2018-00327 - [Campagne Post-Doctorat 2018/CRI PARIS] - Post-Doctoral Research Visit / Scientific computing / Numerical schemes and simulations

**Context**

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).

MATHERALIS originally focused on computational chemistry issues (electronic structure calculations for materials, laser control of chemical reactions) before gradually widening its scope beyond such considerations and their applications, and applying 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 and multiscale simulation of fluid or solid materials in general (including periodic and random homogenization).

MATHERALIS 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, etc.

**Assignment**

The team is currently involved in the study of various numerical methods for electronic structure calculation, molecular and multiscale simulation. Concerning the first theme, the focus is currently on models of defects in crystalline materials. 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. Numerical techniques for stochastic homogenization are also investigated.

Many of these works are made in collaboration with other groups in Paris, in particular CNRS and University Paris 6.

**Main activities**

The postdoctoral fellow will conduct his/her research within the MATHERALIS team, interacting with its permanent members. He/She will write research articles and present his/her work in international conferences.

**Skills**

Candidates are required to have a strong experience in numerical scientific computing.
Benefits package

- Subsidised catering service
- Partially-reimbursed public transport

Remuneration

Additional information

- Location: Paris 12ème
- Gross Salary per month: 2653€ brut/mensuel

Security and defense procedure:

This position is likely to be situated in a restricted area (ZRR), as defined in Decree No. 2011-1425 relating to the protection of national scientific and technical potential (PPST).

Authorisation to enter an area is granted by the director of the unit, following a favourable Ministerial decision, as defined in the decree of 3 July 2012 relating to the PPST. An unfavourable Ministerial decision in respect of a position situated in a ZRR would result in the cancellation of the appointment.