Multi-scale modelling: applications to physicochemical processes

Paris IHP, February 2013, 2 days between 11 and 15 February

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1. Proposal

1.1 Introduction and motivation

The description, comprehension and prediction of physicochemical processes in engineering are based on multi-scale modelling. It starts from *ab initio* molecular simulations to hydrodynamic chemical engineering codes, through molecular dynamics, Monte Carlo simulations, and a large variety of mesoscopic approaches: Brownian dynamics, lattice models, analytical approximations, *etc*. The range of domains covered by such modelling is widely extended: phase separation, liquid-liquid extraction, and all the variety of electrochemical generators, as well as the problem of waste storage, *e.g.* nuclear wastes, carbon dioxide, and heavy metal residuals. It involves now a much larger variety of problems that in the original solid material science features, which remain reference problems, without the complexity of liquid, interfacial and soft matter problems, where the dynamics of the particle is the fundamental point.

1.2 State of the art

Today state of art for the multi-scale modelling for liquid, soft matter and interfacial systems starts from *ab initio* molecular simulations, followed by classical molecular dynamics (MD) or Monte-Carlo (MC). Then, several coarse graining procedures can take place: Brownian Dynamics (BD), lattice models (LM), analytical and thermodynamic model, *etc.* In principle, each approach is exact (or at least self-consistent) and presents advantages and drawbacks when it comes to practical applications, since many approximations, assumptions, and restrictions come to play for real cases. The basic point is to keep all relevant information coming from molecular structure and *ab initio* simulations in the final macroscopic models including hydrodynamic chemical engineering codes. In practice, this goal is only very partially reached and the purpose of the present workshop is to link more completely the different approaches.
For the present discussion meeting, we plan to tackle both theoretical and numerical approaches for the description of different classes of physicochemical processes.

1.3 Objectives

The aim is to gather together experts in complementary fields to share and discuss research that is concerned with all aspects of the multi-scale modelling: engineering processes, multiphase equilibria and extraction, electrical energy and waste storage. Particular emphasis will be given to the problem of nuclear soft matter, with the special constraint to treat very heavy metals, such as actinides. For each topic chosen for this meeting different contributions and points of view are expected. The topics are:

- First principles modelling,

- Brownian models,
- Specific problems for heavy metals,
- Existing physicochemical applications,
- Specific problems for solid and glasses,
- Projects.

A two days meeting will be proposed, the exact dates will be specified as soon as possible.

1.4 Participant List

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2. Financial Support

We ask CFCAM a support for this meeting of the order of 2000€, to cover logistic expanses such as coffee break and first day lunch, and travel expanses for selected young participants.
A support will be given by CEA/DEN/DRCP for participants from the French atomic energy commission, belonging to this department.