2018-00414 - [Campagne doctorants-CRI Paris] Numerical analysis of molecular and multiscale models

Level of qualifications required : Graduate degree or equivalent
Fonction : PhD Position

Context
The MATHERIALS team applies methods of applied mathematics to the field of molecular and multiscale simulation.

The source of many phenomena in physical and life sciences, and in most engineering disciplines, is to be found in microscopic features of the system under consideration. Linking the properties of matter at these different scales is a major challenge, both from the theoretical perspective (understanding how to link a model or an equation at a certain scale to another one at a different scale) and the numerical one (how to couple two consistent descriptions of matter, e.g. atomistic and continuum, using the same code).

MATHERIALS (formerly MICMAC) originally focused on computational chemistry issues (electronic structure calculations for materials, laser control of chemical reactions). The team has next gradually widened its scope beyond such considerations and their applications, and applied its expertise to related topics at very different scales. This has led to studies in molecular dynamics (in situ molecular system evolution), in computational statistical mechanics (computation of ensemble averages), and studies of relationships with more traditional mechanical models at the continuum scale (multiscale simulation of solid materials in general, including periodic and random homogenization of elliptic PDEs, numerical homogenization techniques such as MsFEM, ...).

MATHERIALS currently offers a range of expertise, rarely found on the international scene, in a number of promising topics for numerical simulation and applied mathematics in general: molecular chemistry, solid-state physics, numerical modeling in materials science, highly-oscillatory PDEs, etc.

Assignment
The team is currently involved in the study of various numerical methods for (i) electronic structure calculation, (ii) molecular simulation and (iii) multiscale PDEs. Concerning the first theme, the focus is currently on the design of methods for periodic and aperiodic materials, modelled at the quantum scale. For molecular simulation models, efficient numerical algorithms for accelerating the computation of a long trajectory in molecular dynamics are currently investigated, including parallel algorithms and algorithms dedicated to out-of-equilibrium models. Variance reduction techniques to improve the...
Monte Carlo approaches are likewise of interest. Concerning the third theme, numerical homogenization techniques, that aim at addressing the PDE of interest in a dedicated manner (e.g. using a well-adapted discretization space) are currently investigated. The team has also a long-term interest in theoretical and numerical questions concerning non-periodic homogenization (modelization of defects, variance reduction in stochastic homogenization, ...).

**Main activities**

The project will be made precise together with the candidate, depending on his/her skills and interests, and on the current interests of the team at the time of application.

This position is for a PhD thesis in the MATHERIALS team, and can involve any member of the team. Please contact us before applying to find a match between your interests and the team members.

**Benefits package**

- Subsidised catering service
- Partially-reimbursed public transport

**Remuneration**

Gross Salary per month: 1,982 € the first 2 years and 2,085 € the last year