TNT 2011
Trends in NanoTechnology

November 21-25, 2011
Tenerife - Canary Islands
(Spain)

Satellite Workshop MULT-EU-SIM
November 24, 2011

PHANTOMS foundation

INL International Iberian Nanotechnology Laboratory

Universidad de Oviedo

Universitas Friburgensis

UAM Universidad Autonoma de Madrid

UAB Universitat Autònoma de Barcelona

Universitas Complutensis Matritensis

ibec Institute for Bioengineering of Catalonia

leti

cea

Universitat de Barcelona

CIC nanoGUNE nanoscience cooperative research center

dipc Donostia International Physics Center

Georgia Tech

ULL Universidad de La Laguna

NIMS Nanomaterials Laboratory

Purdue University

MANA

MULT.EU.SIM aims to gather the simulation research community in Europe to establish a joint vision of multiscale modelling and simulation. This will enable to prepare Europe to play a leading role in the opening era of computational sciences where multiscale simulation will profoundly change the scientific and technological practices. This European vision will serve as the foundation for a joint effort with emphasis toward multiscale unified codes and standardized interfaces & workflows in a field that is currently very fragmented. Ultimately, the availability of such a multiscale code toolbox will put Europe's industry in a strong IPR position.

SCIENTIFIC PROGRAMME
Thursday - November 24, 2011

Satellite Workshop MULT-EU-SIM ***Chairman: Thierry Deutsch (CEA, France)***		
15h00-15h15 **p. 1**	**Thierry Deutsch** (CEA / L_Sim, France**)** *"MULT.EU.SIM: A joint vision on the perspectives of multiscale modelling and simulation for nanodevices"*	**O**
15h15-15h45 **p. 9**	**Massimo Macucci** (Universita di Pisa, Italy) *"Analysis of the perspectives of multiscale simulation of devices and circuits"*	**K**
15h45-16h15 **p. 11**	**Pablo Ordejon** (CIN2,Spain) *"Beating the size limits of first-principles calculations in nanoscale systems"*	**K**
16h15-16h45 **p. 3**	**Ricardo Diez Muino** (CFM/CSIC-UPV/EHU, Spain) *"A time-dependent view of electronic excitations in the nanoscale"*	**K**
16h45-17h00 **p. 15**	**Sebastian Radke** (TU Dresden, Germany) *"Charge transport in organic semiconductors: Ab initio charge carrier propagation schemes"*	**O**
17h00-17h30	**Coffee Break**	
17h30-18h00 **p. 13**	**Bernard Querleux** (l'Oreal, France) *"Numerical Modelling at L'Oreal R&I: Present and future"*	**K**
18h00-18h30 **p. 5**	**Maurizio Fermeglia** (Trieste University, Italy) *"Nano tools for macro problems: multiscale molecular modeling of nanostrucured systems"*	**K**
18h30-19h00 **p. 7**	**Geoffroy Hautier** (Universite Catholique Louvain, Belgium) *"High-throughput ab initio computations for materials design"*	**K**
19h00-19h15	**Concluding Remarks**	

INDEX ALPHABETICAL ORDER

K: Keynote / O: Oral

Thierry Deutsch (CEA / L_Sim, France) *"MULT.EU.SIM: A joint vision on the perspectives of multiscale modelling and simulation for nanodevices"*	**O**	**p. 1**
Ricardo Diez Muino (CFM/CSIC-UPV/EHU, Spain) *"A time-dependent view of electronic excitations in the nanoscale"*	**K**	**p. 3**
Maurizio Fermeglia (Trieste University, Italy) *"Nano tools for macro problems: multiscale molecular modeling of nanostrucured systems"*	**K**	**p. 5**
Geoffroy Hautier (Universite Catholique Louvain, Belgium) *"High-throughput ab initio computations for materials design"*	**K**	**p. 7**
Massimo Macucci (Universita di Pisa, Italy) *"Analysis of the perspectives of multiscale simulation of devices and circuits"*	**K**	**p. 9**
Pablo Ordejon (CIN2,Spain) *"Beating the size limits of first-principles calculations in nanoscale systems"*	**K**	**p. 11**
Bernard Querleux (l'Oreal, France) *"Numerical Modelling at L'Oreal R&I: Present and future"*	**K**	**p. 13**
Sebastian Radke (TU Dresden, Germany) *"Charge transport in organic semiconductors: Ab initio charge carrier propagation schemes"*	**O**	**p. 15**

ABSTRACTS

MULT.EU.SIM: « European Multiscale Simulation for the Computational Era »

"MULT.EU.SIM will provide the European Commission with a constructed case allowing it to decide whether or not to launch a proactive initiative in the field of multiscale modelling and simulation for nanoelectronics."

Thierry Deutsch

CEA / L_Sim, France

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A JOINT VISION ON THE PERSPECTIVES OF MULTISCALE MODELLING AND SIMULATION FOR NANODEVICES

Where do we stand?

The last years have seen the emergence of a broad array of novel products based on components structured at the nanoscale. The design of such systems spanning a wide range of length- and time-scales requires models based on realistic descriptions of the nanoscale building blocks. Integrating the quantum effects that dominate at the nanoscale into these models should be easily feasible as ab initio methods are well developed in Europe. However, the larger scales of nanodevices, the evolution of a system consisting of millions of atoms as a whole, cannot be cannot be predicted by means of ab initio. On each length- and time-scale, specific phenomena arise which cannot be described realistically but on their own level of detail. Not all interaction must necessarily be treated within the first principles framework. To succeed in describing the whole nanodevices in their complexity, a hierarchy of level of treatment must be introduced in which ab initio would be treated only as a subsystem, in order to extract relevant information to complete the upper-level model for the full system. A modelling and simulation "toolbox" is therefore called for, combining several models in a multiscale realistic and comprehensive description. Yet, despite much research in this direction, there a few demonstrated examples to date, which address present day R&D requirements of the European industry and research community.

What are we aiming at?

The goal is to achieve integrated modelling suites for nanodevices, bridging across the different scales from first principles to industrial application. The creation of a realistic and comprehensive simulation capability will allow the design of new devices bypassing most of the fabrication test runs, thereby accelerating the pace of development while in the same time sharply reducing the costs (time and money wise), and consequently gaining in competitiveness. Ultimately, the availability of such multiscale methods will put Europe's industry in a strong IPR position.

Those assessments are supported by a strong consensus of the simulation community, stemming from various contributions as well as from a survey conducted by the MULT.EU.SIM consortium. The conclusion of this survey is that multiscale simulation has great potential impact on S&T future progress, provided the (strategic) means of realizing it are given. In addition, the development of key enabling technologies (KETs) such as nanoelectronics, and thus the promotion of design capabilities, have been outlined as priorities in the EU technological strategy.

2

How do we get there?

This European vision will serve as the foundation for a joint effort in a field that is currently very fragmented. The development of multiscale simulation requires first furthering and optimizing the computational resources. Besides increasing the capacity to the petaflop or even the exaflop, it means supporting the progress in codes, theory and numerical algorithms, as these progresses contribute as well to the improvement of the effective computational power. The existing software tools need to be integrated in the multiscale strategy and adapted to reusability and modularity. Conceiving those new design tools implies a strong collaboration across disciplines and between academia and industry. A data-sharing system is notably called for, allowing researchers to use a broader set of information, and ultimately render more accurate models. In addition, empirical testing is still required to complement the computational methods, providing data to validate the key results and fill in the gaps. In the end, collaboration on creating new tools will rapidly increase the pace of innovation. Lastly, this foreseen integrated environment calls for an overall coordination effort (running along the specific projects and housing the transverse numerical effort), of which means the European Commission could be the supplier.

A time-dependent view of electronic excitations in the nanoscale

Ricardo Díez Muiño

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Donostia International Physics Center DIPC, San Sebastián, Spain

Femtosecond and subfemtosecond time scales typically rule electron dynamics in low-dimensional metallic systems. Recent advance in experimental techniques permits now remarkable precision in the description of these processes. In particular, shorter time scales, smaller system sizes, and spin-dependent effects are current targets of interest. In this lecture, we will review some of the distinct aspects that define electron dynamics in the nanoscale, focusing into confinement effects [1]. Using density functional theory and its time-dependent extension, we will show that the screening of localized charges in metal clusters and surfaces is created locally in the attosecond time scale, while collective excitations transfer the perturbation to larger distances in longer time scales. We will also briefly discuss the elastic width of resonances in excited alkali adsorbates on surfaces and the electron – electron scattering in several metallic systems of nanometer size. In addition, we will discuss the role of electron excitations in a different context, namely the elementary reactive processes that take place at metal surfaces [2]. Over the last years, the combination of experimental molecular-beam techniques and refined theoretical calculations based on ab-initio methods have led research on this field to a new stage, in which detailed investigations of the kinetics and dynamics of molecular reactivity at surfaces are possible. The possible relevance of non-adiabatic effects in these processes, as well as the time scale in which the different energy dissipation channels play a role will be discussed.

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Nano tools for macro problems: multiscale molecular modeling of nanostrucured systems

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A current challenge of physical, chemical and engineering sciences is to develop theoretical tools for predicting structure and physical properties of complex organic inorganic nano composite from the knowledge of a few input parameters. This task is particularly crucial in the design and fabrication of nano and bio-nano devices and systems which is the new horizon of nanotechnology for the forthcoming 5 years. Indeed, nanotechnology roadmap is moving from passive nanostructures to active nanostructures and eventually to Nano systems. The complexity of such systems and devices does not allow to follow the try-and-error procedure for the design, due to incredible amount of resources needed to obtain the desired results.

Recent development in computer HW and SW as well as in theories and algorithms allow us to investigate complex systems in the field of material and life science, using the computer as a virtual microscope, allowing us to 'see' the nanostructure and to predict macroscopic properties and behavior, without the need of constructing the nanosystem.

This paper deals with the application of multiscale molecular modeling to different Nano systems selected form the material science and the life science sectors. Despite the very different systems studied and the different application, the multiscale modeling protocol is rather general and applicable with small adjustments from nanostructured plastics to DNA/siRNA therapeutics in cells.

The concept of multiscale molecular modelling is briefly summarized in figure 1 [1], in which it is explained how different methods and algorithms may be integrated to calculate properties at different time and length scale. The challenge is to 'integrate' the methods, so that the ultimate property may be estimated taking into account all the phenomena pertaining at a smaller scale.

The proposed computational procedure of the multiscale simulation and modeling is based on the following ansatz: 1) fully atomistic molecular dynamics simulations are perform to retrieve fundamental structural and energetical information at the molecular level; 2) the data gathered at point 1) are mapped into the corresponding structural and energetical information necessary to run coarse-grained simulations at a mesoscopic level; 3) the main output of point 2), i.e., the system mesoscopic morphologies and density distributions finally constitute the input for finite element calculations and macroscopic properties predictions. The core step in the entire computational recipe is undoubtedly constituted by point 2), or the mesoscale level simulations. In mesoscale modeling, the familiar atomistic description of the molecules is coarse-grained, leading to beads of material (representing the collective degree of freedom of many atoms). These beads interact through pair-potentials which capture the underlying interactions of the constituent atoms [2]. The primary output of mesoscale modeling are phase morphologies with size up to the micron level. These morphologies are of interest per se, although little prediction of the material properties is available with the mesoscale tools. Finite element modeling then comes into play, and the material properties of interest can be calculated accordingly by mapping the material structures formed at the nanometer scale onto the finite element grid and coupling this information with the properties of the pure

components that comprise the complex system. Using standard solvers the finite element code can then calculate the properties of the realistic structured material [3].

In this paper we apply the above mentioned methodology to examples of interest to material science and life science. The first example is related to the enhancement of mechanical and barrier properties if a nanofiller is dispersed into a polymer matrix: the role of multiscale modeling for the development of the material in the stage of screening the best design is evidenced [4]. The second example, important for the opto electronic industry, is related to the prediction of the dispersion of gold nanoparticles into a di block copolymer system forming different nano structures. In this case it is relevant to understand how it is possible to influence the self-assembly of the nanoparticles in the diblock copolymer structure [5]. The third example is about drug delivery using bio compatible di/tri block copolymers. In this case it is relevant to predict the phase behavior of the polymer system and the ability of the polymer to form micelles and the load a drug. The last example is related to nanovectors in which we combined multiscale molecular simulations and experimental approaches to define mode and molecular requirements of the interaction of nucleic acid-based therapeutics and dendrimer/dendron-based delivery agents. This type of investigation can provide valuable information to devise optimal delivery systems that would increase the efficacy of DNA/siRNA therapeutics in cells and laboratory animals and move them toward clinical applications.

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Figures

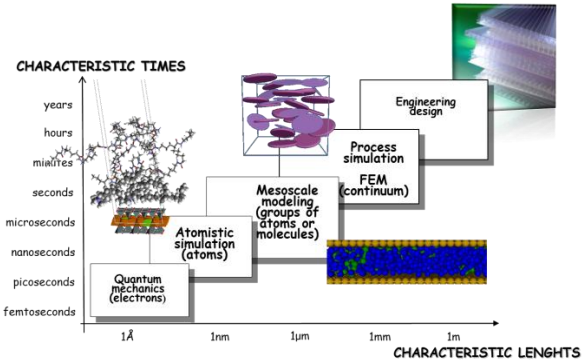

Figure 1: *The concept of multiscale modelling*

High-throughput *ab initio* computations for materials design and the Materials Project database

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Many essential materials properties can nowadays be computed through *ab initio* methods in the density functional theory (DFT) framework. When coupled with the exponential rise in computational power available to research groups, this predictive power provides the opportunity for large-scale computational searches for new materials. Tens of thousands of novel materials can be generated and screened by their computed properties even before their synthesis, focusing experiments on the most promising candidates and exploring rapidly new chemical spaces.

In this talk, I will review the challenges and opportunities for *ab initio* high-throughput computing. The problem of finding new inorganic compounds will be addressed and techniques based on data mining which tackle this problem with reasonable computational budget will be presented. To illustrate the benefits of high-throughput computing, I will present results from a computational search of new Li-ion battery cathode materials. Finally, I will introduce the *materials project*: a large publicly available database of materials properties obtained by *ab initio* high-throughput computing (http://www.materialsproject.org).

Analysis of the perspectives of multiscale simulation of devices and circuits

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Within the Mult.Eu.Sim project we have addressed the community working on device and circuit simulation in order to develop a document containing assessment of the current state of the art in the field of multiscale modeling and a vision of what will be important to pursue in the near future to match the needs of industrial and academic researchers working on the final downscaling of CMOS technology or on the application of emerging device concepts.

The initial core of the document has been written by the participants at a meeting held last spring in Bilbao, the resulting text has then been sent to a large number of researchers operating in the field worldwide. The feedback has been overwhelming, with messages of approval, suggestions for correction and improvement of the contents, submission of new sections covering aspects of multimode modeling that had not been initially included. In this way, the resulting document is backed by a large group of researchers, who are representative of mainly the device community and, in part, also of the circuit community.

The main conclusions are that multiscale modeling will have to provide tools with good predictive capabilities, but relatively straightforward to use also by nonspecialists. To become really attractive for the industry, simulation codes will have to provide insight into deviations of device behavior from what can be predicted by simple intuition.

There are several hints that traditional multiscale approaches, such as those based on the extraction of a compact model from a physics-based device simulation and inclusion of the compact model, defining the relationship among the electrical quantities at the terminals, into a SPICE-like circuit simulator, will not be directly suitable to the description of several types of architectures based on emerging devices. Therefore new hierarchies will have to be defined and validated.

Furthermore, it will be important that future multiscale tools will be able to run on computation facilities available to most interested parties. It is not the time any longer when the computational power of a supercomputer was found five or six years later in a desktop computer. One should in case aim at exploiting low-cost solutions to supercomputation, as in the case of GPU-based systems.

Overall, a close and continuous collaboration with experimental groups will be needed, in order to calibrate and validate the simulation tools all the way through their development.

The expertise currently available in Europe on specific issues very relevant to multiscale modeling, such as ab-initio approaches and integration of electrical and thermal simulation, should be leveraged upon and a critical mass should be reached for a coordinated effort to establish excellence in the development of multiscale TCAD tools for advanced devices.

Beating the size limits of first-principles calculations in nanoscale systems

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The advances in the predictive power, speed and reliability of ab-initio methods has occurred in the last few decades at a very fast pace. Simultaneously, the computing power available through HPC facilities has continued growing exponentially. This combination has brought the paradigm of ab-initio simulations as an invaluable tool to understand and predict the behavior of matter at the nanoscale. First-principles electronic structure methods have advanced in their efficiency to the point where realistic simulations can now be done for systems with many hundreds of atoms [1]. Besides, these methods have been successfully extended to deal with nonequilibrium processes such as electronic transport [2]. Current-voltage characteristics for systems as large as several hundreds of atoms, as those shown in Figure 1, can be currently studied a the fully atomistic and first-principles level [3]. However, enormous challenges are still ahead of us, to be able to extend the range of practical applicability of these methods to the sizes and time scales which are relevant to most of the practical problems in nanotechnology. For instance, many of the processes and properties that make graphene an outstanding material for potential applications are still beyond the reach of these methods, due to the large length or time scales involved. One example is electronic transport, in which the scattering lengths involved are so large that straight first-principles transport calculations are not relevant, because they can still not reach the appropriate length scales. In this talk I will review work done in our group in using first-principles methods for the study of graphene (including electronic transport [3]), and efforts to extend these studies to reach larger length and time scales. In particular, I will describe an implementation of a hybrid QM/MM approach [4] and its application to the immobilization of proteins on graphite surfaces decorated with gold nanoclusters. I will also illustrate the use of first-principles calculations to obtain tight-binding parameters that can be used to compute the transport properties of large samples of chemically modified graphene [5-7].

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Figures

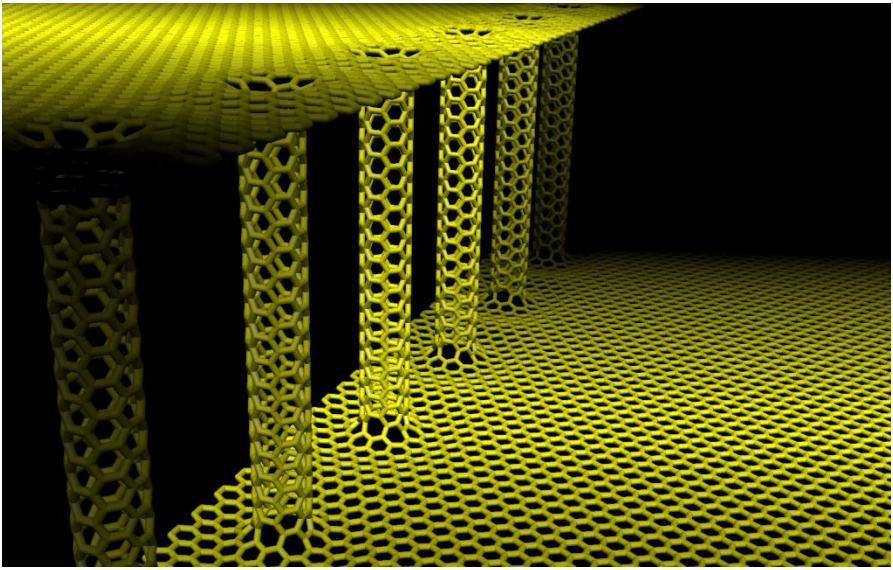

Figure 1: *Pictorial representation of a device consisting in an array of carbon nanotubes linking two semi-infinite graphene sheets. The electronic properties of these arrays were studied using first-principles calculations in Reference [3]*

Numerical Modeling at L'Oréal R&I: Present and Future

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This talk will focus on some topics and challenges which are specific to the cosmetic science in general, and will be illustrated with some of L'Oréal results.

Cosmetic research is characterized by a diversity of topics and needs specialists in over thirty disciplines (chemistry, biology, physics, optics, dermatology, toxicology, genetics, etc.) who attempt to push back the limits of knowledge about hair and skin. They are deepening our intimate understanding at a cellular level and lower, highlighting the biological mechanisms at work in aging, natural color, graying or hair loss, they are synthesizing molecules that act, protect, repair or color, and designing, developing and testing products suited to all types of skin and hair.

For L'Oréal, at the crossroads of several domains, numerical modeling is fast becoming a key factor in the success of its missions:

- *Discovering* new avenues of innovation
- *Predicting* in the field of safety assessment
- *Simulating* to anticipate visible performance

I will present some modeling results at different spatial scales from the atomistic level (molecular modeling) to the macroscopic level (Physically-based model of hair movement), and I will address some challenges requiring a multiscale modeling approach.

Faced with the need to calculate before designing, multiscale modeling will enable L'Oréal and all other cosmetic companies to process all the interactions between *active ingredients*, *formulas* and *cosmetic substrates* within the same time frame.

Charge transport in organic semiconductors: *Ab initio* charge carrier propagation schemes

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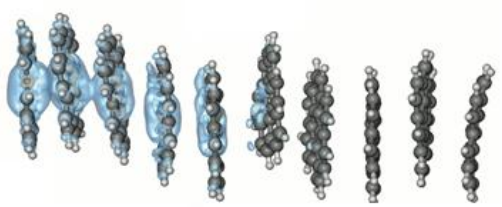
Although π-conjugated, organic semiconductors have been successfully tested in several electronic devices; *e.g.* organic photovoltaic cells [1], organic light emitting diodes [2], and organic field-effect transistors [3]; a full understanding of the precise nature of the underlying charge migration mechanisms is still lacking. In such systems, charge carrier mobilities are dramatically influenced by the structural fluctuations of the molecular stacks, which makes it necessary to take dynamic effects into account beyond purely perturbative treatments. As a result of this strong coupling of the electronic structure to dynamic degrees of freedom, charge transport cannot be described in terms of fully coherent or fully incoherent microscopic mechanisms within the molecular devices' operating temperature range (250 K to 350 K) [4].



In our studies, based on accurate and extensive benchmark calculations, two different propagation schemes are extended and applied to investigate the charge transport mechanisms of molecular systems: A kinetic Monte Carlo scheme based on semi-classical Marcus theory used for the evaluation of the charge transfer rates and a quantum dynamical scheme propagating the charge carrier wave function under explicit consideration of charge effects on the dynamics and the electronic structure of the system. Herewith, charge carrier mobilities are computed for highly ordered molecular systems of different complexity in real-time in a fully *ab initio* matter. Our theoretical investigations open the possibility to achieve quantitative comparisons to transport experiments and are an essential basis for the development of a first-principle materials design.

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