1. TITLE: Hybrid Atomistic Methods for Materials and Biological Systems

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2. SCIENTIFIC CONTENT

2.1 Scientific background

2.1.1 Need for variable precision approaches

Current "standard model" DFT-based first principles methods, although very accurate and general, are notoriously computationally demanding. Their application is thus restricted to relatively small systems and short simulation times. An alternative route to atomistic modelling is provided by parametrized classical potentials, whose domain of application is much less limited in size and time scales. However, the force fields, although they can be built to describe well equilibrium structures and dynamical properties, cannot fulfill the conflicting requirements of accuracy and transferability imposed by chemically complex systems, and thus match the overall quality of first-principles electronic structure based techniques. Thus, variable precision methods, namely embedding schemes where the electronic degrees of freedom are explicitly included in the calculation for a part of the system only, are required for a variety of applications.

2.1.2 Embedding techniques, open problems

These approaches are generally known as QM/MM embedding methods, and their application is especially widespread in biology/biochemistry. In the general, standard approach the system subregion where high accuracy is needed is described by a QM Hamiltonian, and is surrounded by (``embedded" in) a larger zone treated by classical interatomic potentials. The system is thus divided into different parts associated to different models (levels of accuracy/sophistication of the description). The main difficulties are encountered while addressing the issues of how to match different models at the boundary regions, how to treat consistently the long-range interaction between different regions and how to manage situations in which the quantum regions diffuse or experience a flow of atoms/molecules through their boundaries.

2.1.3 Differences between "(Bio)Chemistry" and "Materials" embedding techniques and applications

In biological applications the QM zone is usually well identified before any calculation is performed, and does not change during the simulation of the system. When the QM/MM approach is applied to "Materials Science" applications, traditionally focussing on defect issues such as defect diffusion and mechanical properties (e.g., plasticity, failure, microstructural behaviour) the emphasis shifts to developing techniques useful for fast-moving QM regions (such as the region surrounding a crack tip or a dislocation kink). A third level of description (e.g., a finite element description) is sometimes added to include an external continuum region, needed to represent well the applied stress tensor fields. The applications of this kind to date are, however, more limited in terms of chemical complexity than the biochemical ones. Very little has been done, for example, to apply finite temperature MD techniques to large systems where chemically active subregions determine the elastic/plastic behaviour (stress corrosion processes, subcritical brittle failure in wet conditions, etc.).

2.2 Content,Timeliness of the proposed Workshop

2.2.1 An opportunity to bringing together researchers from two communities

Researchers using embedding hybrid schemes within the biology/biochemistry community and those doing the same within the Materials Science community have much to learn from each other. While specific occasions for this to happen have been sparse, the need for it at this point in time is becoming apparent. This is the main goal of the present workshop.

2.2.2 Useful experience from biochemistry which could help boost electronic structure applications on materials.

Ideally, the Workshop should allow researchers (among which, in particular, junior researchers) of materials science background to interact with people from the biochemistry community who are experienced in (i) chemical termination of QM zones by appropriate radicals (ii) correct modeling of long-range electrostatic interactions between the QM zone and the surrounding MM zone (partial Coulomb charges determination, charge spillage issues, etc.) (iii) rare event techniques associated to chemical reactions. This would represent a very timely benefit, as many recent materials science projects derive their need to include an atomistic modeling activity from the acknowledgment that chemical complexity issues are at the heart of materials behavior, and cannot meaningfully be dealt without electronic structure-accurate techniques. For instance, metal/oxide nterface systems where the fracture toughness of the interface is a key property of, e.g., a thermal barrier, are extremely challenging extended systems with long-range interactions and complex chemistry taking place across various time scales.

2.2.3 Useful experience in solid state/material science which could inspire developments in biochemical applications.

On the other hand, issues like (i) the seamless boundary matching with the embedding regions yielding the correct thermal and mechanical impedance, (ii) dealing with extremely large systems (in the hundred thousand atom range) (iii) dealing with several levels of representation at one time, solving the problem of concurrently matching all the different regions (e.g, matching configurational interaction and density functional to treat open shell impurities, providing a theory and an implementation for appropriate "quantum impedance" pseudopotentials for the atoms used to chemically terminate quantum regions[3]) (iv) developing schemes capable of identifying and dealing with multiple, disconnected QM regions whose number is not a priori fixed (v) modifying at run time the parameters of the interatomic force fields to incorporate the QM information, are all issues which have already been addressed in materials applications. Clearly, much of this acquired experience could inspire progresses in biochemical QM/MM approaches, for which these issues are equally relevant.

2.2.4 possible added value, appropriateness of the chosen format, and organizers' experience in the field.

Finally, with the current upheaval of research in biomimetic and bioactive materials, we would expect that cross-field collaborations may be initiated or strengthened during this Workshop. Timeliness issues aside, we believe that the CECAM venue and workshop format, with its tradition for ample time dedicated to open, in-depth discussions is ideal for bringing together these different

experiences and people active in different fields. At the same time, the Psi-k community has a consolidated access to the scientific communities using hybrid methods for both materials science and biological applications, and is obviously no coincidence that the organizers of the present Workshop proposal include two spokespersons of the Psi-K are active researchers of the field. The Group of Paolo Carloni is very active in the use of QM/MM methods for the investigations of a variety of biological processes, including enzymatic reactions [2]. In addition, one of the organizers, Ursula Rothlisberger, has developed one of the most used hybrid Car-Parrinello MD/classical MD codes [3]. The group of Alessandro De Vita is very active in the field of hybrid methods [4], in close collaboration with the Cambridge TCM group where Gabor Csanyi is based.

3. Tentative list of participants

I. Abarenkov (St.Petersbourg,Russia)
T. Albaret (Lyon,France)
M. Ashby (Cambridge,UK)
N. Bernstein (NRL, US)
P. Ballone (Messina,Italy).
P. Carloni (Trieste, Italy)
L. Colombi Ciacchi (Freiburg, Germany)
G. Csanyi (Cambridge,UK)
A. De Vita (London UK)
F. Ercolessi (Udine, Italy)
S. Estreicher (Lubbock, TX,US)
M. Finnis (Belfast,UK)
S. French (London, UK)
M. Fuxreiter (Budapest, Hungary)
P. Gumbsch (Karlsruhe, Germany)
B. Houraine (Strathclyde, UK)
M. Klein (Upenn,US)
J.-B. Maillet (CEA, France)
A. Magistrato (SISSA, Trieste, Italy)
N. Marzari (MIT US)
J. Mavri (Ljubljana, Slovenia)
F. Mohamed (ETHZ,Switzerland)
F. Montalenti (Milano, Italy)
M. Parrinello (ETHZ, Switzerland)
R. Perez (Madrid, Spain)
D. Pettifor (Oxford, UK)
U. Rothlisberger (EPFL, Switzerland)
K. Scheershmidt (Halle,Germany)
A. Sutton (London, UK)
D. Truhlar (U. Minnesota, US)
J. VandeVondele (ETHZ,Switzerland)

4. Number of participants, Schedule

We propose having approximately 25 speakers, not counting the 4 organizers. The formal part of the workshop is planned for four days, with 7 talks per day on Monday through Wednesday, and 4 talks on Thursday morning, concluding with a focused round-table discussion in the afternoon.

Formal talks will take place Monday through Thursday, closed by a working groups session on Thursday afternoon. Anytime in July August or early September 2006 would be preferred.

5.TUTORIALS

Two "Things you always wanted to know but you never got a chance to hear" in-depth seminars (1.5 hours are allocated for each one, including ample time for discussion) will be given on Tuesday and Wednesday, in a special end-of-afternoon session. These seminars will provide a technical overview on how a number of specific problems are tackled by various recent algorithms, and are actually handled in the corresponding production codes.

In the first seminar Alessandra Magistrato (SISSA,Trieste) and Ursule Rothlisberger (EPFL,Lausanne) will cover biological applications of the QM/MM method.

In the second one Gabor Csanyi (TCM, Cambridge) will address a number of issues on hybrid schemes for materials science applications.

6. BUDGET

The following budget is based on 37 participants: 25 speakers, 4 organizers plus 8 (or more, likely junior) scientists. All attending people (organizers excluded) will need a per diem support for 5 days. The organizers plan to obtain 8000 euro of funding from the Psi-k ESF programme, and 8000 euro from CECAM. The requested Psi-k budget figure appears reasonable for a workshop which will cover the activities of two Psi-k working groups. The organizers will cover their own travel and living expenses on their own funds. In euro:

5 nights	8750	70 x 25 x 5
5 days	3750	30 x 25 x 5
Travel expenses for the overseas participants	2500	
Workshop dinner + incidentals	1500	
Overall funding for attending junior scientists	4000	100 x 8 x 5
Total needed	20500	
Total requested to Psi-K	8000	
Total requested to CECAM	8000	
Total requested to other organizations	4500	

7. Other organizations to which an application for funding will be made.

The remaining 4500 euro will be seeked from the DEMOCRITOS CENTER (Sissa, Trieste), the CENMAT CENTER (University of Trieste) and from King's College London. This will be used to cover the expenses for the attending junior scientists.

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