Frank Noé - Curriculum Vitae

Born May 13, 1975, Zweibrücken, Germany
Citizenship: German
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Professional appointments

2015 - Present	Adjunct Professor, Dept. of Chemistry, Rice University, Houston, TX.
2013 - Present	Professor, FU Berlin - Joint Position between the departments of Mathematics, Physics, and Chemistry
2007 - 2013	Independent Junior Group Leader, DFG Centre MATHEON, FU Berlin
2009	Visiting professor for scientific computing (W2), IWR/University of Heidelberg, Germany
2006 - 2007	Postdoc, "Modelling and Simulation in the Biosciences" initiative, Heidelberg, Germany
2002 - 2005	Graduate student, Interdisciplinary Centre for Scientific Computing, Heidelberg, Germany
2000 - 2002	Lecturer, Computer Science, Cork Institute of Technology, Ireland
1999 - 2000	Scientific software developer, Institute for New Media, Frankfurt, Germany
1996 - 1999	Engineer, Robert Bosch GmbH, Stuttgart and Hildesheim, Germany

Academic education

2006 (Jan 27)	Ph.D. (summa cum laude / with distinction) in Computer Science and Theoretical Biophysics, University of Heidelberg, Germany.
2002	M.Sc. in Computing, Cork Institute of Technology, Ireland.
1999	B.Sc. in Electrical Engineering (highest grade of the year), University of Cooperative Education Stuttgart, Germany.

Institutional Roles and Graduate Programs

2015 - 2019	Initiator, Designer and Dean of Studies, Master program Computational Sciences, FU Berlin
2013 -	Faculty Member, Mathematics and Computer Science, FU Berlin Associated Faculty Member, Physics and Chemistry, FU Berlin
2009 - 2012	Acquired and served as a Founding Director of the CECAM node at FU Berlin
2012 -	Faculty Member, Berlin Mathematical School (BMS)
2008 -	Faculty Member, International Max Planck Research School CBSC, Berlin
2006 - 2010	Mentor, DFG Graduate College 710 "Complex Processes", University of Heidelberg

Research interests

- *Machine Learning in the Sciences*: Development of deep learning architectures and algorithms to address fundamental problems in statistical mechanics, quantum mechanics and theoretical chemistry.
- *Method development and simulation in chemical physics and theoretical chemistry*: Protein molecular dynamics (especially long-timescale simulation), particle-based reaction dynamics for cellular signaling, multiscale modeling between atomistic and cellular scale, integration of simulation and experimental data.
- *Scientific software development for the open-source dissemination of our methods*: Dissemination of research in community-usable software, modular software design, Open source software in Python, C, C++, Java.

Offers and Awards

- 2019 - 2020 **ISI Highly Cited** Researcher (Web of Science)
- 2019 **Simons Fellow** at the Institute of Pure and Applied Mathematics (IPAM)
- 2019 **Early-Career Award** in Theoretical Chemistry of the **Americal Chemical Society (ACS)**
- 2018 - 2022 **ERC consolidator grant** (awarded 2017)
- 2013 Won FU-Berlin internal competition for funding and installation of a new junior faculty group in the field of High-Performance Computing (now hired: Prof. Felix Höfling)
- 2013 - 2017 **ERC starting grant** (awarded 2012)
- 2010 Member of the "Genshagener Kreis", a program for selected junior scientists of the Einstein Foundation Berlin
- 2009 Director of the CECAM node Berlin
- 2007 Fellow, "elite program for postdocs", Federal Foundation of Baden-Württemberg
- 2006 Offered permanent PI position at Oak Ridge National Lab., TN, USA (not realized)
- 2006 Postdoctoral stipend, "Modelling and Simulation in the Biosciences" (BIOMS) initiative (3 years offered, 1 year realized)
- 2000 - 2002 CIT Cork MSc research stipend

Scientific memberships and editorial activities

- Fellow, European Laboratory for Learning and Intelligent Systems (ELLIS)
- Editor, Machine Learning: Science and Technology (IOPscience)
- Editorial Advisory Board, Journal of Chemical Theory and Computation (ACS)
- Member: American Physical Society, American Chemical Society, Biophysical Society.

Workshops organized (including fundraising)

- 2019 "Learning Physics and the Physics of Learning", Long Program, IPAM, UCLA, CA
- 2017 "Surrogate Models and Coarsening Techniques", IPAM, UCLA, CA (co-organizer)
- 2016 "Workshop on Kinetics and Markov State Models in Drug Design", Boston, MA (co-organizer)
- 2009,11,13,15 "Molecular Kinetics", FU Berlin, 100 participants (raised ca. 40K EUR each)
- 2003,05,06 "Methods of Molecular Simulation", Heidelberg, 30-80 participants, (raised 5K EUR each)

Funding from competitively evaluated grants (total: 9,033,000 EUR direct costs)

Duration	Active Grant	EUR (total, direct costs)
2019 - 2021	MATH$^+$ Excellence Cluster	555 000
2020 - 2022	DFG grant NO 825/3-2	250 000
2018 - 2021	DFG GRK DAEDALUS	180 000
2018 - 2022	ERC consolidator grant	1 600 000
2017 - 2019	DFG research group 2518	380 000
2016 - 2020	DFG transregio 186	352 000
2015 - 2018	DFG collaborative research center 1114	450 000
2015 - 2017	DFG grant NO 825/2-2	180 000
2011 - 2019	DFG collaborative research center 958	660 000
Duration	Previous Grant	EUR (total, direct costs)
2013 - 2017	Einstein foundation postdoc fellowship	367 000
2013 - 2017	ERC starting grant	1 395 000
2011 - 2014	DFG grant NO 825/3-1	285 000
2010 - 2018	DFG collaborative research center 740	950 000
2009 - 2011	DFG grant NO 825/2-1	200 000
2009 - 2010	CECAM node FU Berlin	80 000
2008 - 2011	DFG collaborative research center 449	180 000
2008 - 2010	Center of Scientific Simulation	67 000
2007 - 2014	DFG research center "Matheon"	840 000
2007 - 2008	Elite program Landesstiftung Baden-Württemberg	62 000

Postdoctoral fellows (current and *alumni*)

1. A. Kraemer: Generative machine learning molecular dynamics sampling
2. E. Abualrous: Experiment and simulation, immune system
3. S. Kaptan: Modeling of ion channels
4. L. Raich: Computational drug design in collaboration with Bayer AG
5. M. Sadeghi: Membrane mechanics, software development
6. S. Stolzenberg: High-performance molecular dynamics, Markov modeling (*won a temporary Principal Investigator position of the German Science Foundation*)
7. B. Husic: Machine learning for coarse-grained molecular dynamics
8. M. Entwistle: Machine learning for quantum Chemistry
9. *J. Hermann (now **Group Leader** at the Berlin Institute for Learning and Data)*
10. *S. Olsson (now **Assistant Professor** at Chalmers University Gothenborg SE. Won a Humboldt Postdoctoral fellowship*)
11. *J. Zhang* (*now Postdoc in Peking University. Won a Humboldt Postdoctoral fellowship*)
12. *H. Wu (now **Assistant Professor** at Tongji University, Shanghai. Won fellowship in the 1000 talents program of the Chinese government)*
13. *S. Bernhard (now **Professor** at Hochschule Pforzheim)*
14. *B. G. Keller (now **tenured Associate Professor** at FU Berlin)*
15. *A. S. J. S. Mey (now **Christina Miller Fellow** at University of Edinburgh)*
16. *G. Pérez-Hernández: (now Postdoc at Charité Berlin)*
17. *N. Plattner: (now at University of Bern)*
18. *J.-H. Prinz (now Data Scientist at keylight GmbH)*
19. *M. del Razo Sarmina (now independent Postdoc at University of Amsterdam)*
20. *R. Shevchuk (now Postdoc at University of Göttingen)*
21. *A. Ullrich (now Freelancer)*
22. *C. Wehmeyer (now Data Scientist at Statice)*

Ph.D. students and *supervised theses*

1. S. Bandstra (1st year): Machine Learning for super-resolution microscopy
2. Y. Chen (1st year): Machine Learning for implicit solvation
3. M. Dibak (4th year): Graphical models, multiscale simulation
4. K. Elez (2nd year): Machine Learning, cryo-EM reconstruction
5. T. Hempel (4th year): Molecular kinetics, Markov modeling
6. M. Hoffmann (4th year): Sparse learning, software development
7. J. Köhler (2nd year): Deep learning theory
8. L. Klein (2nd year): Deep generative models
9. T. Le (2nd year): Machine learning for drug design
10. A. Mardt (4rd year): Deep learning for dynamical systems
11. Z. Schätzle (1st year): Deep learning for quantum mechanics
12. R. Winter (3rd year): Deep learning for drug development. Collaboration with Bayer AG.
13. *C. Fröhner (now software developer at IVU traffic technologies): Reaction-diffusion systems in and out of equilibrium, PhD thesis, 2019.*
14. *L. Sbailò (now postdoc at Fritz-Haber Institute): Efficient multi-scale sampling methods in statistical physics, PhD thesis, 2019.*
15. *F. Paul (now postdoc at University of Chicago): Markov State Modeling of Binding and Conformational Changes of Proteins, PhD thesis, 2017 (Awarded with summa cum laude, Carl Ramsauer Preis der physikalischen Gesellschaft zu Berlin 2018).*
16. *F. Nüske (now postdoc at Paderborn University): The Variational Approach to Conformational Dynamics, PhD thesis, FU Berlin, 2017 (Awarded with: summa cum laude, Tiburtius dissertation Prize, RAUF postdoctoral fellowship at Rice University, Houston, TX).*
17. *B. Trendelkamp-Schroer: Reversible Markov state models, PhD thesis, FU Berlin, 2016.*
18. *F. Vitalini (now at Mirai Solutions Zürich): Hierarchical Approaches to kinetic models of peptides, PhD thesis, FU Berlin, 2015.*
19. *J. Schöneberg (now **Assistant Professor** at UC San Diego, CA): Reaction-diffusion dynamics in biological systems. PhD thesis, FU Berlin, 2014 (Awarded with: summa cum laude, Tiburtius dissertation Prize, Marie Curie Fellowship).*
20. *J. H. Prinz (now at keylight GmbH): Advanced estimation methods for Markov models of dynamical systems. PhD thesis, FU Berlin, 2012 (Awarded with summa cum laude).*
21. *M. Held (now at HitFox Berlin): Novel concepts for conformation and association dynamics in biomolecules. PhD thesis, FU Berlin, 2012 (Awarded with summa cum laude).*

Supervised M.Sc., Diploma and B.Sc. theses

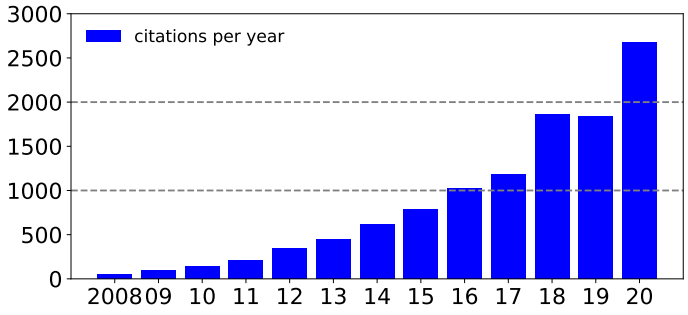
1. Y. Chen: *Extensible and transferable deep learning architectures for implicit solvent models*, MSc Thesis in Comput. Sciences, FU Berlin, 2020
2. B. Miller: *SE(3) Equivariant Neural Networks for Regression on Molecular Properties*, MSc Thesis in Comput. Sciences, FU Berlin, 2020
3. V. Wolf: *EwaldBlocks: Translating the Idea of Ewald Summation to Neural Networks for Global and Local Feature Extraction*, BSc Thesis in Computer Science, FU Berlin (2020)
4. L. Klein: *Exploring new Monte-Carlo Algorithms with Deep Learning Methods*, MSc Thesis in Physics, FU Berlin, 2019.
5. Z. Schätzle: *Solving the Schrödinger Equation with Deep Learning*, MSc Thesis in Physics, FU Berlin, 2019.
6. M. Salomon: *Predicting binding affinities of protein-ligand complexes using SchNet*, MSc Thesis in Comp. Sciences, FU Berlin, 2019.
7. F. Litzinger: *Sparse approximation of generalized eigenvalue problems*, MSc Thesis in Mathematics, FU Berlin, 2017.
8. L. Deecke: *Supervised learning of quantum chemical properties*, MSc Thesis in Physics, FU Berlin, 2017. (Awarded with Study Prize of the Berlin Physical Society 2018)

9. C. Fröhner: *Reversible integrators for particle based reaction-diffusion*, MSc Thesis in Physics, FU Berlin, 2015.
10. K. Colditz: *Adaptive Discretization for Markov Model Construction using HMM*, MSc Thesis in Mathematics, FU Berlin, 2015.
11. J. Biedermann: *Accelerating interacting-particle reaction-diffusion simulations using graphical processing units*, MSc Thesis in Bioinformatics, FU Berlin, 2015.
12. C. Schaller: *STORM microscopy - a mathematical analysis*, MSc Thesis in Mathematics, FU Berlin, 2013.
13. F. Nüske: *A variational approach for conformation dynamics*, MSc Thesis in Mathematics, FU Berlin, 2012.
14. J. Seibert: *Investigation of the reaction-diffusion processes of rod cell disc membrane photoactivation with single-particle resolution*, MSc Thesis in Bioinformatics, FU Berlin, 2010.
15. M. Kavalar: *Conformational Dynamics of a Peptide Ligand in Solvent and in Complex with a MHC-I Protein*, Diploma thesis in Physics, FU Berlin, 2010.
16. A. Azhand: *Diffusion Processes with Hidden States from Single Molecule Experiments*, Diploma thesis in Physics, TU Berlin, 2009.
17. T. Lüdge: *A theoretical model of conformational transitions in biomolecules based on single-molecule Förster resonance electron transfer measurements*, Diploma thesis in Physics, TU Berlin, 2009.
18. M. Fischbach: *Methods for modeling metastable conformational dynamics from trajectory data*, Diploma thesis in Computer Science, FU Berlin, 2008.
19. I. Sakalli: *Parallelization Strategies for a Brownian Dynamics Algorithm*", BSc thesis in Bioinformatics, FU Berlin, 2008.
20. M. Held: *Conformational Studies of UDP-N-Acetyl-Glucosamine in Environments of Increasing Complexity*", MSc thesis in Bioinformatics, FU Berlin, 2007.
21. D. Skanda: *Estimation of equilibrium probabilities of molecular conformations from non-overlapping simulations*", Diploma thesis in Physics, Univ. Heidelberg, 2006.

Citation statistics (based on Google scholar)

Number of citations: 11914
(Mar 3, 2021)

h-index: 54



Books

1. G. Bowman, F. Noé and V. Pande (Editors): "An Introduction to Markov State Models and Their Application to Long Timescale Molecular Simulation.", Advances in Experimental Medicine and Biology, 797. Springer, Heidelberg (2014)

Journal articles

1. J. Hermann, Z. Schätzle and F. Noé. Deep-neural-network solution of the electronic Schrödinger equation. **Nature Chem.** 12, 891-897 (2020)

2. T. Hempel, L. Raich, S. Olsson, N. P. Azouz, A. M. Klingler, M. E. Rothenberg and F. Noé: Molecular mechanism of SARS-CoV-2 cell entry inhibition via TMPRSS2 by Camostat and Nafamostat mesylate. **Chem. Sci.** (in press) DOI: 10.1039/D0SC05064D.

3. T. Le, R. Winter, F. Noé and D.-A. Clevert. Neuraldecipher-Reverse-engineering extended-connectivity fingerprints (ECFPs) to their molecular structures. **Chem. Sci.** 11, 10378-10389 (2020)

4. M. Sadeghi and F. Noé. Large-scale simulation of biomembranes: bringing realistic kinetics to coarse-grained models **Nat. Commun.** 11, 1-13 (2020)

5. B. E. Husic, N. E. Charron, D. Lemm, J. Wang, A. Pérez, A. Krämer, Y. Chen, S. Olsson, G. de Fabritiis, F. Noé and C. Clementi. Coarse Graining Molecular Dynamics with Graph Neural Networks. **J. Chem. Phys.** 153, 194101 (2020)

6. J. Wang, S. Chmiela, K.-R. Müller, F. Noé and C. Clementi. Ensemble learning of coarse-grained molecular dynamics force fields with a kernel approach. **J. Chem. Phys.** 152, 194106 (2020).

7. R. Winter, J. Retel, F. Noé, D. A. Clevert, A. Steffen. grünifai: Interactive multi-parameter optimization of molecules in a continuous vector space **Bioinformatics** 36, 4093-4094 (2020)

8. F. Noé, A. Tkatchenko, K.-R. Müller, C. Clementi. Machine learning for molecular simulation. **Ann. Rev. Phys. Chem.** 71, 361-390 (2020)

9. T. Hempel, N. Plattner and F. Noé. Coupling of conformational switches in calcium sensor unraveled with local Markov models and transfer entropy. **J. Chem. Theory Comput.** 16, 2584-2593 (2020)

10. N. K. Singh, E. T. Abualrous, C. M. Ayres, F. Noé, R. Gowthaman, B. G. Pierce, B. M. Baker. Geometrical characterization of T cell receptor binding modes reveals class-specific binding to maximize access to antigen. **Proteins** 88, 503-513 (2020)

11. F. Noé, G. De Fabritiis, C. Clementi. Machine learning for protein folding and dynamics. **Curr. Opin. Struct. Biol.** 60, 77-84 (2020)

12. S. Klus, B. E. Husic, M. Mollenhauer and F. Noé. Kernel methods for detecting coherent structures in dynamical data. **Chaos** 29, 123112 (2019).

13. F. Noé and E. Rosta. Markov Models of Molecular Kinetics. **J. Chem. Phys.** 151, 190401 (2019).

14. J. K. Noel, F. Noé, O. Daumke and A. S. Mikhailov: Polymer-like model to study the dynamics of dynamin filaments on deformable membrane tubes. **Biophys. J.** 117, 1870-1891 (2019).

15. M. Lehmann, I. Lukonin, F. Noé, J. Schmoranzer, C. Clementi, D. Loerke and V. Haucke: Nanoscale coupling of endocytic pit growth and stability. **Sci. Adv.** 5, eaax5775 (2019)

16. M. Dibak, C. Fröhner, F. Noé, F. Höfling. Diffusion-influenced reaction rates in the presence of pair interactions. **J. Chem. Phys.** 151, 164105 (2019).

17. N. K. Singh, E. T. Abualrous, C. M. Ayres, F. Noé, R. Gowthaman, B. G. Pierce and B. M. Baker. Geometrical characterization of T cell receptor binding modes reveals class-specific binding to maximize access to antigen. **Proteins** doi:10.1002/prot.25829 (2019).

18. J. Zhang, Y. I. Yang, F. Noé. Targeted adversarial learning optimized sampling. **J. Phys. Chem. Lett.** 10, 5791-5797 (2019).

19. F. Noé, S. Olsson, J. Köhler, H. Wu. Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. **Science** 365, eaaw1147 (2019).

20. B. E. Husic, F. Noé. Deflation reveals dynamical structure in nondominant reaction coordinates. **J. Chem. Phys.** 151, 054103 (2019).

21. H. Wu and F. Noé. Variational approach for learning Markov processes from time series data. **J. Nonlinear Sci.**, 30, 23-66 (2019).

22. S. Olsson, F. Noé. Dynamic graphical models of molecular kinetics. **Proc. Natl. Acad. Sci. USA**, 116, 15001-15006 (2019).

23. K. Faelber, L. Dietrich, J. K. Noel, F. Wollweber, A. K. Pfitzner, A. Mühleip, R. Sánchez, M. Kudryashev, N. Chiaruttini, H. Lilie, J. Schlegel, E. Rosenbaum, M. Hessenberger, C. Matthaeus, S. Kunz, A. von der Malsburg, F. Noé, A. Roux, M. van der Laan, W. Kühlbrandt and O. Daumke: Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. **Nature** 571, 429-433, (2019).

24. M. K. Scherer, B. E. Husic, M. Hoffmann, F. Paul, H. Wu, F. Noé: Variational selection of features for molecular kinetics. **J. Chem. Phys.** 150, 194108 (2019).

25. R. Winter, F. Montanari, A. Steffen, H. Briem, F. Noé, D. A. Clevert. Efficient multi-objective molecular optimization in a continuous latent space. **Chem. Sci.** 10, 8016-8024 (2019)

26. F. Paul, H. Wu, M. Vossel, B. L. de Groot and F. Noé. Identification of kinetic order parameters for non-equilibrium dynamics. **J. Chem. Phys.** 150, 164120 (2019).

27. J. Wang, S. Olsson, C. Wehmeyer, A. Pérez, N. E. Charron, G. De Fabritiis, F. Noé and C. Clementi: Machine learning of coarse-grained molecular dynamics force fields. **ACS Central Sci.** 5, 755-767 (2019).

28. C. Ayres, E. Abualrous, A. Bailey, C. A. Arega, L. H. Hellman, S. Corcelli, F. Noé, T. Elliott and B. M. Baker: Dynamically driven allostery in MHC proteins: peptide-dependent tuning of class I MHC global flexibility. **Frontiers Immunol.** 10, 966 (2019).

29. E. Dimou, K. Cosentino, E. Platonova, U. Ros, M. Sadeghi, P. Kashyap, T. Katsinelos, S. Wegehingel, F. Noé, A. J. García-Sáez, H. Ewers and W. Nickel. Single event visualization of unconventional secretion of FGF2. **J. Cell. Biol.** 218, 683-699 (2019).

30. M. Hoffmann, C. Fröhner and F. Noé. ReaDDy 2: Fast and flexible software framework for interacting-particle reaction dynamics. **PLoS Comput. Biol.** 15, e1006830 (2019).

31. M. Hoffmann, C. Fröhner and F. Noé: Reactive SINDy: Discovering governing reactions from concentration data. **J. Chem. Phys.** 150, 025101 (2019).

32. J. Kappler, F. Noé and R. R. Netz. Cyclization and Relaxation Dynamics of Finite-Length Collapsed Self-Avoiding Polymers. **Phys. Rev. Lett.** 122, 067801 (2019).

33. G. Pinamonti, F. Paul, F. Noé, A. Rodriguez and G. Bussi: The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. **J. Chem. Phys.** 150, 154123 (2019).

34. R. Winter, F. Montanari, F. Noé, D. A. Clevert. Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. **Chem. Sci.** 10, 1692-1701 (2019).

35. M. J. del Razo, H. Qian and F. Noé: Grand canonical diffusion-influenced reactions: a stochastic theory with applications to multiscale reaction-diffusion simulations. **J. Chem. Phys.** 149, 044102 (2018).

36. M. Dibak, M. J. del Razo, D. De Sancho, C. Schütte and F. Noé: MSM/RD: Coupling Markov state models of molecular kinetics with reaction-diffusion simulations. **J. Chem. Phys.** 148, 214107 (2018).

37. C. Fröhner, F. Noé: Reversible Interacting-Particle Reaction Dynamics. **J. Phys. Chem. B** 122, 11240-11250 (2018)

38. S. Gerber, S. Olsson, F. Noé and I. Horenko: A scalable approach to the computation of invariant measures for high-dimensional Markovian systems. **Sci. Rep.** 8, 1796 (2018).

39. S. Klus, F. Nüske, P. Koltai, H. Wu, I. Kevrekidis, C. Schütte and F. Noé: Data-driven model reduction and transfer operator approximation. **J. Nonlin. Dyn.** 28, 985-1010 (2018)

40. P. Koltai, H. Wu, F. Noé and C. Schütte: Optimal data-driven estimation of generalized Markov state models for non-equilibrium dynamics. **Computation** 6, 22 (2018)

41. F. Litzinger, L. Boninsegna, H. Wu, F. Nüske, R. Patel, R. Baraniuk, F. Noé and C. Clementi: Rapid calculation of molecular kinetics using compressed sensing. **J. Chem. Theory Comput.** 14, 2771-2783 (2018).

42. A. Mardt, L. Pasquali, H. Wu and F. Noé: VAMPnets: Deep learning of molecular kinetics. **Nat. Commun.** 9, 5 (2018)

43. F. Paul, F. Noé and T. R. Weikl: Identifying Conformational-Selection and Induced-Fit Aspects in the Binding-Induced Folding of PMI from Markov State Modeling of Atomistic Simulations. **J. Phys. Chem. B.** 122, 5649-5656 (2018).

44. B. M. Qureshi, E. Behrmann, J. Schöneberg, J. Loerke, J. Bürger, T Mielke, J. Giesebrecht, F. Noé, T. D Lamb, K. P. Hofmann, C. M. T. Spahn, M. Heck: It takes two transducins to activate the cGMP-phosphodiesterase 6 in retinal rods **Open Biol.** 8, 180075 (2018)

45. M. Sadeghi, T. R. Weikl and F. Noé: Particle-based membrane model for mesoscopic simulation of cellular dynamics. **J. Chem. Phys.** 148, 044901 (2018).

46. R. Schulz, Y. von Hansen, J. O. Daldrop, J. Kappler, F. Noé and R. R. Netz. Collective hydrogen-bond rearrangement dynamics in liquid water. **J. Chem. Phys.** 149, 244504 (2018).

47. D. W. H. Swenson, J.-H. Prinz, F. Noé, J. D. Chodera and P. G. Bolhuis: OpenPathSampling: A Python framework for path sampling simulations. I. Basics **J. Chem. Theory Comput.** 15, 813-836 (2018).

48. D. W. H. Swenson, J.-H. Prinz, F. Noé, J. D. Chodera and P. G. Bolhuis. OpenPathSampling: A Python Framework for Path Sampling Simulations. II. Building and Customizing Path Ensembles and Sample Schemes **J. Chem. Theory Comput.** 15, 837-856 (2018).

49. C. Wehmeyer and F. Noé: Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. **J. Chem. Phys.** 148, 241703 (2018)

50. C. Wehmeyer, M. K. Scherer, T. Hempel, B. E. Husic, S. Olsson and F. Noé: Introduction to Markov state modeling with the PyEMMA software v1.0 **LiveCoMS** 1, 1-12, (2018)

51. F. Paul, C. Wehmeyer, E. T. Abualrous, H. Wu, M. D. Crabtree, J. Schöneberg, J. Clarke, C. Freund, T. R. Weikl and F. Noé: Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. **Nat. Commun.** 8, 1095 (2017).

52. N. Plattner, S. Doerr, G. De Fabritiis and F. Noé: Complete protein-protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modeling. **Nat. Chem.** 9, 1005-1011 (2017).

53. J. Schöneberg, M. Lehmann, A. Ullrich, Y. Posor, W.-T. Lo, G. Lichtner, J. Schmoranzer, V. Haucke and F. Noé: Lipid-mediated PX-BAR domain recruitment couples local membrane constriction to endocytic vesicle fission. **Nat. Commun.** 8, 15873 (2017).

54. S. Olsson, H. Wu, F. Paul, C. Clementi and F. Noé: Combining experimental and simulation data of molecular processes via augmented Markov models. **Proc. Natl. Acad. Sci. USA**, 114, 8265-8270 (2017).

55. F. Noé and C. Clementi: Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods. **Curr. Opin. Struct. Biol.** 43, 141-147 (2017).

56. A. M. Abramyan, S. Stolzenberg, Z. Li, C. J. Loland, F. Noé and L. Shi: The isomeric preference of an atypical dopamine transporter inhibitor contributes to its selection of the transporter conformation. **ACS Chem. Neurosc.** 8, 1735-1746 (2017).

57. L. Sbailò and F. Noé: An efficient multi-scale Green's function reaction dynamics scheme. **J. Chem. Phys.** 147, 184106 (2017)

58. H. Wu, F. Nüske, F. Paul, S. Klus, P. Koltai and F. Noé: Variational Koopman models: Slow collective variables and molecular kinetics from short off-equilibrium simulations. **J. Chem. Phys.** 146, 154104 (2017).

59. M. Wieczorek, E. T. Abualrous, J. Sticht., M. Álvaro-Benito, S. Stolzenberg, F. Noé and C. Freund: Major Histocompatibility Complex (MHC) Class I and MHC Class II Proteins: Conformational Plasticity in Antigen Presentation. **Front. Immunol.** 8, 292 (2017).

60. F. Nüske, H. Wu, C. Wehmeyer, C. Clementi and F. Noé Markov State Models from short non-Equilibrium Simulations - Analysis and Correction of Estimation Bias. **J. Chem. Phys.** 094104 (2017).

61. S. Olsson and F. Noé: Mechanistic models of chemical exchange induced relaxation in protein NMR. **J. Am. Chem. Soc.** 139, 200–210 (2017).

62. G. Pinamonti, J. Zhao, D. Condon, F. Paul, F. Noé, D. Turner and G. Bussi, Predicting the kinetics of RNA oligonucleotides using Markov state models. **J. Comp. Theory Comput.** DOI: 10.1021/acs.jctc.6b00982 (2017).

63. D. Albrecht, C. M. Winterflood, T. Tschager, F. Noé and H. Ewers, Nanoscopic compartmentalization of membrane protein motion at the axon initial segment. **J. Cell Biol.** 215, 37-46 (2016).

64. S. Doerr, M. J. Harvey, F. Noé and G. De Fabritiis, HTMD: High-Throughput Molecular Dynamics for Molecular Discovery. **J. Chem. Theory Comput.** 12, 1845-1852 (2016).

65. F. Nüske, R. Schneider, F. Vitalini and F. Noé Variational Tensor Approach for Approximating the Rare-Event Kinetics of Macromolecular Systems. **J. Chem. Phys.** 144, 054105 (2016).

66. F. Noé and R. Banisch and C. Clementi, Commute maps: separating slowly-mixing molecular configurations for kinetic modeling. **J. Chem. Theory Comput.** 12, 5620-5630 (2016).

67. G. Pérez-Hernández, F. Noé: Hierarchical time-lagged independent component analysis: computing slow modes and reaction coordinates for large molecular systems. **J. Chem. Theory Comput.** 12, 6118-6129 (2016)

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Reviewing service

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Journals: Nat. Methods, Nat. Chem., Nat. Commun., Nat. Mater., Nat. Rev. Chem., Sci. Adv., PNAS, JACS, Phys. Rev. X, Phys. Rev. Lett., Phys. Rev. E, JMB, PCCP, JPC, JCP, JCTC, J. Comput. Chem, SIAM Multiscale Model. Simul., PLoS One, PLoS Comput. Biol., Soft Matter, Drug Discov. Today, NeurIPS, ICML, Mach. Learn. Sci. Tech.

Selected invited presentations (> 130 total)

Nov 17, 2020	Pregl Colloquium, Ljubljiana, SVN
Jul 8, 2020	AI4Science kickoff workshop, Amsterdam, NL
Feb 26, 2020	AI Powered Drug Discovery and Manufacturing Conference, MIT, MA, USA
Dec 5, 2019	Keynote, Culminating workshop of Long Program "Machine learning for physics and the physics of learning", Institute of Pure and Applied Mathematics, UCLA, CA, USA.
Sep 27, 2019	Award lecture, PHYS division, American Chemical Society Meeting, San Diego, CA, USA
Mar 6, 2019	Workshop on Bayesian Statistical Inference for Biophysics, Biophysical Society meeting, Baltimore, MD, USA
Mar 4, 2019	American Physical Society Meeting, Boston, MA, USA
Dec 8, 2018	Workshop on Machine Learning for Materials and Molecules, NeurIPS 2018, Montreal, CAN
Apr 7, 2018	Keynote, Symposium on Biophysics Postgraduate Research HKUST, Hong Kong, CN.
Mar 22, 2018	Crick Chair lecture, UC San Diego, CA, USA
Feb 6, 2018	Center for Theoretical Biological Physics, Rice University, Houston, TX, USA
Sep 15, 2017	Machine learning tutorials, IPAM workshop Complex High-Dimensional Energy Landscapes, UC Los Angeles, CA, USA
Sep 14, 2017	Keynote, Set-Oriented Numerics workshop, UC Santa Barbara, CA, USA
May 25, 2017	SIAM conference on applications of dynamical systems, Snowbird, UT, USA
Mar 14, 2017	Americal Physical Society meeting, New Orleans, LA, USA
Oct 24, 2016	"Collective variables in classical mechanics", IPAM, Los Angeles, CA, USA.
Oct 9, 2016	Erice school on Free Energy Landscapes, Erice, IT
Mar 15, 2016	American Chemical Society meeting, San Diego, USA
July 25, 2016	Gordon Research Conference on Computational Chemistry, Girona, ESP
Feb 17, 2016	CECAM workshop "Models for protein dynamics", Lausanne, CH
Jan 26, 2016	Software for Exascale computing workshop, Munich, GER
Oct 13, 2015	CECAM workshop "Computational Modeling of Gene Expression", Tel Aviv, IL
Jun 15, 2015	"Dynamics and Kinetics from Single Molecules to Cells", Telluride, CO, USA
Jul 19, 2015	European Biophysical Congress, Dresden, GER
Sep 8, 2015	Molecular and Chemical Kinetics, Berlin, GER
Nov 12, 2014	BIRS workshop on particle-based reaction-diffusion dynamics, Banff, CAN
Aug 21, 2014	CECAM workshop "Modeling cellular life", Lausanne, CH
Jun 14, 2014	Coarse-graining as a Frontier of Statistical Mechanics, Santa Fe, NM
Mar 7, 2014	Model-Data Integration in Physical Models, Cambridge, UK
Oct 4, 2013	CECAM workshop "Innovative approaches in drug discovery", Lausanne, CH
Sep 3, 2013	Molecular Kinetics, Berlin, GER
Apr 4, 2013	American Chemical Society meeting, New Orleans, USA.
Nov 29, 2012	CECAM workshop "Machine learning in molecular simulation", Lugano, CH
Sep 5, 2012	CECAM workshop "Protein folding dynamics", Zürich, CH
Jul 19, 2011	Int'l Conference on Industrial and Applied Mathematics (ICIAM), Vancouver, CAN.
Feb 26, 2011	Sanibel Symposium, University of Florida, FL, USA.
Aug, 09, 2011	"Rise of the machines", Telluride, CO, USA.
Mar, 8, 2011	"Mathematical Challenges in Molecular Dynamics", Imperial College, London, UK.
Jan, 10, 2011	nDDB workshop Institut Laue-Langevin, Grenoble, FR
Jun 14-17, 2010	Summer school lecture series at SISSA, Trieste, IT
Jun 3, 2010	CECAM workshop "Complex Energy Landscapes", Zaragoza, ESP
May 26, 2010	Leopoldina Meeting "The complexity connecting biomolecular structure and solvation dynamics", Bochum, GER
Feb 9, 2010	W3 Professor selection symposium "Modelling and simulation of dynamics, structure and function of complex molecular systems", IWR Heidelberg
Sep 8-11, 2009	Lecture Series at National Institute of Health, Bethesda, MA, USA
Dec 12, 2009	Plenary Speaker at "Membranes and Molecules", Berlin, GER
Feb 23, 2009	"Rare Events in High Dimensional Systems", IPAM, Los Angeles, CA, USA