

# Offer #2025-08565

# 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 deép learning models to élucidate 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
- Experiencé in déep 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
- Professional equipment available (videoconferencing, loan of computer equipment, etc.)
- Social, cultural and sports events and activities
- · Access to vocational training
- Social security coverage

<sup>\*</sup>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: 2025-09-02 Duration of contract: 3 years Deadline to apply: 2025-02-17

### Contacts

• Inria Team: AT-LOR PhD Supervisor:

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## **About Inria**

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# 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.