# Application BASTRI
## Fiches Equipes

## NANO-D (SR0849TR)

Algorithms for Modeling and Simulating Nanosystems
NANO-D (SR0640RR)  NANO-D

**Statut:** Terminée

**Responsable :** Sergey Grudinin

**Mots-clés de "A - Thèmes de recherche en Sciences du numérique - 2024" :** *Aucun mot-clé.*

**Mots-clés de "B - Autres sciences et domaines d'application - 2024" :** *Aucun mot-clé.*

**Domaine :** Mathématiques appliquées, calcul et simulation
**Thème :** Schémas et simulations numériques

**Période :** 01/10/2018 -> 31/12/2020
**Dates d'évaluation :**

**Etablissement(s) de rattachement :** <sans>
**Laboratoire(s) partenaire(s) :** <sans UMR>

**CRI :** Centre Inria de l'Université Grenoble Alpes
**Localisation :** Centre de recherche Inria de l'Université Grenoble Alpes
**Code structure Inria :** 071073-2

**Numéro RNSR :** 201822861A
**N° de structure Inria:** SR0849TR

### Présentation

The goal of the team is to help experimental biologists, physicists, and bioinformaticians to predict the structure, conformational heterogeneity and function of various macromolecular machines. This will be made possible thanks to developing novel mathematical, algorithmic, and computational approaches and also by using advances in several research fields, such as various experimental techniques and data science.

### Axes de recherche

Our research axes are:

- **Developing novel physics-based computational methods** for integrative structural biology. These include modeling of scattering experiments (i.e. SAXS and SANS), modeling of cross-link experiments, modeling of FRET experiments, inclusion of Cryo-EM, NMR, and XFEL data, modeling of missing structural fragments (loops and termini), adapting physics-based force-fields, developing and integrating docking algorithms, and using the theory of linear elasticity to model large-scale macromolecular flexibility.
- **Developing novel data-driven algorithms**. These include methods for both the ***analysis*** of genomic and 3D structural databases and also for ***learning*** the models from these data. The ultimate goal of this axis is learning the organization of macromolecules and their complexes at physiological conditions. This includes learning physical models for the interactions within the system under study (the enthalpic contribution), and also the low-dimensional representation of the conformational variability of the system (the entropic contribution).
- **Combining knowledge-based and physics-based approaches together and developing practical user interfaces and applications**. We will primarily develop stand-alone tools and later integrate them into web-based applications.

### Relations industrielles et internationales

#### Contact

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#### En savoir plus

- Site de l'équipe
- Site sur inria.fr
- Site du responsable
- Derniers Rapports d'Activité : 2016 , 2017 , 2018 , 2019

#### Documents sur la structure

- Intranet
- Privés

#### Décisions

- 12979 (11/07/2018) : création
- 14586 (10/12/2020) : fermeture

#### Localisation

- **Adresse postale :** Centre de recherche Inria de l'Université Grenoble Alpes Inovallée 655 Avenue de l'Europe - CS 90051 38334 Montbonnot CEDEX France
- **Coordonnées GPS :** 45.218, 5.807