Offer #2025-08880

Post-Doctoral position at CERMICS: "Computing transition rates: models and algorithms"

Level of qualifications required : PhD or equivalent

Fonction : Tempary Research Position

Main activities

Post-doctoral position: "Computing transition rates: models and algorithms"

Keywords: molecular dynamics, machine learning, rare event sampling

Net salary: Approximately 2400 Euros per month, subject to discussion based on the candidate's experience.

Duration: 12 months, renewable up to 18 months.

Position to be fulfilled as soon as possible. Application from 30th April to 30th June 2025.

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The aim of this project is to efficiently and accurately compute reaction rates of chemical transformations, typically in the field of catalytic chemistry (for instance alcohol isomerization). A first task will be to quantitatively study the limitations of approximate formulas obtained from harmonic transition state theory (Eyring-Kramers or Eyring-Polanyi formulas), by comparing the predictions of these approximate theories to reference results obtained either by direct numerical simulations or using dedicated numerical methods such as the adaptive multilevel splitting (AMS) algorithm [1]. A second task will be to improve the performance of AMS by combining it with importance sampling techniques and building good reaction coordinates, relying on neural networks such as bottleneck autoencoders,

which have proved successful for free energy computations [2,3]. Improved reaction coordinate can be obtained by minimizing the total reaction rate of the associated effective dynamics [4].

This postdoctoral fellowship is funded by the PEPR B-best, through the project MAMABIO, whose overall goal is to develop new numerical methods to study reactions of transformation of biosourced molecules, in collaboration with Hadrien Vroylandt from University of Caen Normandy, IFP Energies nouvelles (Pascal Raybaud, Thomas Pigeon, Manuel Corral-Valero), and the group of Christoph Chipot (CNRS, University of Lorraine).

[1] T. Pigeon, G. Stoltz, M. Corral-Valero, A. Anciaux-Sedrakian, M. Moreaud, T. Lelièvre, P. Raybaud, Computing surface reaction rates by Adaptive Multilevel Splitting combined with machine learning and ab initio molecular dynamics, J. Chem. Theory Comput. 19(12), 3538–3550 (2023) https://doi.org/10.1021/acs.jctc.3c00280

[2] Z. Belkacemi, M. Bianciotto, H. Minoux, T. Lelièvre, G. Stoltz and P. Gkeka, Autoencoders for dimensionality reduction in molecular dynamics: collective variable dimension, biasing and transition states, J. Chem. Phys 159, 024122 (2023) https://doi.org/10.1063/5.0151053

[3] Z. Belkacemi, P. Gkeka, T. Lelièvre, G. Stoltz, Chasing collective variables using autoencoders and biased trajectories, J. Chem. Theory Comput. 18(1), 59-78 (2022) https://doi.org/10.1021/acs.jctc.1c00415

[4] W. Zhang, C. Hartmann and C. Schutte, Effective dynamics along given reaction coordinates, and reaction rate theory, Faraday Discussions, 195, 365-394 (2016) https://doi.org/10.1039/C6FD00147E

Benefits package

- Subsidized meals
- Partial reimbursement of public transport costs
- Leave: 7 weeks of annual leave + 10 extra days off due to RTT (statutory reduction in working hours) + possibility of exceptional leave (sick children, moving home, etc.)
- Possibility of teleworking and flexible organization of working hours
- Professional equipment available (videoconferencing, loan of computer equipment, etc.)
- Social, cultural and sports events and activities

General Information

- **Theme/Domain :** Numerical schemes and simulations
  Scientific computing (BAP E)
- **Town/city :** Paris
- **Inria Center :** Centre Inria de Paris
- **Starting date :** 2025-04-30
- **Duration of contract :** 1 year, 8 months
- **Deadline to apply :** 2025-06-02

Contacts

- **Inria Team :** MATHERIALS
- **Recruiter :**
  Lelièvre Tony / Tony.Lelievre@inria.fr

About Inria

Inria is the French national research institute dedicated to digital science and technology. It employs 2,600 people. Its 200 agile project teams, generally run jointly with academic partners, include more than 3,500 scientists and engineers working to meet the challenges of digital technology, often at the interface with other disciplines. The Institute also employs numerous talents in over forty different professions. 900 research support staff contribute to the preparation and development of scientific and entrepreneurial projects that have a worldwide impact.

Warning : you must enter your e-mail address in order to save your application to Inria. Applications must be submitted online on the Inria website. Processing of applications sent from other channels is not guaranteed.

Instruction to apply

Defence Security :
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.

Recruitment Policy :
As part of its diversity policy, all Inria positions are accessible to people with disabilities.