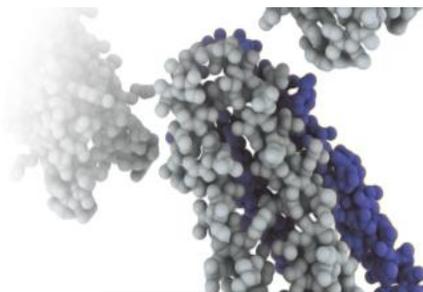


NANO-D

Algorithms for Modeling and Simulation of Nanosystems



Internship Proposal

Interactive deformations of large molecular systems

About the NANO-D research group at INRIA Grenoble – Rhône-Alpes

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.

Modeling and simulation of natural or artificial nanosystems is still a challenging problem, however, for at least three reasons: (a) the number of involved atoms may be extremely large (liposomes, proteins, viruses, DNA, cell membrane, etc.); (b) some chemical, physical or biological phenomena have large durations (e.g. the folding of some proteins); and (c) the underlying physico-chemistry of some phenomena can only be described by quantum chemistry (local chemical reactions, isomerizations, metallic atoms, etc.). The large cost of modeling and simulation constitutes a major impediment to the development of nanotechnology.

The NANO-D team aims at developing efficient computational methods for modeling and simulation of complex nanosystems, both natural (e.g. the ATPase engine and other complex molecular mechanisms found in biology) and artificial (e.g. NEMS - Nano Electro-Mechanical Systems).

In particular, the group develops novel multiscale, adaptive modeling and simulation methods, which automatically focus computational resources on the most relevant parts of the nanosystems under study.

Modeling macromolecules

Numerous molecular structures contain a large number of atoms, hence a large number of degrees of freedom. Because user interaction devices typically contain just a few degrees of freedom (e.g. a mouse, a haptic device, etc.), it is non-trivial to define an *effective mapping* between these devices and the molecules. In other words, it is difficult for a user to interactively perform large-scale deformations that involve numerous degrees of freedom using simple interaction devices.

Research internship details

The goal of the internship will be to develop a series of user interaction methods that will make it easy to edit and deform large molecules. During the first part of the internship, the successful applicant will study the state of the art of interaction methods able to handle large sets of particles that are subject to an interaction force-field (the deformed molecules should preserve their structures). In the second part, the intern will develop one or more interactive tools for large-scale deformation. In the third stage, the proposed algorithms will be validated by testing their ability to reproduce signal transduction scenarios and their ease of use when fitting flexible protein structures into cryo-EM maps. The proposed tools will be integrated into SAMSON, the platform being developed in the NANO-D group (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems).

Please contact Stephane Redon (stephane.redon@inria.fr) for more details.

Salary

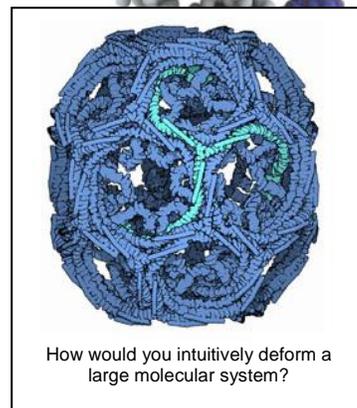
Around 1100 Euros net per month, for 5 months (part of an ANR contract).

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.

Contact information

Stephane Redon
INRIA Rhône-Alpes Research Center
655 avenue de l'Europe - Montbonnot
38334 Saint Ismier Cedex - France
+33 4 76 61 55 69
stephane.redon@inria.fr
<http://nano-d.inrialpes.fr/~redon>



How would you intuitively deform a large molecular system?