Offer #2025-08831

Post-Doctoral Research Visit F/M
Deciphering conformational dynamics in macromolecular complexes

Contract type : Fixed-term contract

Level of qualifications required : PhD or equivalent

Fonction : Post-Doctoral Research Visit

Level of experience : From 3 to 5 years

Context

This postdoc position is funded for two years by the grant from Programme Inria Quadrant (PIQ). The main goal is to develop a graph neural network architecture to investigate conformational dynamics of macromolecular complexes. The Postdoc researcher will be in connection with **Yasaman Karami** (Chargee de recherche, Inria) with expertise in proteins conformational dynamics and allostery, and will be hosted in the Delta team within the Inria center at the Universite de Lorraine. Our team consists of two permanent researchers with several PhD and postdoc members, and is expected to grow by hiring new members. It provides a multidisciplinary and international environment, and benefits from experts in structural bioinformatics, as well as in computer science and deep learning. Our main goal is to develop deep learning models, to study, and predict protein structure, interactions, function and to further design synthetic molecules. The team has access to computational resources, including efficient GPUs and CPUs, from different cluster centers including Grid5000, Jean Zay, etc.

Assignment

Biomolecules such as proteins and nucleic acids are at the heart of virtually all fundamental cellular processes. They adopt complex dynamic behavior and their functions are directly linked to the arrangement of atoms in 3D and dynamics. Therefore, characterizing the structure, dynamics and conformational changes of biomolecules can help understand the molecular mechanisms of underlying diseases. We recently developed **ComPASS**, a large-scale computational method designed to study communication networks in protein-protein and protein-nucleic acid complexes [1]. ComPASS has been applied to different biological systems, facilitating the interpretation of the conformational dynamics. In a recent study, we highlighted the role of cysteine hyperoxidation in Nucleosome [2,3]. Moreover, we took major steps in learning conformational dynamics by proposing **DynamicGT**, a novel architecture that combines cooperative graph neural networks with a graph transformer, to predict binding sites [4].

The main goal of this Postdoc is to elucidate the conformational dynamics of macromolecular complexes and to develop a method for understanding their communications. The main idea is to take another major step, taking advantage of the recent developments of AI and propose a novel approach to uncover distinct mechanisms in macromolecular systems. The post-doctoral researcher will also help supervise the team's students working on computational biology problems.

[1] Bheemireddy S, Gonzalez-Aleman R, Bignon E, Karami Y. Communication pathway analysis within proteinnucleic acid complexes. bioRxiv, 2025.

[2] Karami Y, Bignon E. Cysteine hyperoxidation rewires communication pathways in the nucleosome and destabilizes the dyad. Computational and Structural Biotechnology Journal, 2024, 23, 1387-1396.

[3] Karami Y, Gonzalez-Aleman R, Duch M, Qiu Y, Kedjar Y, Bignon E. Histone H3 as a redox switch in the nucleosome core particle: insights from molecular modeling. bioRxiv, 2024.

[4] Mokhtari O, Grudinin S, Karami Y, Khakzad H. DynamicGT: a dynamic-aware geometric transformer model to predict protein binding interfaces in flexible and disordered regions. bioRxiv, 2025.

Main activities

1. Implementing the deep learning architecture
2. Contributing into training data collection and curation
3. Validating the method and analysing the results over SOTA benchmarks

4. Supervising Master students and teamwork with PhD students, collaborating with other teams

5. Writing scientific articles, software development and participating in international conferences

Skills

- PhD degree in Computer Science, or Bioinformatics
- Proficiency in Python and good coding practices is mandatory
- Experience in deep learning (PyTorch) is mandatory*
- Knowledge in protein biochemistry
- Ability to work independently and also to work in a team
- Excellent oral and written English skills

*Applications with no computer science/deep learning background will not be considered.

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 (after 6 months of employment) and flexible organization of working hours
- Professional equipment available (videoconferencing, loan of computer equipment, etc.)
- Social, cultural and sports events and activities
- Access to vocational training

- Social security coverage

Remuneration

From 2788 € gross/month

General Information

- **Town/city :** Villers lès Nancy
- **Inria Center :** Centre Inria de l'Université de Lorraine
- **Starting date :** 2025-10-01
- **Duration of contract :** 2 years
- **Deadline to apply :** 2025-05-17

Contacts

- **Inria Team :** AT-LOR AE
- **Recruiter :**
  Karami Yasaman / yasaman.karami@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.