



**Offre n°2025-08634**

## **Engineering structural bioinformatics applications: algorithms and code optimization**

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

**Type de contrat :** CDD

**Niveau de diplôme exigé :** Bac + 5 ou équivalent

**Autre diplôme apprécié :** PhD

**Fonction :** Ingénieur scientifique contractuel

### **Contexte et atouts du poste**

SCIENTIFIC CONTEXT. Biomolecules, particularly proteins and nucleic acids (DNA and RNA), are essential to biological processes. Their study is typically divided into two main aspects: the structural level, which focuses on their (meta-)stable conformations, and dynamics, which evaluates the stability of these conformations and the rates at which they interconvert. AlphaFold, the program developed by Deepmind, made a very significant step for structural predictions of structured proteins, and its two leaders were co-awarded the 2024 Nobel prize in chemistry. But the question of fast and accurate predictions of dynamical properties remains open. This is a particularly important problem to understand the strength of interactions at the molecular level, with potentially far reaching applications in medicine. The goal of the project EMINENCE–molEcular dynaMics In iNtErNal CoordinatEs, funded by France 2030–see below, is to deliver state-of-the-art modeling tools geared towards biomolecular dynamics, within the Structural Bioinformatics Library.

**SOFTWARE:** the Structural Bioinformatics Library. The Structural Bioinformatics Library (SBL, <https://sbl.inria.fr>) is a comprehensive software environment to model biomolecules, with a unique and versatile design. It jointly provides (i) low level algorithm classes, (ii) biophysical models, and (iii) applications solving specific problems in structural bioinformatics. Applications are ascribed to two principal categories respectively targeting static and dynamic models, see <https://sbl.inria.fr/applications/>. To foster genericity, re-usability, efficiency and robustness, the SBL is mainly developed in generic (template based) C++, and consists of ? 100 C++ packages, 2/3 in the Core, and 1/3 for Applications.

**FRANCE 2030.** France 2030 is an investment plan aiming at supporting innovative technologies and the ecological transition <https://www.economie.gouv.fr/france-2030>. The project EMINENCE is supported by the Inria Quadrant Program and receives national funding through The French National Research Agency as part of the France 2030 plan under the reference « ANR24-RRII-0002 », operated by the Inria Quadrant Program. In the framework of France 2030 and the Digital program agency Digital Program Agency - Algorithms, software and usage operated by Inria, the Inria Quadrant Program selected by the General Secretariat for Investment (SGPI) and the Directorate-General for Research and Innovation (DGRI) aims to support scientific risk-taking and to address current and future challenges in research and innovation for and through digital sciences and technology. See <https://piq.inria.fr/>.

## **Mission confiée**

### **ENGINEERING POSITION AND TASKS: ALGORITHM ENGINEERING FOR BIOMOLECULAR DYNAMICS.**

In modeling biomolecules, internal coordinates in general and torsion angles in particular are much more effective than Cartesian coordinates to generate large amplitude conformational changes. However, using torsion angles is more challenging mathematically, in several respects: necessity to solve inverse problems of the loop closure type, non local effects, sampling biases. We have recently developed several algorithms to explore energy landscapes, and sample loops as well as multiloop systems.

- \* Main goals/specific tasks
- \*\* Optimizing loop and multiloop samplers.
- \*\* Optimizing energy landscape explorers.
- \*\* Optimizing binding affinity estimators.

## **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

## Informations générales

- **Thème/Domaine** : Biologie numérique  
Calcul Scientifique (BAP E)
- **Ville** : Sophia Antipolis
- **Centre Inria** : [Centre Inria d'Université Côte d'Azur](#)
- **Date de prise de fonction souhaitée** : 2025-03-01
- **Durée de contrat** : 1 an, 7 mois
- **Date limite pour postuler** : 2025-12-27

## Contacts

- **Équipe Inria** : [ABS](#)
- **Recruteur** :  
Cazals Frédéric / [Frederic.Cazals@inria.fr](mailto:Frederic.Cazals@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'efforce ainsi de répondre aux enjeux de la transformation numérique de la science, de la société et de l'économie.

## L'essentiel pour réussir

- \* Requirements: education and skills
- \*\* PhD in computer science, algorithms, machine learning, bioinformatics, biophysics.
- \*\* Expertise in software development, including C++, python, git.
- \*\* Expertise in algorithm engineering (implementation, optimization, profiling and experimental evaluation).
  
- \* Main Conditions
- \*\* Position for 18 months, at Centre Inria d'Université Côte d'Azur, Algorithms-Biology-Structure, SophiaAntipolis.
- \*\* Small and vibrant group.
- \*\* Work on a potentially high impact project.
- \*\* Net salary per month before taxes: 3000 - 4600, depending on experience.
  
- \* Applying: email Frederic.Cazals@inria.fr with: vitae, a cover letter, and two references.

**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.