

# Sergei Grudin

CNRS RESEARCH SCIENTIST, CR1 CNRS

Nano-D team of Inria, Minatec Campus, 17 rue des Martyrs, 38054 Grenoble, France

☎ (+33) 04 38 78 16 91 | ✉ Sergei.Grudin@inria.fr | 🏠 nano-d.inrialpes.fr/~grudin | 📧 Sergei Grudin | 🌐 R<sup>G</sup> Sergei\_Grudin

## Education

### FZJ Jülich (Forschungszentrum Jülich)

Juelich, Germany

PH.D. IN COMPUTATIONAL STRUCTURAL BIOLOGY

2002 - 2005

- Thesis Title "Computer simulations of membrane proteins bacteriorhodopsin and sensory rhodopsin II".
- Supervised by Georg Büldt, Valentin Gordeliy, and Artur Baumgaertner.

### MIPT (Moscow Institute of Physics and Technology)

Moscow, Russia

M.S. IN APPLIED PHYSICS AND MATH FROM THE DEPARTMENT OF GENERAL AND APPLIED PHYSICS

2000 - 2002

### MIPT (Moscow Institute of Physics and Technology)

Moscow, Russia

B.S. IN APPLIED PHYSICS AND MATH FROM THE DEPARTMENT OF GENERAL AND APPLIED PHYSICS

1996 - 2000

## Professional Academic Experience

### CNRS / Inria / Nano-D team

Grenoble, France

RESEARCH SCIENTIST, CR CNRS

Oct. 2009 - Now

### Inria / Nano-D team

Grenoble, France

POSTDOC

Oct. 2007 - 2009

- Development of adaptive multi-scale methods for long-range interactions (adaptive FMM, etc).

### FZJ Jülich (Forschungszentrum Jülich)

Jülich, Germany

POSTDOC

Jan. 2006 - Sep. 2007

- Development of implicit solvation schemes for biomolecules.

## Honors & Awards

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| 2017 | <b>Cover publication</b> , "A novel fast Fourier transform accelerated off-grid exhaustive search method for cryo-electron microscopy fitting" | <i>J Appl Cryst</i> , 50, 1036         |
| 2017 | <b>Cover publication</b> , "NOLB: Nonlinear Rigid Block Normal Mode Analysis Method"   | <i>J Chem Theory Comput</i> , 13, 2123 |
| 2016 | <b>Cover publication</b> , "Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry"                         | <i>J Appl Cryst</i> , 49, 158          |
| 1996 | <b>1st Prize</b> , All-Russian Physics Olympiad  | Orel, Russia                           |
| 1995 | <b>2nd Result</b> , All-Russian Mathematics Olympiad, Siberia and Far-Eastern region   | Kemerovo, Russia                       |

## Publications

- 39 Journal peer-reviewed publications
- 7 Conference proceedings articles
- 1 International patent

See more at 📧 Sergei Grudin | 🏠 team.inria.fr/nano-d/team-members/sergei-grudin/ | 🌐 R<sup>G</sup> Sergei\_Grudin

## Referee for Scientific Journals and Conferences

- Nature Communications
- Bioinformatics
- Current Opinion in Structural Biology
- FEBS Journal
- Journal of Chemical Information and Modeling
- Journal of Computational Chemistry
- Journal of Computer-Aided Molecular Design
- PLoS Computational Biology
- PLoS ONE
- Scientific Reports
- Proteins: Struct., Funct., Bioinf.
- Journal of Physical Chemistry
- European Biophysics Journal
- BMC Bioinformatics
- BMC Research Notes
- Spectrochimica Acta
- Crystal Growth and Design
- Journal of Bioinformatics
- Chemical Research in Toxicology
- Biomedical Signal Processing and Control
- BCB'17
- ISBRA'11
- WAFR'10

## Research Projects

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- **Computational Tools for Scattering**, Novel tools for small-angle scattering – supported by Inria and MIPT internship programs 2015–
- **Ph.D. Maria Kadukova**, Development of novel computational tools for structure-based drug design – Ministry grant 2016–2020
- **NewOptogeneticsTools**, ANR-DFG project on computational and experimental design of new optogenetics tools 2016–2020
- **Ph.D. Guillaume Pâges**, Development of novel computational tools for protein design – ANR grant + local fundings 2016–2019
- **PPI-3D**, Associate team between Nano-D Inria and Stony Brook University, New York, USA with the goal to speed up docking approaches to tackle genome-scale problems 2014–2017
- **Machine-learning applications in structural biology**, Development of knowledge-based potentials and convex optimization-based exploration techniques – supported by Inria, MIPT and Skoltech internship programs 2010–2017
- **Ph.D. Alexandre Hoffmann**, Development of novel computational tools for flexible protein-protein interactions – Ministry grant 2014–2017
- **PEPSI**, Polynomial Expansions of Protein Structures and Interactions - development of novel algorithmic techniques for structural bioinformatics – ANR Modèles Numériques (MN) project, two postdoctoral positions 2011–2016
- **Ph.D. Petr Popov**, Development of new sampling techniques for protein-protein interactions – ANR fundings 2011–2015
- **Cryo-CA**, Exploratory project of Computational algorithms for biomolecular structure determination by cryo-electron microscopy – ANR in the program Projets Exploratoires Pluridisciplinaires (PEPS) Bio-Maths-Info (BMI) 2012–2013
- **Ph.D. Georgy Derevyanko**, Development of new FFT and machine-learning based algorithms for protein-protein interactions – External funding 2011–2014
- **Ph.D. Ivan Gushchin**, Computational and experimental studies of protein-protein interactions – External funding 2011–2014

## Software Packages

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### STAND-ALONE

- 2015–2017 **Knodle**, KNOWledge-Driven Ligand Extractor [team.inria.fr/nano-d/software/Knodle/](http://team.inria.fr/nano-d/software/Knodle/)
- 2014–2017 **NOLB**, Nonlinear Rigid Block Normal Mode Analysis [team.inria.fr/nano-d/software/nolb-normal-modes/](http://team.inria.fr/nano-d/software/nolb-normal-modes/)
- 2013–2015 **Sam**, Fast FFT-based protein docking program specifically designed to assemble protein complexes with arbitrary point group symmetry [sam.loria.fr](http://sam.loria.fr)
- 2014 **RigidRMSD**, Open-source library for constant-time computations of the RMSDs corresponding to rigid-body molecular motions [team.inria.fr/nano-d/software/rigidrmsd/](http://team.inria.fr/nano-d/software/rigidrmsd/)
- 2014–2017 **RapidRMSD**, Open-source library for constant-time computations of the RMSDs corresponding to flexible molecular motions [team.inria.fr/nano-d/software/rapidrmsd/](http://team.inria.fr/nano-d/software/rapidrmsd/)
- 2014–2016 **Pepsi-Dock**, Protein docking method with a very detailed FFT-accelerated data-driven potential [team.inria.fr/nano-d/software/pepsi-dock/](http://team.inria.fr/nano-d/software/pepsi-dock/)
- 2014– **Pepsi-SAXS**, Multipole-based SAXS profile computation method [team.inria.fr/nano-d/software/pepsi-saxs/](http://team.inria.fr/nano-d/software/pepsi-saxs/)
- 2012–2014 **DockTrina**, Protein docking method for modeling the 3D structures of nonsymmetrical triangular trimers [team.inria.fr/nano-d/software/DockTrina/](http://team.inria.fr/nano-d/software/DockTrina/)
- 2010–2014 **HermiteFit**, Docking algorithm for rapid fitting atomic structures into low-res maps using 3D orthogonal Hermite functions [team.inria.fr/nano-d/software/HermiteFit/](http://team.inria.fr/nano-d/software/HermiteFit/)
- 2014–2017 **OffGridFit**, Novel FFT-based exhaustive search method extended to off-grid translational and rotational degrees of freedom [team.inria.fr/nano-d/software/OffGridFit/](http://team.inria.fr/nano-d/software/OffGridFit/)
- 2010–2017 **Convex-PL**, Knowledge-based scoring function for protein-ligand interactions [team.inria.fr/nano-d/software/Convex-PL/](http://team.inria.fr/nano-d/software/Convex-PL/)
- 2010–2017 **SBROD**, Smooth Backbone-Reliant Orientation-Dependent scoring function for protein quality assessment [team.inria.fr/nano-d/software/SBROD/](http://team.inria.fr/nano-d/software/SBROD/)

### SAMSON AND SAMSON-RELATED MODULES

- 2009– **SAMSON**, Software platform for computational nanoscience [www.samson-connect.net](http://www.samson-connect.net)
- 2014– **Several SAMSON Elements**, Symmetry detection, SAXS, NMA, docking, and force-fields [Link to the Elements page](#)