VIRT&L-COMM

Electronic Magazine for Virtual
Innovation, Research,
Teaching & Learning Communities

Vol. 1 (2012)

Published by:
MASTER-UP S.R.L.
Frequency: 2 issues per year
ISSN: 2279-8773

Virt&l-Comm is a new international online electronic scientific magazine offering a forum for presenting the work carried out by Virtual Innovation, Research, Teaching & Learning Communities. This magazine is the result of a joint endeavour of the COMPCHEM Virtual Organization (VO), of the European Chemistry Thematic Network (ECTN) Association and of the University of Perugia spinoff Master-Up.

Virt&l-Comm is a scholarly open access online Magazine requiring no payment neither from the authors nor from the readers.

Virt&l-Comm publishes at present two issues per year to promote Molecular and Materials Science, Teaching and Learning, Computer Science research. The magazine is also specialized in education and innovation and focuses on Service Oriented approaches. Therefore, in addition to articles, news, projects, reports of (successful or failed) attempts to build services relevant to the field of interest, lists of best practices, products used, the advantages and disadvantages of the solutions adopted will be considered for publication. In particular, all the information useful to build the puzzle of innovative complex applications in education (EDU), information and communication tecnology (ICT) and research and development (R&D) in Molecular and Materials science are welcome.

Table of contents

Part I

EDU: educational

WP5 Virtual Campus

ANTONIO LAGANÀ
Department of Chemistry, University of Perugia, Italy

Attachment: https://www3.compchem.unipg.it/virtl-comm/sites/default/files/virtlcomm12_v1_p2_attach.pdf

Activities planned in the original proposal for the tasks of developing a CoP environment and designing and developing a software for the distributed management of learning objects have been successfully carried out in the first two years of the project thanks also to the exploitation of the outcomes of some ICT European projects (EGEE and COST) as indicated in the WG reports (twice a year), in the WG sessions at the annual meetings, in the network newsletter and in four scientific publications.

Part II

R&D: research and development

Theoretical study of chemical bond in heterogeneous gold catalysis

GIOVANNI BISTONI, FRANCESCO TARANTELLI
Department of Chemistry, University of Perugia, Italy

Attachment: https://www3.compchem.unipg.it/virtl-comm/sites/default/files/virtlcomm12_v1_p4_attach.pdf

In 1987 Haruta and co-workers [1] discovered that very small gold nanoparticles are active for the CO oxidation. In the same years Ito et al. reported the first example of a catalytic asymmetric aldol reaction [2] using a gold(I) catalyst in homogeneous conditions. After this discoveries, the catalytic ac- tivity of gold has been the subject of increasing interest by the scientific community and now is one of the fastest growing fields in chemical research. Gold capabilities in catalysis were summarized in several reviews (see for instance [3]) but such is the frequency of current discoveries that new re- views are required regularly. Over the years, gold has shown astonishing activity in heterogeneous catalysis in which gold nanoparticles, supported or unsupported, are active catalysts in a wide range of reactions. At the same time also homogeneous gold catalysis has proven to be a valuable tool in the hands of chemists [4, 5, 6, 7, 8, 9]. [...]

A research project on gas molecule flux through single wall carbon nanotubes

DILARA OKSUZ[a], NOELIA FAGINAS LAGO[b]
[a]Faculty of Sciences, Gazi University, Turkey
[b]Department of Chemistry, University of Perugia, Italy

Attachment: https://www3.compchem.unipg.it/virtl-comm/sites/default/files/virtlcomm12_v1_p5_attach.pdf

The storage of hydrogen by adsorption using various new forms of carbon-based materials has recently gained widespread attention as one of the key components of a future hydrogen economy. The emerging use of proton exchange membrane (PEM) fuel cells for stationary power generation and for vehicle applications depends on efficient hydrogen storage. Carbon-based materials are typically lightweight, due to the low atomic mass of carbon, which helps improve gravimetric energy storage density [1]. According to the US Department of Energy, a carbon material needs to store 6.5% of its own weight in hydrogen to make fuel cells practical in cars [2]. [...]

A research project on ion permeability and selectivity through molecular pores using functional groups

HANIF MUHAMMAD KHAN, LEONARDO PACIFICI
Department of Chemistry, University of Perugia, Italy

Attachment: https://www3.compchem.unipg.it/virtl-comm/sites/default/files/virtlcomm12_v1_p6_attach.pdf

Waters and ions are essential for life. Hence, understanding of ion permeability and selectivity gives us better insight for scientific investigations, including biological research since ion permeability through molecular pores determines many properties of cell membranes. Investigations of the electrical properties of the membrane of excitable cells are of great interest for neuroscientists and to develop the model for ionic transport through such small-scale pores [1]. Another potential application may be for desalination technology [2]. The major pathway for ion transport through the membrane of excitable cells is represented by voltage-gated ion channels [3]. These are transmembrane proteins endowed with an aqueous pore that allows the passage of certain ions, while excluding others, a property called selectivity. For example the neuronal action potential, the electrical message propagating throughout the nervous system, involves the sequential opening of two types of voltage-gated ion channels, respectively selective to Na+ and K+ ions. It is, therefore, important for physiological studies to single out the structural determinants governing the passage of ions through ion channels, and to identify the mechanism by which they select the various ions. It also indicates that selectivity properties can be implemented on other industrial applications such as desalination technology [2]. Also, Ion selectivity under different radii hydrophobic pores has been investigated [4]. CNTs have been already used for modeling micropores and their properties [2,4-8]. [...]

Part III

ICT: information and communications technology

A gem of user

NEASAN O'NEILL
EGI Regional Dissemination Coordinator

From EGI Newsletter.

How much grid does one person need? Well one man, Professor Ernesto Garcia Para, apparently needs a lot. He has used over **15 millions** hours of CPU on the European grid since he started in the year 2006 and his work is expected to still go strong doing **5 millions** alone this year.

Based at the University of the Basque Country in Vitoria, Prof. Garcia and his team are interested in investigating what is going on at the atomic level in chemical reactions. This is obviously a very wide field and the reactions studied have many applications. Prof. Garcia's recent results have mostly studied reactions in our atmosphere including how they are affected by carbon emissions or their impact on spacecraft re-entry.

Back in **A YEAR** Prof. Garcia started using the grid, "**We couldn't do our research without computers, the days of the back of an envelope or the blackboard are well gone. However doing detailed calculations of reactions takes a long time on the standard resources available to us. To be honest when I was first shown the grid I was a little sceptical but decided that if it delivered on its promises it would be a boon to our field**".

Prof. Garcia combines cutting edge theoretical chemistry with computer modelling, with the aim of examining, and making predictions about, real world scenarios. Taking into account as many variables as possible to produce something that obeys theory but also matches experimental results requires enormous computing resources. As prof. Garcia explains "**On the face of things some of the reactions we are investigating look quite simple but saying A+B give you C+D hides a huge amount of complexity. What are the intermediate steps, what part does the local conditions play, can the reaction go backwards? This made even a "simple" reaction that involves only 3 atoms extremely problematic and sometimes assumptions needed to be made to interpret crossed molecular beam experiments, adding errors to the final results**."

Thankfully the professor and his team are not alone. Computational chemistry was one of the first communities outside high-energy physics that saw the potential of grid and so there were applications already there for them to try out. As the infrastructure has matured so have these tools. Prof. Garcia

has seen this progress first hand and is very thankful "**When we started the tools were useful but slightly crude. Now the guys at the University of Perugia have developed the Grid Empowered Molecular Simulator (GEMS), which makes my life a lot easier".**

One of the people at Perugia is **Prof. Antonio Lagana** from the university's Department of Chemistry coordinating a joint team of Molecular and Computer scientists, "**The grid is powered by virtual organisations (VO), collections of users and institutes with a common research interest. I think one of the most important steps was the creation of the COMPCHEM VO. This gave new, wary, users instant access to resources and applications but more importantly it gave them a support network and a way for them and developers to communicate**".

At the heart of the GEMS application is its "blocks", making it modular and customisable for each user. Each block performs a certain kind of calculation and can be used or discarded, as the user wants. More importantly the user determines the code/algorithm each block uses, so that they are working with what they know. It has also tackled another problem, "**The lack of standard data formats has plagued this community for years**", says **Prof. Lagana**, "**This has made collaboration difficult as the different codes people use just simply can't talk to each other. During our work on GEMS we have made some progress on this. We needed the different blocks and codes to be able to exchange information so we have developed and adopted standards that will benefit even the non-grid users in our community**".

HIPEG: a project for a High Performance Grid bridging HTC and HPC in scientific computing

ANTONIO LAGANÀ[a], CARLO MANUALI[a],
ALESSANDRO COSTANTINI[a], ELDA ROSSI[b], MARCO CARPENÈ[b],
ANTONIA GHISELLI[c], MARCO CECCHI[c]
[a]Department of Chemistry, University of Perugia, Italy
[b]CINECA, Casalecchio di Reno, Italy
[c]CNAF-INFN, Bologna, Italy

Attachment:
https://www3.compchem.unipg.it/virtlcomm/sites/default/files/virtlcomm12_v1_p10_attach.pdf

The project aims at developing a tool suited to redirect transparently the jobs or job sections (submitted by the COMPCHEM community to the Grid) to the most appropriate platform by choosing between the machines of the Grid and those of the Large Scale Facilities partner of the project according to the resource request of the job. The proposed tool (to be developed as a WfMS integrating the GriF framework of COMPCHEM or any other software suited for that purpose) will facilitate the use of the Grid for scientists unwilling (or unable) to deal with the technicalities of the middleware. For testing and validating the implemented tools two types of applications requiring either high throughput first and then high performance computing or high performance first and then high throughput computing will be implemented.

Tools for VRCs

JAMIE SHIERS
CERN, Genève, Switzerland

Attachment: https://www3.compchem.unipg.it/virtlcomm/sites/default/files/virtlcomm12_v1_p11_attach.pdf (freely derived from D.6.4 EGI Inspire documents)

In order to perform production and analysis tasks across a highly distributed system crossing multiple management domains, powerful and flexible monitoring systems are clearly needed. The Experiment Dashboard monitoring system was originally developed to support the four main LHC experiments (LHCb, CMS, ATLAS, ALICE). This framework not only supports multiple grids / middleware stacks, including gLite (EGEE), VDT (OSG) and ARC (NDGF), but is also sufficiently generic to address the needs of multiple user communities including, but not limited to HUCs.

Furthermore, the system covers the full range of the experiments computing activities (job monitoring, data transfer, site commissioning etc.) and addresses the needs of different categories of users (computing teams of the LHC VOs, VO and WLCG management, site administrators and VO support at the sites, users running their computational tasks on the grid infrastructure etc.)

Experiment Dashboard applications are widely used by the LHC experiments for their everyday work and receive over a thousand unique visitors every day and this number is steadily growing.

Heavy Users Communities

JAMIE SHIERS
CERN, Genève, Switzerland

Attachment:
https://www3.compchem.unipg.it/virtlcomm/sites/default/files/virtlcomm12_v1_p12_attach.pdf
(freely derived from D.6.4 EGI Inspire documents)

HUCs are Virtual Research Communities (VRCs) that have been using EGEE and EGI routinely and thus have become more structured and advanced in terms of grid usage. These communities focus on domain specific issues, such as how to access High Energy Physics applications on EGI, how to enable new physics experiments on EGI and so on. On the one hand these teams are operated by external projects, such as WLCG, but on the other hand have members in the WP6 work package (also called SA3) of EGI-InSPIRE. The effort of the distributed WP6 team of EGI-InSPIRE is targeted towards the provision of shared services that will ease the porting of new applications from these scientific domains to the wider grid by detecting and exploiting commonalities between VOs and driving the implementations to a generic direction. At the same time inter-VO collaboration results typically not only in more powerful solutions, but also saves significant amounts of manpower in the long run. Such benefits would be unlikely to be achieved with generic support structures, both for individual large communities such as HEP (which could otherwise develop multiple similar solutions to basically common problems), as well across disciplines. In conclusion HUCs offer benefits not only to new adopters of grid technology but also to each other. This continues to be demonstrated, both by the adoption of tools initially developed for one community spreading to others, as well as at the conceptual level: less optimal but offering a more pragmatic solution for existing communities.