Research Internship Opening

- **Title** : Modelling of molecular flexibility using the theory of continuous linear elasticity
- **MSc thesis advisor** : Sergei Grudinin, sergei.grudinin@inria.fr, Phone: +33 4 38 78 16 91
- **Laboratory** (+working place) : Nano-D, Inria Grenoble,

Minatec Campus 17 rue des Martyrs, 38054 Grenoble France, https://team.inria.fr/nano-d/

- **If PhD position is possible** : yes

Duration: 4-8 months

Internship presentation :

Macromolecules such as proteins are flexible, and this flexibility plays an important role in their function. In most of the cases, the flexibility of a protein can be described with only a few collective degrees of freedom. Theses can be computed with normal mode analysis (NMA), which is computationally inexpensive technique [1-2]. NMA solves exactly a linear approximation of Newton's equation of motion. The approximate differential equation is then solved by diagonalizing the Hessian matrix of the potential function. The eigenvectors of the Hessian matrix are called the normal modes. The normal modes corresponding to the lowest eigenvalues, or frequencies, can be used to represent collective motions of a molecule.

Internship objectives:

The goal of this internship is to apply the linear elasticity equations (Navier-Cauchy) [3-4] to a continuous medium given by the electron density functions,

$$\rho \frac{\partial^2 \vec{u}}{\partial t^2} = \mu \Delta \vec{u} + (\lambda + \mu) \nabla (\nabla . \vec{u}) \quad \forall x \in \Omega \quad \forall t \in \mathbb{R}^{+*}$$

Discretization of this equation leads to a sparse eigenproblem, similar to those solved in classical molecular NMA, which needs to be solved very efficiently.

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), and possibly QT will be an asset.

References:

[1] A. Hoffmann & S. Grudinin. NOLB : Non-linear rigid block normal mode analysis method. Journal of Chemical Theory and Computation, 2017, 13 (5), pp.2123-2134.

[2] https://team.inria.fr/nano-d/software/nolb-normal-modes/.

[3] http://www.maths.manchester.ac.uk/~mheil/Lectures/Elasticity/Material/Chapter5.pdf

[4] http://www.bo.ingv.it/~garcia/research/RadiationPropertiesGarcia/