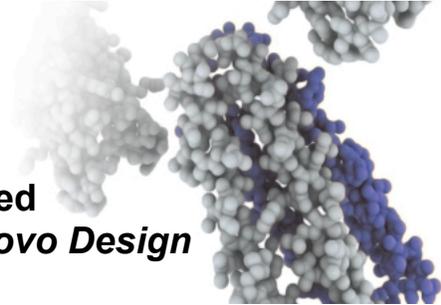


# NANO-D

Algorithms for Modeling and Simulation of Nanosystems

## Development of Formulation for a Coarse-Grained Potential Function for *Protein Folding* and *De Novo Design*



INRIA Grenoble - Rhône-Alpes  
NANO-D research group

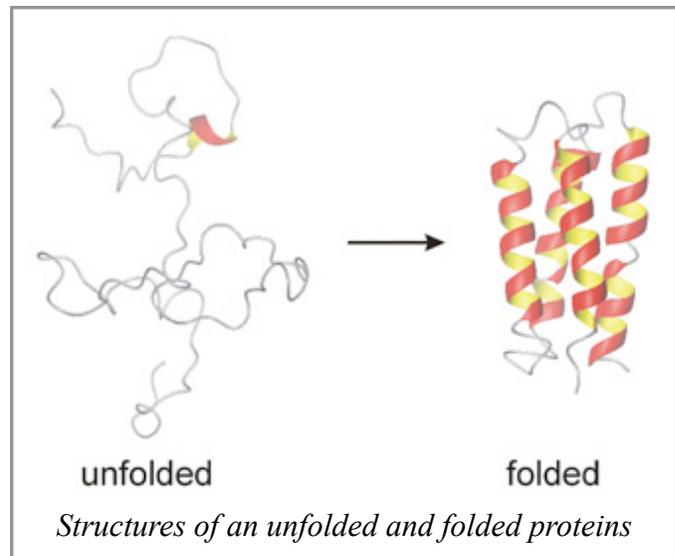
### About NANO-D

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 that are used to model and simulate molecular structures. Applications of these methods are molecular structure predictions via folding, docking and refinement algorithms.

### Protein Folding

Protein folding is the physical process by which a [polypeptide](#) folds into its characteristic and functional [three-dimensional structure](#) from [random coil](#). If structures of one or more [homologous](#) proteins are known, [homology modeling](#) or [protein threading](#) predictions can produce an ensemble of structural models starting from a particular [amino acid sequence](#). In order to assess and optimize different structures from such ensemble, specially designed potentials are used as [energy functions](#). The most successful potentials are derived from the knowledge-base of known protein structures in the [Protein Data Bank](#).

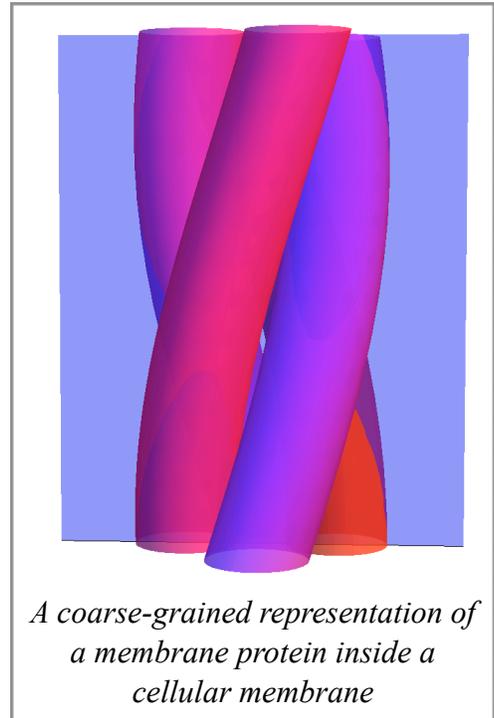


## Research Internship Details

We have recently developed a new *isotropic* (i.e., direction-independent) formulation for the potential function for interactions between proteins. We would like to extend this formulation to a class of *anisotropic* (i.e., direction-dependent) potential functions for the recognition of native protein folds.

The goals of the internship are:

- develop a pairwise-additive angular-dependent potential function that predicts native protein folds
- deduce coefficients for the potential from the knowledge-base (i.e., SCOP database)
- treat water-soluble and membrane proteins independently
- study the effect of several angular basis sets, as well as several radial basis sets on the quality of the potential
- validate the potential on a set of structures of high resolution extracted from the Protein Data Bank



*A coarse-grained representation of a membrane protein inside a cellular membrane*

## 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

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