A WELCOME TO QRS: THE ITINERARY TO A VIRTUAL COMMUNITY

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The editors of Virt&l-Comm are happy to host the contributions submitted by the participants to the 2022 edition of the Quantum Reactive Scattering (QRS) workshop organized by Gyorgy Lendvay (GL). The abstracts confirm the evolution of the focus of the workshop towards larger and more complex chemical systems as well as towards higher levels of handling reactive chemical dynamics research and applications as well. Accordingly, as editors of Virt&l-Comm, we suggest the authors to submit as soon as possible the relevant extended papers for which we shall adopt a simplified publishing track. At the same time, we provide below some indications on how the members of the QRS group may organize themselves as members of a Virtual International Research, Teaching & Learning Community (whose acronim is indeed VIRT&L COMM) to the end of getting involved in the provision of relevant Cloud Enabled Services within the European Open Science Cloud (EOSC) initiatives.

1) TOWARDS DISTRIBUTED COLLABORATIVE COMPUTING CLUSTERS – The structuring of the European distributed computing infrastructures occurred through projects built and nurtured by the European initiatives Enabling Grids for E-sciencE (EGEE) [https://eu-egee-org.web.cern.ch/], first, and then consolidated by the European Grid Infrastructure (EGI) [https://www.egi.eu/] starting from the beginning of the present century. Indeed, Chemistry activities aimed at establishing research and innovation networks called Metalaboratories *(clusters of geographically distributed Laboratories working in a co-ordinated way on a common project by sharing manpower, hardware and software to foster innovative solutions for chemical applications and a new paradigm for collaborative research)* started to be supported by the European COST (COoperation in Science and Technology) Initiative by funding the **D23** COST action **METACHEM** [https://www.cost.eu/actions/D23/] (17/10/2000-18/07/2005). In order to make Metacomputing evolve into the grid based computing of EGI, the **D37** COST Action **GRIDCHEM** [https://www.cost.eu/actions/D37/] (06/07/2006-05/07/2010) was later started. The D37 Action was articulated into 5 clusters of laboratories with a large participation of the members of the QRS group:

- PHOTODYN: **Computational Photochemistry and Photobiology** - H. Lischka (Vienna), W. Gansterer (Vienna), T. Muller (Julich), V. Bonacic-Koutecky (Berlin), J. Pittner (Prague), H.D. Meyer (Heidelberg), H. Koppel (Heidelberg), M. Persico (Pisa), P.G. Szalay (Budapest), H.P. Luthi (Zurich), S. Leutwyler (Berne), Z. Maksic (Zagreb);

- QDYN: **Quantum Dynamics Engine for Grid Enabled Molecular Simulators** - A. Lagana (Perugia), G. Balint-Kurti (Bristol), E. Garcia (Vitoria), J.M. Launay (Rennes), G. Lendvay (Budapest), U. Manthe (Bielefield), S. Farantos (Crete), G. Nyman (Goteborg);

- ELAMS**: E-science and Learning Approaches in Molecular Science** - O. Gervasi (Perugia), M. Valle (Manno), A. Gomes (Santiago de Compostela), P. Mimero (Lyon), J. Froelich (Vienna), E. Varella (Thessaloniki);

- DECIQ: **Code Interoperability in Computational Quantum Chemistry** - E. Rossi (Bologna), G.L. Bendazzoli (Bologna), S. Evangelisti (Toulouse), M. Kallay (Budapest), K. Baldridge (Zurich), R. Kenneth (Tromso), R. Cimiraglia (Ferrrara), V. Vallet (Lille), J. Sanchez-Marin (Valencia);

- CCWF: **Computational Chemistry Workflows and Data Management** - T. Steinke (Berlin), H.P. Luthi (Zurich), M. Brandle (Zurich), T. Clark (Erlangen), P.M. Rust (Cambridge), H. Rzepa (London), A.M. Marquez Cruz (Sevilla), J. Fernandez Sanz (Sevilla).

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2) FROM COLLABORATIVE CLUSTERS TO A VIRTUAL ORGANIZATION – As a result of the collaborative activities carried out within the COST Actions, the above mentioned clusters reorganized themselves as a not-for profit Virtual Organization (VO). The VOs use a Service Oriented Approach (SOA) relying on machine-machine interoperability based on the Simple Object Access Protocol (SOAP) [https://www.w3.org/TR/soap/]. The services are software components with well defined implementation independent interfaces. In this way the service interface (the what) can be used by clients (consumers) who do not need to care about its implementation (the how). This allows the utilization of services offered by other users (persons, institutions, organizations, etc.) acting as Providers. The monitoring of services (both internal and external to the VO) either used or provided allows to build an economy of debits and credits. For this purpose a Java based Grid Framework (GRIF) [1] has been implemented. As an example, we show below in Fig. 1 the scheme of GEMS (the Grid Empowered Molecular Simulator) [http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/96] of interest for QRS members (blue boxes are services provided by QDYN) when undertaking reactive scattering investigations.

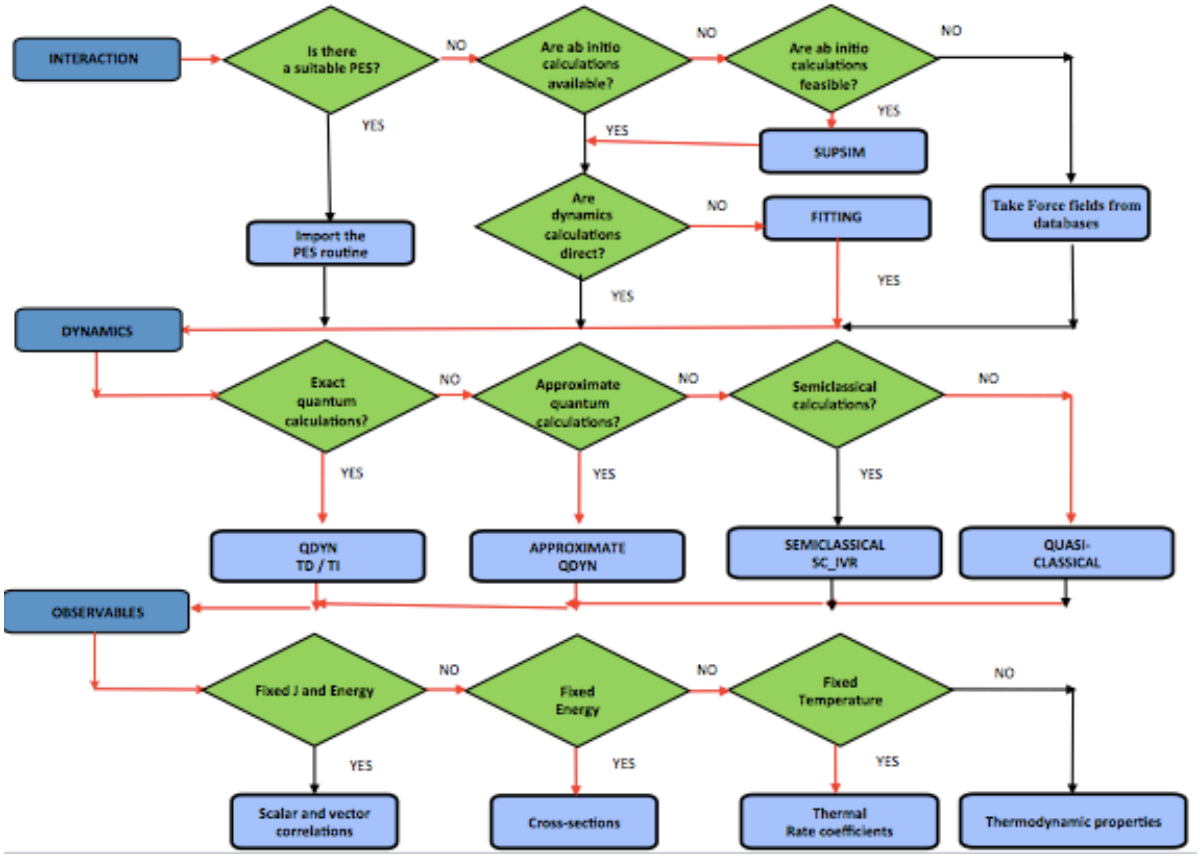

Fig. 1 - The block diagram scheme of GEMS

3) PROSUMER MODEL IMPLEMENTATION OF EDUCATIONAL SERVICES – An analogous approach has been adopted to the end of providing as services the educational products developed by the European Chemistry Thematic Network (**ECTN)** by referring in particular to the activity of its Virtual Education Community (VEC) committee levering. In particular we refer here to the use of interoperable technologies based on advanced networking and semantic web approaches developed by the above mentioned **ELAMS** cluster in order to carry out extended e-assessment tests of Chemistry competences (EChemTest®) to virtually all member Universities of ECTN. Using an extension of the SOA called Prosumer (Producer-Consumer) in some countries a National Test Centre (NTC or, shortly, TC) coordinating, where

feasible, various Accredited Test Sites (ATS)s for local activities it has been possible to conjugate the activities of creating and extending the service. Data accumulated by the TC/ATSs on the Chem Learn portal while carrying out the EChemTest® activities are shown in Fig 2 where 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). [http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/257].

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

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

4) THE VO AND THE EUROPEAN OPEN SCIENCE CLOUD (EOSC) INITIATIVE – At present relevant computational activities of the VO have been transferred into the European Open Science Cloud (EOSC) Initiative in order to make them accessible to the Molecular Science community at large. To this end a cloud platform was activated at the University and the CNR SCITEC Section of Perugia, and its OpenStack cloud image (VHERLA) was implemented at the GARR Cloud node of Palermo as a Virtual Data Center. VHerla services are intended to produce/discover datasets querying metadata, access/download datasets, run/check/terminate experiment/computations using downloaded data, intermediate data, incorrect/useless runs, preserve correct results for further use, support reproducibility of extremely large and streaming data when input data set(s) cannot be stored, annotate, curate, preserve produced data by cycling from raw measured data, to annotated experimental data and metadata for a better re-use, to simulation based formulation of mechanism and observables for consistency checks. The cycle is repeated to a satisfactory convergence for validated availability in cloud. This is meant to operate on behalf of MOSEX (the Molecular Simulator Enabled Cloud Services being implemented on VHerla) to the end of supporting the above described GEMS. [http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/278]

References

1]_C. Manuali, A. Lagan\`a: GriF: A New Collaborative Framework for a Web Service Approach to Grid Empowered Calculations, Future Generation Computer Systems, 27(3), 315-318 (2011).