

## Job Offer

### Job Summary

<b>Title, Job Position</b>	<b>Postdoctoral position:</b> <b>Generalized Langevin equations and stochastic sampling</b>
<b>Research Field</b>	Applied mathematics
<b>Employer</b>	Sorbonne Université Institut des sciences du calcul et des données
<b>Location :</b>	Paris, France
<b>Application Deadline / Timezone</b>	15-02-2020 11:00AM Paris (GMT+01 :00)
<b>Salary</b>	depending on skills and experience
<b>Type of Contract</b>	Temporary (fixed term) 18 months
<b>Job Status</b>	Full-time
<b>Envisaged Starting Date</b>	Between 15 April and 15 June 2020

### Hiring Organisation

#### Organisation

Sorbonne Université was created on January 1st, 2018 from the merger of Paris-Sorbonne and Pierre and Marie Curie (UPMC) universities. As a public institution, it fulfils the public service calling of French higher education, research and innovation.

Sorbonne University is a multidisciplinary and research-intensive university with world-famous origins. Continuing the humanist tradition of the Sorbonne, it is devoted to meeting the scientific challenges of the 21st century and spreading the knowledge created in its laboratories by its research teams and transmitted to its students and to society as a whole. Sorbonne University's three faculties in humanities, medicine and science each with the wide-ranging autonomy necessary to conduct its ambitious programs in both research and education. The University's 53,500 students, 3,400 professor-researchers and 3,600 administrative and technical staff members who help it run every day contribute to a University that is diverse, creative, innovative, and with a global outlook.

#### Organisation Type

Higher Education Institute

#### Department

Institut des sciences du calcul et des données, FED 3

The institute of computing and data sciences (ISCD (<http://iscd.sorbonne-universite.fr/>)) is dedicated to exploring and developing the potential of computational and data-driven research and training across science, humanities and medicine at Sorbonne Université. Our research teams use the power of algorithms and visualisation to solve problems in biology, chemistry, mathematics, computer science, medicine, and the digital humanities. Our history of supporting collaboration goes back more than 10 years when the institute was created to support areas where methods and means of approaching challenges spilled over the disciplines. and were profoundly transforming research.

## Offer Description

## Description

**Scientific context.** Molecular simulation is the main tool for the prediction of kinetic properties of physico-chemical systems in computational physics and materials science. The most satisfactory framework to describe and understand the dynamics of metastable transitions consists in projecting the high-dimensional trajectory of the system (thousands of Cartesian atomic coordinates) onto a low-dimensional space of collective variables. This dimensional reduction leads to a stochastic differential equation (SDE) – a so-called effective dynamic – which should in general be non-Markovian (generalized Langevin equation).

**Scientific environment.** The post-doctoral project is part of the new **MAESTRO** interdisciplinary team, within the Institute for Computing and Data Sciences (ISCD) in Sorbonne Université. By joining forces between mathematicians, physicists and physical chemists, the long-term goal of the team is to investigate materials for energy through stochastic sampling and high-performance computing.

**Scientific objectives.** The objective of the first phase (2 years) of the project is the development of a systematic approach to construct accurate Langevin models of dynamical processes in complex materials, employing as input data extensive molecular dynamics trajectories. These trajectories are often too short to obtain accurate statistics, and we need a model to compute long time dynamics.

The main challenges to solve in this direction are the development of efficient stochastic optimization, unbiased statistical estimators and variance reduction techniques, as well as the definition of general strategies (e.g. variational principles) to identify optimal collective variables and to tackle non-Markovian memory effects.

The study will primarily focus on simple “toy” models, in order to identify the key steps and overcome the mathematical bottlenecks without being limited by the numerical cost and physical complexity. The results will then be transferred to challenging systems in materials science.

**Project PI:** A. Marco SAITTA

**Postdoc supervisors:** Pierre MONMARCHE – Ludovic GOUDENEGE – Fabio PIETRUCCHI – Benjamin ROTENBERG

## Appointment Term

Eighteen months appointment starting as soon as possible.

**Keywords:** Generalized Langevin diffusion; colored noise; effective/coarse-grained dynamics; sampling methods; material science; numerical simulation; molecular dynamics

*As part of your duties, you may be required to provide internal training related to your business expertise.*

## Profile Requirements

### Required Education Level

Expertise in probability, statistics and stochastic algorithms. Monte-Carlo methods and Bayesian statistics. Stochastic optimization.

### Skills / Qualifications

- Applicants must have a recent Ph.D. in Mathematics
- Prior experience and proficiency in numerical algorithms and stochastic optimization
- Applicants should be hard working, analytical and have excellent writing and communication skills necessary to author technical and scientific reports, publications, and deliver scientific presentations, seminars, meetings and/or teaching lectures
- Experience collaborating effectively with a team of scientists of diverse backgrounds

### Specific Requirements

- This position involves a significant amount of numerical code development
  - Therefore the candidate will have prior scientific programming experience combined with an enthusiasm for scalable computing.

### Required Languages

English

### Required Research Experience

PhD/previous postdocs in research-intensive labs, significant publication record

## Work Location

### Institute

Institut des sciences du calcul et des données

Equipe-projet “Maestro” (The **MA**aterials for **E**nergy through **ST**ochastic sampling and high **peR**formance **cO**mputing) – PI: A. Marco SAITTA



### Country

France

### Location

Sorbonne Université

Campus Pierre et Marie Curie

4, place Jussieu

Paris

## How to apply ?

### Required Application Materials

1. Cover letter with current and future research interests
2. Most recent curriculum vitae
3. Copy of first author publications
4. Names and contact for three referees

### How to submit

Interested candidates should

- Contact for additional information about the offer:  
Pr. Pierre Monmarché ([pierre.monmarche@sorbonne-universite.fr](mailto:pierre.monmarche@sorbonne-universite.fr)),  
Pr. Ludovic Goudenège ([ludovic.goudenège@math.cnrs.fr](mailto:ludovic.goudenège@math.cnrs.fr))  
Pr. Fabio Pietrucci ([fabio.pietrucci@sorbonne-universite.fr](mailto:fabio.pietrucci@sorbonne-universite.fr))
- submit the required application materials to:  
Pascal Frey, Agnieszka Miskiewicz ([iscd@sorbonne-universite.fr](mailto:iscd@sorbonne-universite.fr))  
with the tile "ISCD Fellowship Application".

## Selection Procedure

### Selection process

The Institute's selection process is based on an email submission.

Candidates are evaluated by faculty reviewers in their own academic fields and from other disciplines. Reviewers will evaluate candidates according to their academic accomplishments and their potential for research.

The selection process is organized in four stages.

1. Eligibility check: candidate's compliance with the requirements of the offer will be checked on the basis of the information provided by the applicant.
2. Evaluation of CV: applicant's CV and research proposals will be evaluated and ranked according to their merit.
3. Interviews of candidates: **short listed** candidates will be invited for an interview conducted by the selection committee.
4. Final decision: the selected candidate will be proposed the position. A reserve list of candidates may be identified in case of withdrawal of the selected candidate.

Please note that priority in individual applicant selection will be given to first-time fellows.