Offre n°2025-08831

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

Le descriptif de l'offre ci-dessous est en Anglais

Type de contrat : CDD

Niveau de diplôme exigé : Thèse ou équivalent

Fonction : Post-Doctorant

Niveau d'expérience souhaité : De 3 à 5 ans

Contexte et atouts du poste

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.

Mission confiée

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.

Principales activités

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

Compétences

- 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.

Avantages

- 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

Rémunération

From 2788 € gross/month

Informations générales

- **Ville :** Villers lès Nancy
- **Centre Inria :** Centre Inria de l'Université de Lorraine
- **Date de prise de fonction souhaitée :** 2025-10-01
- **Durée de contrat :** 2 ans
- **Date limite pour postuler :** 2025-05-17

Contacts

- **Équipe Inria :** AT-LOR AE
- **Recruteur :**
  Karami Yasaman / yasaman.karami@inria.fr

A propos d'Inria

Inria est l'institut national de recherche dédié aux sciences et technologies du numérique. Il emploie 2600 personnes. Ses 215 équipes-projets agiles, en général communes avec des partenaires académiques, impliquent plus de 3900 scientifiques pour relever les défis du numérique, souvent à l'interface d'autres disciplines. L'institut fait appel à de nombreux talents dans plus d'une quarantaine de métiers différents. 900 personnels d'appui à la recherche et à l'innovation contribuent à faire émerger et grandir des projets scientifiques ou entrepreneuriaux qui impactent le monde. Inria travaille avec de nombreuses entreprises et a accompagné la création de plus de 200 start-up. L'institut s'e?orce ainsi de répondre aux enjeux de la transformation numérique de la science, de la société et de l'économie.

Attention: Les candidatures doivent être déposées en ligne sur le site Inria. Le traitement des candidatures adressées par d'autres canaux n'est pas garanti.

Consignes pour postuler

Sécurité défense :
Ce poste est susceptible d'être affecté dans une zone à régime restrictif (ZRR), telle

que définie dans le décret n°2011-1425 relatif à la protection du potentiel scientifique et technique de la nation (PPST). L'autorisation d'accès à une zone est délivrée par le chef d'établissement, après avis ministériel favorable, tel que défini dans l'arrêté du 03 juillet 2012, relatif à la PPST. Un avis ministériel défavorable pour un poste affecté dans une ZRR aurait pour conséquence l'annulation du recrutement.

Politique de recrutement :
Dans le cadre de sa politique diversité, tous les postes Inria sont accessibles aux personnes en situation de handicap.