- **Title** : User-assisted modelling of macromolecular complexes guided by low-resolution scattering profiles
- **MSc thesis advisor** : Sergei Grudinin, sergei.grudinin@inria.fr, Phone: +33 4 38 78 16 91
- **Group leader** : Stephane Redon, stephane.redon@inria.fr
- **Laboratory** (+working place) : NANO-D, INRIA Rhone-Alpes Research Center Minatec Campus 17 rue des Martyrs, 38054 Grenoble France, https://team.inria.fr/nano-d/
- **If a PhD is forseen** : yes

**Internship presentation** :
Small-angle scattering is one of the fundamental techniques for structural studies of biological systems. Small-angle X-ray scattering (SAXS) is a type of small-angle scattering where X-rays scatter elastically from the sample and are then collected at very small angles. Compared to other structure determination methods, SAXS experiments are very simple conceptually and thanks to advances in instrumentation [1], the SAXS technique is becoming very popular in the recent years as a complement to other methods in structural biology [2]. Over the years, a number of computational tools have been developed for the analysis of SAXS curves, calculation of theoretical profiles and low-resolution reconstruction of model shapes. Many efforts have been spent to reduce the running time of these tools without degrading the quality of their approximations. The most prominent of them is the ATSAS package developed at EMBL Hamburg [3]. Very recently, however, we developed a new tool called Pepsi-SAXS that outperformed all the competitors in both speed and accuracy [4]. On average, Pepsi-SAXS is about ten to fifty times faster compared to all other methods and significantly more precise.

**Internship objectives**:
The overall research topic of the PhD proposal is to extend the state-of-the art computational methods for small-angle (both SAXS and SANS) scattering experiments. More precisely, it includes development and validation of novel user interaction methods with intuitive feedback for both the guided search and providing the constraints. All the tools will be integrated into the SAMSON (https://www.samson-connect.net) modular software platform developed in the NANO-D team of Inria, providing an intuitive user-friendly interface and integration with other modules.

**Additional information:**
This is envisaged as a joint project between ESRF/EMBL and the NANO-D research group at INRIA.

**Requirements** :
We are looking for candidates from a computer science / applied math background with strong knowledge of applied maths and physics and an interest in biophysics. Knowledge of C++, Python, parallel programming (e.g. GPU/multi-threading), QT, and possibly signal processing or rigid-body mechanics will be an asset.

## References:


[1] Spilotros, A. & Svergun, D. I. (2014). Encyclopedia of Analytical Chemistry, pp. 1–34.
[2] Graewert, M. A. & Svergun, D. I. (2013). Current opinion in structural biology, 23(5), 748– 754.
[3] Petoukhov, M. V., Franke, D., Shkumatov, A. V., Tria, G., Kikhney, A. G., Gajda, M., Gorba, C., Mertens, H. D., Konarev, P. V. & Svergun, D. I. (2012). Journal of applied crystallography, 45(2), 342–350.
[4] S. Grudinin, M. Garkavenko & A Kazennov, “Pepsi-SAXS : an adaptive method for rapid and accurate computation of small angle X-ray scattering profiles.” Submitted to Acta Crystallographica Section D.