EMINENCE–molEcular dynaMics In iNtErNal CoordinatEs

Opening of an engineering position:

- **Boosting the dissemination of biomolecular apps.**

Country	France
Organisation/Company	Centre Inria at Université Côte d'Azur, French Riviera
Department	Algorithms-Biology-Structure
	Web: `http://team.inria.fr/abs`
Research Field	Computer science, Simulation engineering, Computational Structural Biology
Positions' type	Research engineers
Application deadline	Positions are open, apply asap
Type of contract	Temporary, 18 months
Job status	Full-time
Mission and conditions	See details below

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 « ANR-24-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/`.

Engineering position 1: **Boosting the dissemination of biomolecular apps.** Applications in structural bioinformatics are typically made available via two channels, namely web sites, and plugins/apps within environments such as VMD (`https://www.ks.uiuc.edu/Research/vmd/`) or Pymol (`https://pymol.org/`).

The mission entrusted to the engineer will consist of two main tasks. The first one will be to boost the dissemination and the adoption of the application packages of the SBL, both via dedicated web sites and plugins for VMD and Pymol. The second one will consists of animating the community by preparing tutorials and courses.

●**Main goals/specific tasks**

- Design of a generic GUI graphical interface for SBL applications.

- Dissemination of applications for biomolecular static analysis.

- Dissemination of applications for biomolecular dynamic analysis.

- Outreach: tutorials and training for the community.

●**Requirements: education and skills**

- Master/PhD in bioinformatics, biophysics.

- Expertise in software development, including C++, python, git, GUIs.

- Expertise in scientific computing and/or visualization and/or biomolecular modeling.

●**Conditions**

- Position for 18 months, at Centre Inria d'Université Côte d'Azur, Algorithms-Biology-Structure, Sophia-Antipolis.

- Small and vibrant group.

- Work on a potentially high impact project.

- Net salary per month before taxes: 2700 - 3500, depending on experience.

●**Applying**

- Email Frederic.Cazals@inria.fr with: vitae, a cover letter, and two references.