HPC-Europa2 Newsletter: June 2009
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HPC-Europa2

Pan-European Research Infrastructure on High Performance Computing

Welcome to the fifth edition of the HPC-Europa2 newsletter! This issue is edited by CINECA and focuses on the research that one of GENCI-CINES's HPC-Europa2 visitors has performed using the HPC facility at GENCI-CINES.

--- NEWS ---

The image on the right is a snapshot of the Volume 'Science and Supercomputing in Europe – report 2008' that will be published in June.
All of the authors will automatically receive a copy.
Please contact us if you are interested in receiving a copy or to inform us of anychanges of address.
We are also working on the CD version, which that will also be published very soon.

Snapshot of the cover of the Volume 'Science and Supercomputing in Europe – report 2008' that will be published in June

Timetable for 2009 Virtual Surgeries

6 Jul	**BSC**	**Programming with StarSs***
Aug	**EPCC**	OpenMP 3.0
Sep	**CSC**	Workshop on application porting and optimization
Oct	**TCD**	Parallel Linear Algebra
Nov	**EPCC**	Parallel Fast Fourier Transforms
9 Dec	**CINECA**	Parallel I/O tools for scientific data

* Abstract:
STARSs is a programming model that enables sequential programming and dynamic exploitation of applications' inherent functional parallelism on parallel resources. Dynamic data-dependence analysis, data renaming and locality aware task scheduling are some of the features implemented in the available runtimes for STARSs. BSC has been developing different flavours of StarSs for computational grids and clusters (GRIDSs, COMPSs) and for heterogeneous and homogeneous multicores (CellSs, SMPSs). In the talk, we will outline the characteristics of this programming model and also how they can be combined towards a more hierarchical programming model that can cope with grids/clusters of multicores.

Next 2009 call **deadlines**:
15 September 2009
15 November 2009

--- UPCOMING EVENTS ---

HPCEuropa2 workshop on application porting and optimization at CSC
The goal of this workshop is that after the course the participants will havetheir codes ported, compiled, profiled, tuned and ready for efficient production runs. The specific platform is CSC's flagship machine, a Cray XT4/XT5 Louhi, but the discussed strategies are applicable to other platforms too.
Further information at
http://www.csc.fi/csc/kurssit/arkisto/crayworksho p09

edited by CINECA

GENCI (www.genci.fr) and CINES (www.cines.fr) are very proud to be part of HPC-Europa2 program. The installation of JADE, Tier 1 HPC platform, ranked 14th in the Top 500 list, offers an ultimate simulation platform for the applicants. The openness and the exchange involved are a real opportunity for CINES to create new contacts and partnerships.

The First HPC-Europa2 applicant hosted at CINES is Marco Smerieri, from the department of physics of Genova University. A description of his scientific progress and results is given by Dominique Costa. We note with satisfaction that the use of the HPC platform led to a scientific progress and validation. It illustrates perfectly the fact that besides the two historical thrusts of science, theory and experimentation, a third is now available: simulation.

Eric Boyer (*Intensive Computing Department* – CINES)

Scanning Tunnelling Microscopy is a fascinating technique which allows "images" of a surface to be recorded at the nanometer scale, up to atomic resolution. Last generation low temperature STMs are characterized by a high stability, which allows the same small groups of atoms or molecules to be investigated for several hours and thus to explore all possible measuring conditions. In spite of that, this technique suffers of some limits: due to the fact that recorded "images" corresponds to the density of states of the surface, not always coinciding with its topography, and due to the lack of chemical contrast when used as a pure microscopic tool, STM may present some difficulties in the interpretation of images. At this point the use of a complementary technique becomes important to extract precious information, and the computational approach is extremely valuable in this respect. Taking as an example the HPC Europa project I developed in the spring of 2009, I had very good STM images showing different self assembled structures of Glutamic Acid (GA) on Ag(100). I had made a qualitative analysis of these experimental data and I could suppose some qualitative models. However, I was not able to verify these models and to determine the chemical state of GA at the surface (neutral, anionic, zwitterionic). The presence of several structures with different density (forming depending on substrate temperature during GA deposition) could also be indicative that GA is stable on the Ag surface in different chemical states depending on experimental conditions. To clarify all this, I moved to Paris and joined the group of Dr. Dominique Costa at ENSCP. We simulated the GA/Ag(100) system using the VASP software and the computation power offered by the super-computer JADE (provided by CINES). We modeled the GA/Ag(100) system starting from the two simplest structures, the "squares" (see fig. 1a) and the isolated rows. The main results are summarized by my French host. What I wish to point out here is the usefulness of this experience for my scientific formation. I could indeed face complementary aspect of the same problem, matching information obtained by theory and experiment to get a complete unitary picture of the system. Besides that, I could understand the mechanisms which are behind simulated images and this will be of great help also for a better understanding of theoretical and simulated results on other systems.

Marco Smerieri

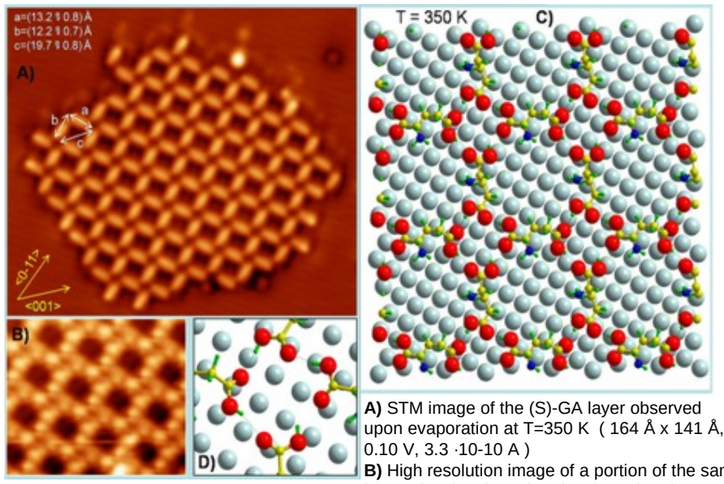
Mario Rocca
Letizia Savio
and
Luca Vattuone
University of Genova (Italy)
Surface Science Spectroscopy Group

Dominique Costa
CR1
Laboratoire de Physico-Chimie des Surfaces
ENSCP Chimie ParisTech

Frederik Tielens
Maître de Conférences
Laboratoire de Réactivité de Surface
UPMC Paris

The starting point of modeling is the elaboration of a realistic and representative model. In computational chemistry, the model translated in the "input file", is the nature, number and relative position of the atoms on which the calculation is performed. The construction of the model is therefore of utmost importance, and is often based on several assumptions, such as chemical intuition, experience, and hypothesis of the researcher himself. Nevertheless, models have two serious limits: they might be too "simple" or not representative enough of the real system. And models depend strongly on the imagination and creativity of the researcher himself.
At this point, experiments performed on controlled systems, especially with atomic resolution, may bring to the theoretician precious information about his "input file". A recent HPC-Europa stay illustrates this point. Marco Smerieri is a phD student working with Dr. Letizia Savio in the surface science group of Prof. Mario Rocca at the Department of Physics of the University of Genova. He has evidenced by low temperature scanning tunneling microscopy (LT-STM) amazing structures of glutamic acid forming a well organized patterns on a silver surface: squares (Figure 1a, b), rows, even "flowers", have been formed regularly on the surface, depending on the experimental conditions. Such structures were hardly imaginable.

Marco visited the Laboratoire de Physico-Chimie des Surfaces, in Paris, to work with me, in collaboration with Dr. Frederik Tielens from the Laboratoire de Réactivité de Surface, Paris, to model by first principles methods the obtained structures. We could unravel the story behind this self-organizing adsorption process: since the amino acid was found to interact poorly with the Ag(100) surface, silver being a noble metal, the driving force of the adsorption has to lie on the attractive adsorbate-adsorbate interactions. In a first step of the modeling, glutamic acid molecules form lines. Then, allowing the system to relax, with the use of ab initio molecular dynamics, glutamic acids reoriented at the surface to form rugby –ball-like nanostructures, followed by squares of four molecules, as illustrated on the Figure 1c. Simultaneously, the energy of the system was lower, indicating stabilization. The final structure presents, at the boundary of four squares, a cycle of hydrogen bonds between the glutamic acids (Figure 1d), demonstrating the power of the chemistry of the amino acids as building blocks, behind the diversity of life.



A) STM image of the (S)-GA layer observed upon evaporation at T=350 K (164 Å x 141 Å, 0.10 V, 3.3 ·10-10 A)
B) High resolution image of a portion of the same layer, showing the submolecular units of GA molecules. (60 Å x 50 Å, 0.10 V, 3.3 ·10-10 A)
C) Corresponding simulated model by VASP.
D) Detail of simulated model: OH ring.

Dominique Costa - *Laboratoire de Physico-chimie des surfaces – ENSCP Chimie Paris Tech*
Frederic Tielens - *Laboratoire de réactivité de surface UPMC Paris*

Brief Curriculum Vitae

Marco Smerieri was born in Genova (Italy) on May 26, 1979.
He got his degree in physics at the University of Genoa in October 2006. He discussed a thesis on low temperature STM investigation of the hydroxilation of O-precovered Ag(110), under the supervision of Dr. Letizia Savio and Prof. Mario Rocca.
In January 2007 he started his Ph.D. in physics at the University of Genoa, under the supervision of Dr. Luca Vattuone and Prof. Mario Rocca. His research consists in a low temperature STM investigation on self-assembling of glutamic acid molecules at Ag(100) and in the molecular dynamics simulations of the same system. This part of the thesis was done in collaboration with Dr. Dominique Costa in the frame of a HPC project.