Offer #2025-08634

Engineering structural bioinformatics applications: algorithms and code optimization

Contract type : Fixed-term contract

Level of qualifications required : Graduate degree or equivalent

Other valued qualifications : PhD

Fonction : Temporary scientific engineer

Context

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/.

Assignment

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.

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

General Information

- **Theme/Domain :** Computational Biology
  Scientific computing (BAP E)
- **Town/city :** Sophia Antipolis
- **Inria Center :** Centre Inria d'Université Côte d'Azur
- **Starting date :** 2025-03-01
- **Duration of contract :** 1 year, 7 months
- **Deadline to apply :** 2025-12-27

Contacts

- **Inria Team :** ABS
- **Recruiter :**
  Cazals Frédéric / Frederic.Cazals@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.

The keys to success

* 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.

> **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.