Curriculum Vitae - Frank Noé

Personal Data

Name	Frank Noé
Date of birth	13 / 05 / 1975
Place of birth	66482 Zweibrücken
Citizenship	German
Office Address	FU Berlin, Arnimallee 6, 14195 Berlin, Germany
Office Phone	+49 - 30 - 838 75354
Private Address	Nymphenburger Straße 11, 10825 Berlin, Germany
Private Phone	+49 - 30 - 22 19 0800
E-Mail	noe@math.fu-berlin.de

Academic Degrees

2006	Ph.D. in Computer Science (summa cum laude), University of Heidelberg, Germany. Advisors: Jeremy C. Smith and Gerhard Reinelt.
2002	M.Sc. in Computing, Cork Institute of Technology, Ireland. (Advisor: Paul Rothwell).
1999	B.Sc. in Electrical Engineering (best grade of the year), University of Cooperative Education Stuttgart, Germany. (Advisor: Alexander Götz)

Professional Experience

since 2007	Junior Group Leader in DFG Center "Matheon - Mathematics for key technologies" at FU Berlin.
2006 - 2007	Postdoctoral fellow in the "Modeling and Simulation in the Biosciences" initiative, Heidelberg, Germany
2002 - 2005	Graduate student at the Interdisciplinary Center for Scientific Computing, Heidelberg, Germany
2000 - 2002	Lecturer in Computer Science at the Cork Institute of Technology, Ireland.
1999 - 2000	Scientist at the Institute for New Media, Frankfurt, Germany
1999	Scientist at the Robert Bosch GmbH, Hildesheim, Germany

Memberships and Awards

2008	Steering Comittee Member in FU Berlin Priority Program "Center of Scientific Simulation"
2008 - 2010	Member in SFB 449 "Structure and Function of Membrane Receptors".
2006	Offered permanent research group leader position at Oak Ridge National Laboratory, TN, USA (not realized)
2006	Postdoctoral stipend in the "Modeling and Simulation in the Biosciences" (BIOMS) initiative (3 years offered, 1 year realized)
2006	Prize for best Poster (out of 70) in Workshop "Computer Simulation and Theory of Macromolecules", Hünfeld, Germany.
since 2002	Member in the Graduate College 710 "Complex Processes"
2000 - 2002	CIT Cork: Research grant (14000 EUR)

Invited Lectures (last 3 years)

23 / 09 / 2009	Plenary Speaker at "Rare Events in High Dimensional Systems", Institute for Pure and Applied Mathematics, Los Angeles, CA, USA.
02 / 07 / 2008	"European Conference of Mathematical and Theoretical Biology", Edinburgh, UK
27 / 06 / 2008	Group of Ulrich G. Nienhaus, Ulm, Germany.
19 / 04 / 2008	Workshop "Computer Simulation and Theory of Macromolecules", Hünfeld, Germany
11 / 12 / 2007	IMPRS, MPI for Molecular Genetics, Berlin, Germany
07 / 09 / 2007	Conference "Operations Research 2007", Saarland University, Germany
17 / 07 / 2007	Group of Ken A. Dill, UC San Francisco, CA, USA
15 / 07 / 2007	Group of Vijay S. Pande, Stanford University, CA, USA
31 / 05 / 2007	Group of Helmut Grubmüller, MPI for Biophysical Chemistry, Göttingen, Germany
18 / 05 / 2007	DPG Biophysics Section Meeting, Hünfeld, Germany
06 / 10 / 2006	Oak Ridge National Lab, TN, USA
24 / 06 / 2006	Group of Ken A. Dill, UC San Francisco, CA, USA
22 / 06 / 2006	Oak Ridge National Lab, TN, USA
19 / 05 / 2006	Workshop "Computer Simulation and Theory of Macromolecules", Hünfeld, Germany
04 / 05 / 2006	Group of Massimilano Aschi, University of l'Aquila, Italy
14 / 09 / 2005	Group of Andrea Amadei, University Tor Vergata, Rome, Italy
19 / 07 / 2005	"European Conference of Mathematical and Theoretical Biology", Dresden, Germany
07 / 04 / 2005	"International Conference Sequence-Structure-Function Relationships", Warsaw, Poland

Reviewing

National Science Foundation (NSF)
Journal of Molecular Biology
Journal of Computational Chemistry
Proceedings of the German Conference on Bioinformatics

Workshops Organized (chairman of organization committee)

May 2009	Modeling Molecular Kinetics (currently organized)
20-22 / 09 / 2006	Methods of Molecular Simulation 2006 (80 participants)
25-27 / 07 / 2005	Methods of Molecular Simulation 2005 (80 participants)
16-18 / 10 / 2003	Methods of Molecular Simulation 2003 (50 participants)

Teaching

WS 2008	Lecture Computer Simulation of Biomolecules I, FU Berlin (2+2 SWS) Lecture Time Series Analysis (2+2 SWS)
SS 2008	Lecture Computer Simulation of Biomolecules II, FU Berlin (2 SWS)
WS 2007	Lecture Computer Simulation of Biomolecules I, FU Berlin (2+2 SWS)
SS 2004/05/06	Molecular Dynamics and Reaction path lectures in "Computer Modeling of Proteins", University of Heidelberg (2 SWS)
WS 2005	Lecture Discrete Optimization in Molecular Simulation, University of Heidelberg (1 SWS)
SS 2001, WS 2001	Computer Programming lectures and exercises, Cork Institute of Technology, Ireland (4+2 SWS)

Fundraising (total: 512000 EUR)

2008	Center of Scientific Simulation (40000 EUR)
2008 - 2010	DFG collaborative research center 449 (180000 EUR)
2007 - 2010	DFG research center "Matheon" (180000 EUR)
2007 - 2008	Elite program Landesstiftung Baden-Württemberg (62000 EUR)
2006 - 2009	DFG graduate college 450 (50000 EUR, as co-PI)

Supervision

Postdoctoral students	Dr. Stefan Bernhard (FU Berlin)
	Dr. Hao Wu (FU Berlin)
Ph.D. students	Jan Wigger (FU Berlin)
	Martin Held (FU Berlin)
	Martin Fischbach (FU Berlin)
	Thomas Splettstößer (University of Heidelberg)
	Jan-Hendrik Prinz (University of Heidelberg)
	Emal Alekozai (University of Heidelberg)
Diploma students	Martin Fischbach (Computer Science, FU Berlin)
	Torsten Luedge (Physics, TU Berlin)
	Arash Azhand (Physics, TU Berlin)
	Thomas Splettstößer (Biology, University of Heidelberg)
	Dominik Skanda (Physics, University of Heidelberg)
Interns	Ilkay Sakalli (FU Berlin).
	Evan Molinelli, Hans Fritz, Harmuth Henkel, Tilman Bünder (University of Heidelberg)
	Markus Stöhr (Institute for new Media, Frankfurt)

Collaborations:

1. Vijay S. Pande, Stanford University, USA: Folding@Home.
2. Ken A. Dill (Chemistry), UC San Francisco, USA: Protein folding kinetics.
3. Helmut Grubmüller, Max-Planck Institute Göttingen, Germany: Multiscale modeling of biological nanomachines.
4. Andrea Amadei, University Tor Vergata, Rome, Italy: Statistical mechanics.
5. Christof Schütte, Free University of Berlin, Germany: Metastability.
6. Thomas Weikl, Max-Planck Institute Potsdam, Germany: Pin WW protein folding
7. Jeremy C. Smith, University of Heidelberg, Germany: Protein dynamics (several projects)
8. Gerhard Reinelt, University of Heidelberg, Germany and Martin Skutella, TU Berlin, Germany: Graph theory
9. Ulrich Nienhaus, University of Ulm, Germany: Single molecule FRET experiments
10. Ulrike Alexiev, FU Berlin, Germany: Fluorescence experiments

1. P. Metzner, F. Noé and C. Schütte: "Estimation of Transition Matrix distributions by Monte Carlo sampling", *Phys. Rev. E*, submitted.

2. T. Splettstößer, F. Noé and J. C. Smith: "Nucleotide-dependence of G-actin conformation from multiple molecular dynamics simulations and observation of a putatively polymerisation-competent superclosed state", *J. Mol. Biol.*, submitted.

3. C. Schütte, F. Noé, E. Meerbach, P. Metzner and C. Hartmann: "Conformation Dynamics", *Proceedings of the ICIAM 2007*, in press.

4. F. Noé, I. Daidone, J.C. Smith, A. di Nola and A. Amadei: "Statistical Mechanics of the Conformational States of a Peptide by means of the quasi-Gaussian Entropy Theory" *J. Phys. Chem. B*, in press.

5. F. Noé: "Probability Distributions of Molecular Observables computed from Markov Models", *J. Chem. Phys.*, 128, 244103 (2008).

6. F. Noé and S. Fischer: "Transition Networks for Modeling the Kinetics of Conformational Change in Macromolecules", *Curr. Opin. Struct. Biol.*, 18, 154-162 (2008).

7. F. Noé, M. Oswald and G. Reinelt: "Optimization in Graphs with Limited Information on the Edge Weights", In: "Operations Research Proceedings 2007". J. Kalcsics and S. Nickel (Eds), 435-440, Springer (2007).

8. I. Horenko, C. Hartmann, C. Schütte and F. Noé: "Data-based parameter estimation of generalized Langevin processes". *Phys. Rev. E* 76, 016706 (2007).

9. F. Noé and J.C. Smith and C. Schütte: "A network-based approach to biomolecular dynamics". In: "From Computational Biophysics to Systems Biology". U. H. E. Hansmann and J. Meinke and S. Mohanty and O. Zimmermann (Eds), 247-250, John von Neumann Institute for Computing, Juelich (2007).

10. F. Noé, I. Horenko, C. Schütte and J.C. Smith: "Hierarchical Analysis of Conformational Dynamics in Biomolecules: Transition Networks of Metastable States". *J. Chem. Phys.*, 126, 155102 (2007).

11. F. Noé and J.C. Smith: "Transition Networks: A Unifying Theme for Molecular Simulation and Computer Science". *Mathematical Modeling of Biological Systems*, Volume I. A. Deutsch, L. Brusch, H. Byrne, G. de Vries and H.-P. Herzel (eds). Birkhäuser, Boston, 125-144 (2007).

12. P. Imhof, F. Noé, S. Fischer and J.C. Smith: "AM1/d Parameters for Magnesium in Metalloenzymes". *J. Chem. Theo. Comput.* 2, 1050-1056 (2006).

13. F. Noé, D. Krachtus, J.C. Smith and S. Fischer: "Transition Networks for the Comprehensive Characterization of Complex Conformational Change in Proteins.". *J. Chem. Theo. Comput.* 2, 840-857 (2006)

14. F. Noé, M. Oswald, G. Reinelt, J.C. Smith and S. Fischer: "Computing Best Transition Pathways in High-Dimensional Dynamical Systems" *Multisc. Model. Sim.* 5, 393-419 (2006).

15. F. Noé: “Transition Networks: Computational Methods for the Comprehensive Analysis of Complex Rearrangements in Proteins.” Ph.D. thesis, University of Heidelberg, 2006.

16. F. Noé, J.C. Smith and S. Fischer: “Automated Computation of Low-Energy Pathways for Complex Rearrangements in Proteins: Application to the conformational switch of Ras p21.” *Proteins*. 59, 534-544 (2005).

17. T. Becker, S. Fischer, F. Noé, A.L. Tournier, G.M. Ullmann, V. Kurkal and J.C. Smith: “Physical and functional aspects of protein dynamics.” In: “Soft Condensed Matter Physics in Molecular and Cell Biology”, Poon & Andelman (Eds), 225-241, Taylor & Francis (2006).

18. F. Noé, S.M. Schwarzl, S. Fischer and J.C. Smith: “Computational tools for analysing structural changes in proteins in solution.” *Applied Bioinformatics*, 2, 11-17 (2003).

19. T. Becker, S. Fischer, F. Noé, M. Ullmann, A. Tournier and J.C. Smith: “Protein Dynamics: Glass Transition and Mechanical Function.” *Advances in Solid State Physics 43*. Ed. B. Kramer. Springer-Verlag Heidelberg, 677-694 (2003).

20. F. Noé: “The Evolution of Cell Colonies in Volvocacean Algae: Investigation by theoretical analysis and computer simulation”. Master of Science thesis, Cork Institute of Technology, Ireland (2002).

21. F. Noé: “Components for a PC-based Driver-Information System”. Bachelor of Science thesis, University of Cooperative Education, Stuttgart, Germany (1999).