Editorial

THE HIGH PERFORMANCE COMPUTING AND THE MATERIALS SCIENCE

"The sciences do not try to explain, they hardly even try to interpret, they mainly make models. By a model is meant a mathematical construct, which, with the addition of certain verbal interpretations, describes observed phenomena. The justification of such a mathematical construct is solely and precisely that it is expected to work."
John Von Neumann

The main goal of the material science is the design of new materials and the development of new and efficient methods for the controlling and the optimisation of the material properties (mechanical, chemical, electrical, magnetic, thermal, acoustical, optic) by the manipulation of their composition and structures. It involves advanced experimental and analytical investigations of the combined mechanic and physicochemical characteristics of the materials under various thermodynamic conditions and external excitations. The material science is a multidisciplinary field, which is based on knowledge and methods that are coming from various fields as physics, chemistry, geology and biology with a large support from mathematics and computer science.

The traditional couple theory - experiment enables us to understand the interaction mechanisms and the phenomena that take place in materials, as well as to establish the analytical equations and to characterize material properties. The classical way to investigate the properties of the materials is the so-called top-down approach. The system is seen as a black box and the investigation is oriented to break down the system, to gain insight into its compositional sub-systems without considering the structural details of any first-level subsystems. In the subsequent stages the subsystems are refined in more details, until the entire specification is reduced to the basic elements.

The evolution of the experimental methods (especially, the progresses in the synthesis of the nanosystems and in the high-resolution microscopy) and the development of the theory made possible to understand the matter on atomic scale, which supports the change in the view on materials, such as in the so-called bottom-up approach: the elements of the system are considered organized in a hierarchical manner. The atoms are considered linked together to form functional larger subsystems (molecules, clusters, nanosystems, macromolecules, molecular self-assembly, grains), until a complete top-level system is formed. The combination of atoms and molecules in larger entities endows the resulting materials with properties that depend not only on the chemical nature of the atomic and molecular constituents, but also on their interactions in the bulk of the material and on its surfaces. The electronic structure of the system plays an important role in the formation or the breaking of the chemical bonds between atoms, and a quantum approach is required. Atomic and molecular physics provide the theoretical background for quantum chemistry in

understanding the chemical reactivity, while solid-state physics is responsible for the studies on the periodic systems.

The very rapid development of the software and hardware technologies facilitates the use of the symbolic and the numeric calculations in the reduction of the linear equations, but the large number of variables and the nonlinearity of the differential/integral equations enable analytical solutions only in a few cases. Even then a model of system is required to overcome and to solve these problems by using models that imitate objects, processes, phenomena, concentrating on the essentials objects and their interactions. The physical models are described in mathematical equations that can be simplified by analytical or numerical approximations. The modern computer infrastructure (hardware/ software) may help us also to calculate the values of various physical-chemical parameters based on the equation of states and models of a given system. The computers provide us in the organization, the management and the rationalization of the obtained data. Some derivatives or integrals can be numerically evaluated and their parameters could be obtained from experimental measurements. This field has become very consistent in the last fifteen years and has got into a mature investigation instrument in the material investigation called Computer Material Science - CMS.

CMS is a branch of material sciences that uses theoretical concepts and models from chemistry, physics, geology, mineralogy, as well as biology and includes them into software applications in order to calculate the structure and the properties of molecules, gases, liquids and condensed matter. The validation of the methods and the determination of the used parameters are made by using experimental results. The computer simulations get additional information despite those obtained experimentally, and can predict some still undiscovered phenomena. The numerical simulations are not and will never be a substitute of the experimental devices and equipments, but it can offer experimentally unavailable information, such as the electronic density or the electronic charge. From the experimental measurements we get a system response as a consequence of an outside excitation. This complex signal is a sum of simple responses from different types of chemical species, localized in different areas and is averaged over time, depending on the resolution of the recording device. CMS allow the determination of instantaneous microscopic values that are determining the macroscopic response of the material systems, enabling the understanding of the mechanism of complex phenomena, and establish an equation of state and transformation of the system. On the other hand, improving and testing the quality of the materials involves knowledge about the relationship structure-properties, knowledge that is available by understanding the interactions at the microscopic level. Simulations are useful in suggesting new kinds of experiments, in data analysis as a result of an experiment, replacing costly (equipment, team of scientists, materials, time consumption) or dangerous (explosions, drugs, pesticides) or contaminating experiments.

CMS has evolved in such way that it can determine with high accuracy the values of different properties with microscopic origin, allowing the analysis of the phenomena and the identification of the mechanisms. CMS is a powerful analysis tool, which allows the investigations of the geometry optimizations, energetical investigations, the prediction of material proprieties and the determination of thermodynamic parameters. Thus we can: (i) understand the nature of the processes at the molecular level, (ii) describe the interatomic and intermolecular interactions, (iii) predict the mechanical and the thermal properties, (iv) characterize the molecular, crystalline structures and surfaces, (v) establish the relation between structure and properties, (iv) decrease the experimental effort in finding and

characterizing new systems. CMS allows the access to some experimentally unavailable parameters (energy density, electronic density, density of states). It facilitates the access in pressure and temperature domains that are inaccessible by experiment, and permits the analysis of the macroscopic-parameter function of the contribution of different regions and/or components of the investigated system. It has an interdisciplinary character, as it uses various knowledge and methods from different fundamental sciences (mathematics, physics, chemistry, geology, biology, crystallography, mineralogy) and computer science (programming languages and techniques, operating systems and computer networking). Nowadays, with the support of the high performance computing resources, the CMS plays an important role in all the aspects of material science, especially in the dynamic domains such as surface science, nanoscience, electronics, biology and drug design. It establishes a direct relationship between structure and properties, delivering theoretical solutions that may guide us to synthesize new advanced materials, with new properties.

The accuracy of the CMS in the prediction of the material properties is constrained by the maximum size of the system (reflected in the number of atoms that make up the system), since a physically large enough system that wishes to simulate the behaviour of a bulk system will incorrectly reproduce the system interaction and its dynamics. By using more powerful computers, developing efficient algorithms and using other programming methods the computational effort can be reduced. Significant experience in developing algorithms (adapted to a parallel programming) and programs has been gained. The entire capacity of the modern computers with parallel architecture can be used. The parallel programming is focused on partitioning the problems in jobs for each processor and synchronizing the jobs. CMS can benefit from the parallel architecture of the computers: forces and other components of the total energy are separately and simultaneously calculated on different processors under the same conditions. Finally the processor that launched the execution collects the results. The short-distance interaction allows the parallelization of the code by assigning a subset of atoms to each processor, regardless of their position in space-time, each processor having a copy of the positions of all atoms (ADM atom-decomposition-method). Thus, bond forces of type 2 -, 3 - and 4-body can be calculated by dividing the molecular topology directly on the processors. In order to reduce the communication time between processors, the force matrix can be decomposed into blocks (force-decomposition method) and not along the lines, like in ADM. The communication can be even faster by associating each processor to sub-regions of the system (domain-decomposition method).

CMS is the scientific field that requires the most computational power: the bigger computational resources allow the use of higher-level methods for a greater accuracy, as well as the study of the phenomena that occur at larger scales of time and of space. The computational effort can be reduced by carefully choosing theoretical models and algorithms. It requires good computational environment with high computation speed, large amount of memory, and efficient numerical libraries with the support of the parallel programming.

The access of the Romanian researchers to powerful computers was restricted in the past due to the embargo imposed by the western countries. Today, the access to supercomputers is financially limited because of their very high prices. Fortunately, there is a lower cost solution by developing the so-called computer cluster, which is a group of usually identical personal computers or in more energetic efficient blade systems.

*Recently, within the framework of the project **ASSG - Virtual Atomic Scale Simulation Group in Material Science** (Capacities Project 84 CpI/13.09.2007 - National Authority for Scientific Research - NASR, Bucharest) a network of three clusters has been developed as integrated platform of three HPC clusters based on IBM Blade nodes: 67 at the Institute of Physical Chemistry "Ilie Murgulescu", Romanian Academy (project manager: **Dr. Viorel Chihaia**); 33 at the Faculty of Automatic Control and Computers, Polytechnic University of Bucharest (project co-coordinator: **Prof. Dr. Ing. Nicolae Tapus**) and 8 at the National Institute of Materials Physics, Magurele (project co-coordinator: **Dr. Petru Palade**). Each node is equipped with two Intel XEON processors quad-core, with 16 Gb memory and 146 Gb HDD. The operating systems are of Linux type: Scientific Linux 5.2 on first two clusters and SUSE 10 on the last one. More details about ASSG infrastructure may be found under **http://www.hpc-icf.ro**.*

The general objective of the project is the development of the CSM infrastructure made available for the scientific community, considering the existing infrastructure (computer networks, software for simulation and visualization, documentation) and the experience of the group members. ASSG is designed as an open group for new members and it will try to play an important role in gathering together the scientists who work with similar methods and algorithms in different fields and to present to the Romanian scientific community in the field of material science the abilities and the advantages of the atomic-scale simulations. The aim of the project is the investigation of the phenomena that occur on large time scale in low dimensional systems (order of tens of Å), nano and extended systems (10-1000 Å) and infinite systems (1D chains of atoms; 2D-surfaces, interfaces and thin films; 3D-crystals, amorphous, liquids and gases), with ideal structures or with local and extended defects. The phenomena that have place at mesoscopic and macroscopic scale will be also approached by the use of the specific methods for molecular structure and methods of the finite elements.

*In parallel, the **Center for Molecular Modeling and Computational Quantum Chemistry - CMMCQC** was created at Babes-Bolyai University by the project 130/14.09.07 that was financed by NASR. The nodes are composed of 70 IBM blade servers with XEON processors, each server having two quad-core processors, 8 GB of RAM and 2x146 GB HDD 10 K in two racks that also contain a storage system (of 2.1 TB) and a communication server. The link between the two racks is through UTP cable at 1MBps, and the communication between the two partner-institutions is made through optical fiber (for details see: **http://chem.ubbcluj.ro/pagini/anorganica/isi/capacitati/en/index-en.html**).*

*The main objective of this project was the building of a cluster/grid calculation platform, in order to use it in molecular modelling and modelling on the meso and macroscopic level of complex materials. The project was coordinated by the Babes-Bolyai University (project manager – **Prof. Dr. Ioan Silaghi-Dumitrescu),** in a partnership with the Technical University in Cluj Napoca (project co-coordinator- **Dr. Ovidiu Nemes**).*

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