Internship Opening
Symmetry detection in electron densities and molecular structures

About the NANO-D research group at INRIA

The NANO-D group, led by Stephane Redon at INRIA, develops novel multiscale, adaptive modeling and simulation methods, which automatically focus computational resources on the most relevant parts of the nanosystems under study. All algorithms developed by the group are gathered into SAMSON, an open-architecture software platform designed by NANO-D (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems).

During the twentieth century, the development of macroscopic engineering has been largely stimulated by progress in numerical design and prototyping: cars, planes, boats, and many other manufactured objects are nowadays designed and tested on computers. Digital prototypes have progressively replaced actual ones, and effective computer-aided engineering tools have helped cut costs and reduce production cycles of these macroscopic systems.

The twenty-first century is most likely to see a similar development at the atomic scale. Indeed, the recent years have seen tremendous progress in nanotechnology - in particular in the ability to control matter at the atomic scale. Similar to what has happened with macroscopic engineering, powerful and generic computational tools will be employed to engineer complex nanosystems, through modeling and simulation.

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Point group symmetry

The basic point group symmetries are the cyclic group $C_n$ with a single $n$-folded axes and the dihedral group $D_n$ with one $n$-folded axis and $n$ two-folded axes of symmetry. Figure on the right illustrates higher symmetry groups. The tetrahedral group has four 3-fold rotational symmetry axes and three 2-fold rotational axes. The octahedral group has three 4-fold rotational symmetry axes, four 3-fold rotational axes, and six 2-fold rotational axes. Finally, the icosahedral group has twelve 5-fold rotational symmetry axes, twenty distinct 3-fold rotational axes, and fifteen 2-fold rotational axes. The number of monomers in high-order group is twice the number of edges in the corresponding platonic solid. Thus, we have 12 monomers for the T (tetrahedron solid) group, 24 monomers for the O groups (cube and octahedron solids), and 60 monomers for I (dodecahedron and icosahedron solids).
**Goal of the internship**

Symmetry is a frequent structural trait in molecular systems. For example, most of the water-soluble and membrane proteins found in living cells are composed of symmetrical subunits, and nearly all structural proteins (such as microfilaments, intermediate filaments, and microtubules in eukaryotic cells) form long oligomeric chains of identical subunits. Almost all homodimeric proteins obey a certain point-group symmetry. Furthermore, electron densities of a medium-to-high resolution proteins obtained with cryo-electron microscopy are necessarily symmetric. Finally, protein structures obtained with X-ray crystallography often have contacts between molecules in the asymmetric unit with molecules in their symmetrical replicas.

The goal of the internship is to develop a new algorithm for point-group symmetry detection of an electron density map. It should be based on rotational invariants computed with Spherical Harmonics. The developed method will be useful for a variety of medical and biological applications. Particularly, we will apply it for symmetry detection in Cryo-electron microscopy, crystallographic protein structures, etc. Cryo-EM is getting very popular in structural biology, mainly due to the fact that it allows the observation of specimens that have not been stained or fixed in any way, showing them in their native environment, in contrast to X-ray crystallography. The method will be tested and validated on a number of Cryo-EM and PDB examples.

**References:**


**Desired profile**

We are looking for creative, passionate and hard-working individuals with exceptional talent for computer science and mathematics. The successful applicant will be in the process of obtaining a Master’s degree in computer science / applied math or an equivalent level. Excellent oral, written and interpersonal communication skills are essential (the working language will be English – knowledge of French is a plus).

**Requirements**

- **Strong** computer science background
- **Strong** knowledge of applied math (linear algebra, signal analysis, Fourier space)
- Knowledge of applied physics and structural biology is a plus
- **Strong** oral, written and interpersonal communication skills (working language: English – knowing French is a plus)
- Good knowledge of C++
- Ability to work independently and with a team

**Salary**

Depends on the type of the internship but is fixed by the Government’ rules.

**About Grenoble**

Grenoble is the capital city of the French Alps. Combining the urban life-style of southern France with a unique mountain setting, it is ideally situated for outdoor activities. The Grenoble area is today an important centre of industry and science (second largest in France). Dedicated to an ambitious policy in the arts, the city is host to numerous cultural institutions. With 60,000 students (including 6,000 foreign students), Grenoble is the third largest student area in France.

**To apply**

Send an email to Sergei Grudinin (sergei.grudinin@inria.fr) with:

- A resume
- A motivation letter

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- A scan of your Bachelor’s degree transcript and Master’s degree transcript (if you are still a Master student at the time of application, please provide the list of classes that you have taken and the grades you have obtained, as well as the list of classes that you will attend before the internship begins)