

Química, computació i societat, a la JOCS'11

La desena edició de la Jornada Catalana de Supercomputació, organitzada biennalment pel CESCA, ha tingut lloc a la Universitat de Barcelona (UB) sota el lema “Química, computació i societat”. La jornada, que ha comptat amb una sessió de pòsters, ha tractat sobre els reptes de la química computacional, el seu futur i com la seva aplicació contribueix a la millora de la nostra societat.

Els encarregats d'obrir la trobada han estat Pere Lluís Cabot, degà de la Facultat de Química de la UB, i Josep Maria Martorell, director general de Recerca de la Generalitat de Catalunya. Cabot ha destacat que l'edició d'enguany de la JOCS coincideix amb la celebració de l'Any Internacional de la Química, que “té entre els seus objectius la transmissió a la societat de la importància de la divulgació d'aquesta disciplina”. “És indubtable que estem envoltats de química –ha afegit– i en aquest sentit cal transmetre la seva importància, així com els seus beneficis”.

Martorell, qui es va llicenciar a la Facultat de Física de la UB, a tocar de la de Química, ha recordat el seu pas per aquest centre “ple de bons records”, i ha destacat el bon lloc de la ciència a Catalunya i el fet que el Govern ha tingut i té el compromís que aquesta posició es continuï mantenint els propers anys, seguint amb les línies bàsiques de les polítiques científiques dutes a terme tot i els canvis de govern.

Citant el conseller Mas-Colell, el director general ha afirmat que “la sensació és que hem pujat de la planta baixa a un primer pis, hem pujat per les escales, amb uns graons ben alts, ara tenim 2 o 3 anys per descansar, però després hem de pujar al segon pis”. Per a Martorell, “el 2012, en matèria de recerca, no serà un mal any, tot i que no serà de creixement” i ha afegit que “com a Govern tenim clar que aquest és un àmbit prioritari”.

El director general ha destacat el paper del CESCA i de la Xarxa de Referència Química Teòrica i Computacional (XRQTC). “Si parlem de ciència i computació, tenim dos grans exemples: XRQTC i CESCA”. “Els processos d'agregació estalvien molts diners –ha comentat– i el CESCA és un bon exemple de consorci de serveis”. Martorell ha afirmat que “ha estat una molt bona iniciativa, ja que la compartició ha permès tenir el doble de serveis per la meitat del preu”.

La cloenda ha estat a càrrec de Francesc Illas, de la XRQTC, i Miquel Duran, de

la UdG. Illas ha afirmat que “la química teòrica computacional és un camp saludable, almenys tant com la química, formada per una comunitat àmplia i activa”. Duran, qui ha coincidit amb Illas en agrair als organitzadors aquesta jornada que ha definit com a “exitosa”, ha fet un breu repàs de les dues sessions “on s'ha parlat d'oportunitats, d'algoritmes, de computació quàntica...”. Duran ha destacat el rol del CESCA “proveïdor des de 1991 de recursos computacionals, amb suport i consultoria, però també d'altres serveis, com les comunicacions i l'e-Administració”.

La JOCS'11 s'ha dividit en dues sessions. La primera, moderada per Jean-Didier Maréchal, de la UAB, ha donat una visió sobre l'estat de la química computacional, els seus grans reptes, el nou paradigma per a l'adaptació en paral·lel de dinàmica molecular i sobre el futur de la química quàntica als supercomputadors. Hi han intervingut Joseph S. Francisco, de l'ACS; Erik Lindahl, de Gromacs, i Jürg Hutter, de cp2k.

La segona sessió ha estat moderada per Ramon Crehuet, del CSIC, i s'ha centrat en la relació de la química amb el medi ambient, la biotecnologia, la nanotecnologia i la ciència dels materials. Ha comptat amb les ponències de Josep M. Anglada, d'IQAC-CSIC; Leonardo De Maria, de Novozymes; Josep M. Poblet, de la URV, i Carlos Alemán, de la UPC.

La JOCS ha estat possible gràcies a la tasca duta a terme pel comitè de programa format per Miquel Duran, Francesc Illas, Ramon Crehuet, Jean-Didier Maréchal i Miquel Huguet, del CESCA, i ha comptat amb la col·laboració de la UB, la XRQTC i Bull. ■



A l'obertura, Josep M. Martorell i Pere Lluís Cabot. A la cloenda, Francesc Illas i Miquel Duran.

Meeting Societal Grand Challenges with Computational Chemistry: The Road Ahead

Joseph S. Francisco

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We continue to see that accelerated technological, environmental, societal and financial drivers are pushing the chemical enterprise worldwide, and chemists working in it, to increasingly think and collaborate globally. There are challenges and opportunities for our shared discipline and its enterprise. This presentation has looked at the increasing connectivity, integration, and interdependence of economies, societies, technologies, and cultures spheres across the world. The effect that globalization has had on the chemical enterprise and chemical education to date and what it could look like in the years ahead has also been discussed.

The current research information infrastructure is being transformed into a global collaboration infrastructure. The essential underpinnings of such a transformation exist in research networking and distributed research collaborations, and the talk has discussed how computational chemistry is fostering global collaborative interactions.

Copernicus: Automatic Parallel Adaptive Molecular Dynamics

Erik Lindahl

Gromacs



Biomolecular simulation is a core application on supercomputers, but it is exceptionally difficult to achieve the strong scaling necessary to reach biologically relevant timescales. Biomolecular systems are frequently large enough to be reasonably efficiently parallelized, with 100-500 particles assigned to each core in high-performance molecular dynamics (MD) packages such as Gromacs when run on a system with sufficiently low interconnect latency.

However, at this point the time required for a step is approaching 100 μ s of wallclock time, and there simply aren't enough floating-point operations in a single simulation to achieve order-of-magnitude improvements in scalability. While molecular dynamics can achieve close to perfect weak scaling, this will put hard bounds in strong scaling and limit the accessible run lengths for biomolecular simulation.

Here, we present a new paradigm for parallel adaptive molecular dynamics and

a publicly available implementation: Copernicus. This framework combines performance-leading molecular dynamics parallelized on three levels (SIMD, threads, and message-passing) with kinetic clustering, statistical model building and real-time result monitoring.

Copernicus enables execution as single parallel jobs with automatic resource allocation. Even for a small protein such as villin (9,864 atoms), Copernicus exhibits near-linear strong scaling from 1 to 5,376 AMD cores. Starting from extended chains we observe structures 0.6 Å from the native state within 30 h, and achieve sufficient sampling to predict the native state without a priori knowledge after 80-90 h. To match Copernicus' efficiency, a classical simulation would have to exceed 50 microseconds per day, currently infeasible even with custom hardware designed for simulations.

Is There a Future for Quantum Chemistry on Supercomputers?

Jürg Hutter

Physical Chemistry
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The main task of quantum chemistry is the calculation of the electronic structure of molecules. From the electronic structure one can derive properties and reactivity and can make connections to experimental results or predictions for unknown substances. Over the years a large set of methods have been developed that allow more accurate and efficient calculations. Until recently computer programs using these methods to investigate standard chemistry problems were major users of supercomputer resources.

Forced by the exponential growth of computational power available on supercomputers and aided by the shift to massively parallel computer architectures we currently see a change of types of applications. Whereas the more standard applications can be performed on personal computers or on grid computer resources,



L'auditori durant la ponència de Jürg Hutter en la primera sessió de la JOCS.

molecules in complex environments that are studied using quantum chemistry combined with statistical mechanics methods require supercomputers. These new methods allow to investigate the chemistry of important systems related for example to clean energy production and storage or human health issues.

Theoretical Chemistry and Environment

Josep M. Anglada

IQAC-CSIC



Environment has different meanings for different people, depending on how different people approach this diverse area of knowledge. One way of studying the environment comes from Chemistry and from Atmospheric Science. The Earth atmosphere is an open system which is fed by sun radiation and by the release of enormous amounts of matter from the earth surface, including both, biogenic and anthropogenic sources. The matter emitted to the atmosphere is oxidized mainly by OH and by O₃ in day-time, and by NO₃ in night-time, and the products of this oxidation are organic and inorganic acids, aldehydes, carbon dioxide, carbon monoxide or highly reactive radicals, among others. Moreover, many products of the oxidation of atmospheric species can form aerosols or can be taken up by clouds and be eliminated by rain. These oxidation processes dominate the chemistry of air pollution, causing a direct effect on human health. In addition, species like carbon dioxide, methane or ozone are greenhouse gases, having a direct impact on climate change.

Theoretical and computational chemistry is a useful tool for the study of atmospheric chemistry. It contributes to understand and to rationalize the processes occurring in the atmosphere and, in many cases, it can provide thermodynamic and kinetic data with a high level of accuracy so that they can be used in atmospheric models. Let us take two examples to illustrate this fact.

The first one is the oxidation of formic acid by OH that can affect the concentration of atmospheric CO₂. If the acidic hydrogen is abstracted, then HCOO is formed, ultimately yielding H + CO₂, if the formyl hydrogen is abstracted, then HO-CO is formed, and will break down into OH + CO. This reaction has been well studied experimentally and, unexpectedly, shown to prefer abstraction of the acidic hydrogen. The theoretical work has been able to rationalize this process and it has shown that the preference of the acidic hydrogen abstraction is due to the fact that the reaction undergoes a proton coupled electron transfer reaction. Furthermore, theoretical studies predict that, in presence of water vapor, about 10% of formic acid will react with OH abstracting the formyl hydrogen rather than the acidic hydrogen, changing thus the product distribution.

The second one is related to the reaction of ozone with alkenes in a process that leads to the formation of carbonyl oxides (RR'COO) and aldehydes. The atmospheric fate of carbonyl oxides is of great interest as they have been experimentally shown to be both a day and night time source of OH radicals, H₂O₂, organic acids and hydroperoxides. The theoretical studies have been key in determining the reaction mechanisms involved in this process and in predicting a further atmospheric formation of hydroxyl radical, which is the main oxidizing species in the atmosphere.

Chemistry and Biotechnology

Leonardo De Maria

Novozymes



Novozymes is the world market leader in bio-innovation, with its core business centered on industrial enzymes, microorganisms, and biopharmaceutical ingredients. With over 700 products used in 130 countries, Novozymes' bio-innovations improve industrial performance and safeguard the world's resources by offering superior and sustainable solutions for tomorrow's ever-changing marketplace. Novozymes'

natural solutions enhance and promote everything, from removing trans fats in food to advancing biofuels to power the world tomorrow.

The *Candida antarctica* lipase B (CALB) has found very extensive use in biocatalysis reactions. Long molecular dynamics simulations of CALB in explicit aqueous solvent confirmed the high mobility of the regions lining the channel that leads into the active site, in particular, of helices α5 and α10. The simulation also confirmed the function of helix α5 as a lid of the lipase. Replacing it with corresponding lid regions from CALB homologues resulted in two new CALB mutants. Characterization of these revealed substantially improved catalytic properties. The research process leading to the improved CALB variants exemplifies clearly how do supercomputers support the enzyme optimization tasks within a leading biotech company.

Computational Modelling of Nanostructures: The Case of Molecular Metal Oxides

Josep M. Poblet

URV



The continuous progress of computers in general, and quantum chemistry software in particular, has enabled to quantum chemists to develop strategies to rationalize electronic and structural properties of large complex systems. Polyoxometalates are molecular metal oxide anions mainly formed by tungsten, molybdenum and vanadium atoms and mixtures of them. Typical polyoxometalates contain between 12 and 30 metal atoms but large structures have been characterized with more than 300 metal atoms and the corresponding oxygen atoms, with applications in catalysis, in the synthesis of nanoparticles or in medicine among many others. A distinctiveness of polyoxometalates is that almost any element of the periodic table can be incorporated in its structure allowing tuning the properties of the anion. For example, typical polyoxometalates

have been used to bleaching of wood pulp in a benign technological process, or very recently polyoxometalates containing ruthenium or cobalt atoms are used to oxidize water in a green process.

From a computational point of view the computational modeling of polyoxometalates presents serious difficulties because of the size of the compounds, their complex electronic structure and the relevance of the stabilizing effects of solvent and counterions ions in solution and counterions in solid state. These compounds are a good example to show the challenges that the computational chemistry must face in nanoscience: nucleation mechanisms; modeling of electrochemical properties; transport of nanosystems, reactivity in solution or in solid state, etc. We are persuaded that Computational Chemistry and Supercomputer Centers will have in the coming years an essential role in the development of nanosciences and nanotechnologies.

Jürg Hutter
“The majority of standard quantum chemistry applications can be performed on small and medium systems”

Chemistry and Materials Science

Carlos Alemán
UPC



It can be stated that, although Chemistry and Materials Science followed separated ways for a long time, the collaborative relationships between these two disciplines started in the early twentieth century. At that time chemists provided useful information about the structure and composition of many new materials as well as the about the processes to apply and synthesize them. These achievements converged with the classical concepts of Materials Science. As a result, Chemistry is now playing a predominant role in Materials Science.

The simplest way to discuss the benefits that the relationships between Chemistry and Materials Science provoke on the society is from an historical perspective. Thus, the collaboration between the two disciplines can be divided in three stages, each one with its own relevant and characteristic features. The first stage extends from the early twentieth century to the eighties and corresponds to the period in which chemists discovered many

new materials and processing methods, like for plastics that still are of fundamental importance for the society.

At around eighties, chemists described a wide number of cases in which different combinations of materials produced different but very interesting properties. This was the nucleus of the second stage, which resulted in a massive development of blends and composites. Moreover, advances in computer architectures and software developments were so impressive that Computational Chemistry became, by its own, in another branch of the Chemistry. Computational Chemistry started to play a very significant role in the relationships between Chemistry with Materials Science.

Finally, we have recently started a new stage in the collaboration between the two disciplines. This arises from the development of synthetic methods to prepare and characterize molecular hybrid conjugates, in which molecular fragments of very different chemical nature are covalently linked. As the preparation and manipulation of these new materials are very complex, Computational Chemistry is currently playing a leadership role in the collaboration between Chemistry and Materials Science. ■

All the presentations are available at www.cesca.cat/jocs



Els ponents i el comitè de programa de la JOCS'11.