PROSUMER model, but it can even produce positive outcomes (or credits for further actions) as is the case of the NTC.PL of Krakow.

## 6 Conclusions

In the present paper, we discuss the impressive evolution of networked computer activities into a worldwide extended highly interacting grid of collaborating entities that has at present led to the establishing of open science clouds and tightly collaborating virtual communities. We are pleased to conclude by mentioning that there are undergoing attempts to extend the online ECHEMTEST General Chemistry Self-Evaluation Sessions of ECTN to upper secondary schools. As a matter of fact, it is a pleasure for the author of the paper to mention that some ECHEMTEST sessions have been officially performed by the Donegani Technical Institute of Crotone, IT, by appointing a local ECTN advisor (LEA) (Lasta and Maggiore 2021). In that case, the quality of its students wishing to access the General Chemistry 1 level was certified with the technical support of the University of Perugia Test Center. We are pleased also to mention that, as shown in Table 2, there has been for a certain number of years a European contest for students wishing to access the European chemistry studies. Relevant outcomes have been reported at a recent meeting of the Italian Accademia dei Lincei in Rome, March 27–28, 2023 where it was suggested to promote the establishing of some common cloud educational-scientific clusters of universities, research centers and upper secondary schools.

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## Declarations

**Conflict of interest** The author declares no conflict of interest.

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