

Offer #2025-08954

PhD Position F/M PhD position: Geometric deep learning models to study intrinsically disordered proteins

Contract type: Fixed-term contract

Level of qualifications required : Graduate degree or equivalent

Fonction: PhD Position

Context

This PhD position is part of the **IDPFold** project (2025-2029) recently funded by the French National Research Agency (ANR). The main goal is to develop geometric deep learning models to study intrinsically disordered proteins (IDP). The PhD candidate will be supervised by Hamed Khakzad (Junior Professor, Inria). Our team consists of two permanent researchers with several PhD and postdoc members, and is expected to grow by hiring new members. 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

IDPs are a large subset of proteins with no stable 3D structure on isolation. They are involved in various cellular processes, and protein-protein interactions (PPIs). One of the key aspects of IDPs is their ability to undergo disorder-to-order transition upon binding to a target structure. While understanding this mechanism is essential, it remains an open problem in the field. Novel approaches based on deep learning have started to make remarkable advances in protein structure and complex prediction. However, the performance of these methods on PPI prediction where

IDPs are involved is still lagging behind, mostly due to the complexity imposed by flexible regions. This PhD position aims to develop geometric deep learning models to elucidate this complex mechanism and will be potentially built on on-going research efforts in the team. The PhD candidate will have the possibility to be involved in international collaborations and will work closely with permanent researchers of the lab on this topic.

Main activities

- 1. Implementing deep learning models
- 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

- Master 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

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

^{*}applications with no computer science/deep learning background will not be considered.

Remuneration

2200 € 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: 3 years
Deadline to apply: 2025-06-26

Contacts

Inria Team : AT-LORPhD Supervisor :

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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.