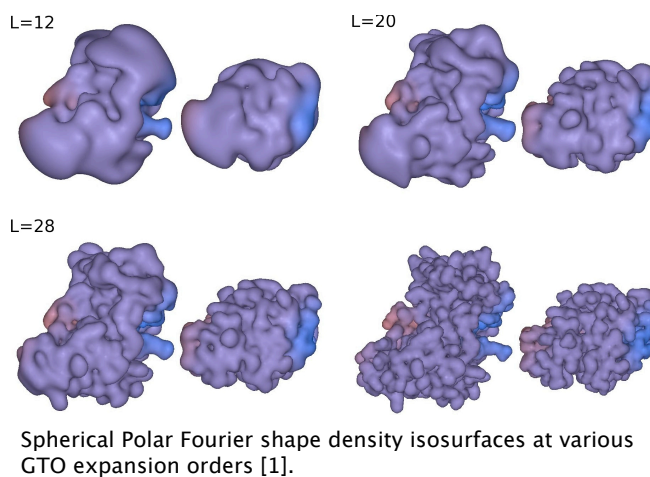# *Research* **Internship Opening**

- **Title** : Matching and reconstruction of 3D shapes using high-order special functions
- **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 :

Shape modelling is a very active research topic in computer graphics and there has been big progress in this field recently. Generally, shapes can be represented in multiple ways, for example, as a set of 2D projections taken from multiple angles, as a 3D mesh or a 3D volumetric map. In physics-based applications, however, shapes are very often represented using 3D polynomial bases, such as Cartesian or spherical Fourier expansions [1]. This allows to formulate the shape matching problem as a search in 6D space of rigid-body motions of one shape with respect to another. For example, this problem may be defined in terms of one intermolecular distance and five

Spherical Polar Fourier shape density isosurfaces at various GTO expansion orders [1].

Euler rotation angles, which allows to match shapes via rotational FFT correlations [1]. In the context of a 6D search space, this is much more efficient than using translational FFTs because only one forward Fourier transform is required.

Internship objectives:

The first goal of the internship is to develop a new representation of 3D objects using 3D orthogonal polynomials (for example those used in scattering [2-3] with spherical harmonics for the rotational part [4]). The second goal is to develop an efficient shape matching algorithm based on the chosen polynomial basis. This step will most probably involve the Fast Fourier transform and the correlation theorem [1]. The method will be validated on a number of simulated and experimental examples collected from the protein data bank.

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. multi-threading), and possibly signal processing and rigid-body mechanics will be an asset.

References:

[1] Ritchie, David W., and Graham JL Kemp. "Protein docking using spherical polar Fourier correlations." Proteins: Structure, Function, and Bioinformatics 39.2 (2000): 178-194.
[2] S. Grudinin et al. Pepsi-SAXS : an adaptive method for rapid and accurate computation of small-angle X-ray scattering profiles. Acta Cryst., 2017, D73, pp.449 – 464.
[3] J. Navaza : "On the three-dimensional reconstruction of icosahedral particles.", J. Struct. Biol. (2003). 144, 13-23
[4] https://en.wikipedia.org/wiki/Spherical_harmonics