Jeffrey K. Noel, Ph.D.

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Current Address: 1012NK Amsterdam, Netherlands

I am a Ph.D. physicist with 16 years of experience in biomolecular computational physics and quantitative software development. I have led physics-based modeling activities in both the academic and industrial spheres. My interests generally lie in protein folding and protein-membrane interaction. In particular, 1) I work to extend and enhance our SBM software (SMOG, https://smog-server.org), 2) study the assembly and function of the polymeric protein filaments formed by dynamin related proteins, and 3) study the folding and function of knotted proteins.

Education

Ph.D. in Physics	University of California, San Diego	June 15, 2012
Thesis title:	Development and Application of All-Atom Structure-based Models for Studying the Role of Geometry in Biomolecular Folding and Function	
Bachelor of Science	University of Wisconsin, Madison	June 6, 2005
	Major: Applied Math, Engineering, and Physics (Computer Engineering focus)	

Research Experience

Modelling Team Lead and Modelling Expert, Electric Ant Lab, Amsterdam, Netherlands 2021-2023

- Leading the modeling effort for our product Rheocube, a SaaS chemical simulation software geared toward experimental scientists working in the chemical industry. Leading a team of seven Ph.D.s.

Humboldt Fellow, Max-Delbrück Center, Berlin (PI: Oliver Daumke and Alexander Mikhailov) 2016-2021

- Used various techniques (soft matter physics, all-atom simulations, coarse-grained simulations, biochemical experiments) to understand the molecular mechanism of the dynamin molecular motor, a polymeric GTPase machine that catalyzes membrane scission during endocytosis.

Postdoctoral Fellow, Center for Theoretical Biological Physics, Rice University (PI: José Onuchic) 2013-2015

- Applied all-atom structure-based models and explicit solvent simulations to study large-scale molecular rearrangements in the ribosome and influenza hemagglutinin

Awards and Honors

Alexander von Humboldt Postdoctoral Fellowship	2016-2018
Guest Researcher of the Max Planck Society	2015-2018
Robert A. Welch Foundation Postdoctoral Fellow	2014-2015
NIH Molecular Biophysics Training Grant	2007–2009
San Diego Fellowship	2005–2007
AMEP Leadership Award	2005
NSF REU Grant	2003 & 2004

Computing Awards

XSEDE Grant MCB140274 for 4.6MSUs (Co-PI)	2014
National Research Council (NRC) Anton Grants PSCA00062P, PSCA14037P, PSCA15061P, and PSCA16067P (Co-PI)	2011-2017

Summary of Scientific Impact

43 peer-reviewed publications, 20 as a first or corresponding author, H-index 25, 2600 total citations (Google Scholar). Authored 3 invited reviews and 2 book chapters. Given 29 invited seminars. Reviewer of more than 30 manuscripts for Nature Comms, PNAS, Proteins, Nucl. Acid Res., Biophys. J, others

Workshops Co-organized

RNA Dynamics: Going from In Vitro to In Silico. RNA Institute Workshop, Albany, NY — Mar 2015

Structure-based Models with SMOG@ctbp. International Conference on Biological Physics, San Diego, CA — Jun 2011

Protein Dynamics: Going from In Vitro to In Silico: A Center for Theoretical Biological Physics Workshop. University of California, San Diego, CA — May 2007

Scientific Service

Reviewer of more than 30 manuscripts for Nature Comms, PNAS, Proteins, Nucl. Acid Res., others
Postdoc-to-PhD mentor program, Max Delbruck Center — 2019
Berlin Long Night of Science (public engagement) — 2015-2019
Software packages maintained for the community: SMOG and WHAM.jar

Peer-Reviewed Publications

* shared authorship # corresponding author

43. Melo AA, Sprink T, **Noel JK**, Vazquez Sarandeses E, Van Hoorn C, Loerke J, Spahn C, Daumke O (2022) Cryo-electron tomography reveals structural insights into the membrane remodeling mode of dynamin-like EHD filaments. Nature Communications 13 [link]

42. Bock-Bierbaum T, Funck K, Wollweber F, Lisicki E, Laborenz J, **Noel JK**, Hessenberger M, von der Malsburg A, von der Malsburg K, Bernert C, Kunz S, Riedel D, Lilie H, Jakobs S, van der Laan M, Daumke O (2022) Structural insights into crista junction formation by the Mic60-Mic19 complex. Science Advances 8(35). [link]

41. Oliveira AB, Contessoto V, Hassan A, Byju S, Wang A, Wang Y, Rojas EGD, Mohanty U, #**Noel JK**, #Onuchic JN, #Whitford PC (2021) SMOG 2 and OpenSMOG: Extending the limits of structure-based models. Protein Science. [link]

40. Liu J, Alvarez FJD, Clare DK, **Noel JK**, and Zhang P (2021) CryoEM structure of the super-constricted two-start dynamin 1 filament. Nature Comms. 12(1), 5393–11. [link]

39. Ganichkin O, Vancraenenbroeck R, Rosenblum G, Hofmann H, Mikhailov AS, Daumke O, #***Noel JK** (2021) Quantification and demonstration of the collective constriction-by-ratchet mechanism in the dynamin molecular motor. Proc. Natl. Acad. Sci. USA 118, e2101144118 [link]

38. Liu J, Tassinari M, Souza DP, Naskar S, **Noel JK**, Bohuszewicz O, Buck M, Williams TA, Baum B, Low HH (2021) Bacterial Vipp1 and PspA are members of the ancient ESCRT-III membrane-remodeling superfamily. Cell 184(14):3660-3673.e18) [link]

37. Danielsson J, **Noel, JK**, Duggan B, Oliveberg M, Onuchic JN, Jennings PA, Haglund E (2020) The pierced lasso topology leptin has a bolt on dynamic domain composed by the disordered loops I and III. J. Mol. Bio., 432, 3050-63. [link]

36. #**Noel JK**, Noé F, Daumke O, and Mikhailov AS (2019) Polymer-like model to study the dynamics of dynamin filaments on deformable membrane tubes. Biophys. J. 117, 1870-91. [link]

35. Faelber K, Dietrich L, ***Noel JK**, *F Wollweber, *A-K Pfitzner, et al., M van der Laan, W Kuhlbrandt, and O Daumke (2019) Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. Nature 571, 429–33. [link]

34. Levi M, #**Noel JK**, #Whitford PC (2019) Studying ribosome dynamics with simplified models. Methods, 162, 128-40. [link]

33. Liu JW, **Noel JK**, Low, HH (2018) Structural basis for membrane tethering by a bacterial dynamin-like pair.

Nature Comms., 9, 3345. [link]

32. Lin X, **Noel JK**, Wang Q, Ma J, Onuchic JN (2018) Atomistic Simulations of the Loop to Coiled-Coil Functional Transition of the B-loop Domain of Influenza Hemagglutinin. Proc. Natl. Acad. Sci. USA 115, E7905–E7913. [link]

31. Sun L, **Noel JK**, Levine H, Onuchic JN (2017) Molecular simulations suggest a force-dependent mechanism of vinculin activation. Biophys. J. 113(8), 1697–710. [link]

30. Yang H, **Noel JK**, Whitford PC (2017) Anisotropic Fluctuations in the Ribosome Determine tRNA Kinetics. J. Phys. Chem. B 121, 10593-601 [link]

29. **Noel JK**, Whitford PC (2016) How EF-Tu can enable efficient proofreading of aa-tRNA by the ribosome. Nature Comms. 7, 13314. [link]

28. *Lin X, ***Noel JK**, Wang Q, Ma J, Onuchic JN (2016) Lowered pH Leads to Fusion Peptide Release and a Highly-dynamic Intermediate in Influenza Hemagglutinin. J. Phys. Chem. B 120, 965460. [link]

27. **Noel JK**, Levi M, Raghunathan M, Lammert H, Hayes RL, Onuchic JN, Whitford PC (2016) SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLOS Comput. Biol. 12, e1004794. [link]

26. **Noel JK**, Morcos F, Onuchic JN (2016) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000Res 5, 1-7. [link]

25. Cheng RR, Raghunathan M, **Noel JK**, Onuchic JN (2016) Constructing sequence-dependent protein models using coevolutionary information. Protein Sci. 25, 111—22. [link]

24. Lammert H, **Noel JK**, Haglund E, Schug A, Onuchic JN (2015) Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures. J. Chem. Phys. 143, 243141. [link]

23. Fisher KM, Haglund E, **Noel JK**, Hailey KL, Onuchic JN, Jennings PA (2015) Geometrical frustration in Interleukin-33 decouples the dynamics of the functional element from the folding transition state ensemble. PLOS One 10, e0144067. [link]

22. Ramirez-Sarmiento CA, **Noel JK**, Valenzuela SL, Artsimovitch I (2015) Interdomain contacts control native state switching of RfaH on a dual-funneled landscape. PLOS Comp. Biol. 11, e1004379. [link]

21. Hayes RL, **Noel JK**, Mandic A, Whitford PC, Udayan M, Sanbonmatsu KY, Onuchic JN (2015) Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Phys. Rev. Lett. 114, 258105. [link]

20. Sun L, **Noel JK**, Sulkowska JI, Levine H, Onuchic JN (2014) Connecting thermal and mechanical protein (un)folding landscapes. Biophys. J. 107, 2941-52. [link]

19. **Noel JK**, Chahine J, Leite VBP, Whitford PC (2014) Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome. Biophys. J. 107, 2872-81. [link]

18. Lin X, Eddy NR, **Noel JK**, Whitford PC, Wang Q, Ma J, Onuchic JN (2014) Order and disorder control the functional rearrangement of influenza hemagglutinin. Proc. Natl. Acad. Sci. USA, 111, 12049-54. [link]

17. Haglund E, Sulkowska JI, **Noel JK**, Lammert H, Onuchic JN, Jennings PA (2014) Pierced Lasso Bundles are a New Class of Knot Motifs. PLOS Comp. Biol. 10: e1003613. [link]

16. **Noel JK**, Whitford PC (2014) How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Isr. J. Chem., 54, 1093–107. [link]

15. Hayes RL, **Noel JK**, Whitford PC, Udayan M, Sanbonmatsu KY, Onuchic JN (2014) Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophys. J. 106, 1508-19. [link]

14. *Ozenne V, ***Noel JK**, Heidarsson PO, Brander S, Poulsen FM, Jensen MR, Kragelund BB, Blackledge M, Danielsson J (2014) Exploring the minimally frustrated energy landscape of unfolded ACBP. J. Mol. Biol. 426, 722-34. [link]

13. **Noel JK**, Onuchic JN, Sulkowska JI (2013) Knotting a protein in explicit solvent. J. Phys. Chem. Lett. 4, 3570-3. [link]

12. Lammert H, **Noel JK**, Onuchic JN (2012) The Dominant Folding Route Minimizes Backbone Distortion in SH3. PLOS Comput. Biol. 8, e1002776. [link]

11. *Sulkowska JI, ***Noel JK**, Onuchic JN (2012) Energy landscape for knotted protein folding. (2012) Proc. Natl. Acad. Sci. USA, 109, 1778388. [link]

10. Hayes RL, **Noel JK**, Mohanty U, Whitford PC, Hennelly SP, Onuchic JN, Sanbonmatsu K (2012) Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. J. Amer. Chem. Soc., 134, 12043-53. [link]

9. **Noel JK**, Whitford PC & Onuchic JN (2012) The Shadow Map: A General Contact Definition for Capturing the Dynamics of Biomolecular Folding and Function. J. Phys. Chem. B, 116, 86928702. [link]

8. **Noel JK**, Schug A, Verma A, Wenzel W, Garcia AE & Onuchic JN (2012) Mirror images as naturally competing conformations in protein folding. J. Phys. Chem. B, 116, 6880-8. [link]

7. *Suzuki Y, ***Noel JK** & Onuchic JN, (2011) A semi-analytical description of protein folding that incorporates detailed geometrical information. J. Chem. Phys., 135, 245101. [link]

6. **Noel JK**, Sułkowska JI & Onuchic JN (2010) Slipknotting upon Native-like Loop Formation in a Trefoil Knot Protein. Proc. Natl. Acad. Sci. USA, 107, 15403-15408. [link]

5. **Noel JK**, Whitford PC, Sanbonmatsu KY & Onuchic JN (2010) SMOG@ctbp: simplified deployment of structure-based models in GROMACS. Nucleic Acids Res. 38 W657–61. [link]

4. Whitford PC, **Noel JK**, Gosavi S, Schug A & Onuchic JN (2009) An All-atom Structure-Based Potential for Proteins: Bridging Minimal Models with Empirical Forcefields. Proteins: Structure, Function, Bioinformatics. 75 430-441. [link]

3. Suzuki Y, **Noel JK** & Onuchic JN (2008) An analytical study of the interplay between geometrical and energetic effects in protein folding. J. Chem. Phys., 128 025101. [link]

2. Vano JA, Wildenberg JC, Anderson MB, **Noel JK** & Sprott JC (2006) Chaos in low-dimensional Lotka-Volterra models of competition. Nonlinearity. 19, 2391-2404. [link]

1. Sprott JC, Vano JA, Wildenberg JC, Anderson MB & **Noel JK** (2005) Coexistence and chaos in complex ecologies. Phys. Let. A, 335 (2-3) 207-212. [link]

Reviews and Chapters

5. Levi M, Bandarkar P, Yang H, Wang A, Mohanty U, **Noel JK**, Whitford PC (2018) Using SMOG 2 to simulate complex biomolecular assemblies. Chapter in: Methods in Molecular Biology, Springer Nature (in press) [link]

4. **Noel JK**, Morcos F, Onuchic JN (2016) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000Res 5, 1-7. [link]

3. **Noel JK**, Whitford PC (2014) How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Isr. J. Chem., 54(8-9), 1093–107. [link]

2. Sulkowska JI, **Noel JK**, Ramirez-Sarmiento CA, Rawdon EJ, Millett KC, Onuchic JN (2013) Knotting pathways in proteins. Biochemical Society Transactions 41, 523–527. [link]

1. **Noel JK** & Onuchic JN, The many faces of structure-based potentials: From protein folding landscapes to structural characterization of complex biomolecules. Chapter 2 in Computational Modeling of Biological Systems; Dokholyan, N. Ed., Springer: New York, 2012. [link]

Invited Talks

"Dynamin Works as a Nanomuscle in Remodeling of Biomembranes" Quantitative Biosciences Institute, UCSF, USA (zoom)	Oct 2020
"Mesoscopic modeling of membrane deformation by dynamin oligomers" Institute for Advanced Simulation, Jülich, Germany (zoom)	Sept 2020
"Mesoscopic modeling of membrane deformation by dynamin oligomers" 9th International Conference Engineering of Chemical Complexity, Potsdam, Germany	Jun 2019
"The operation of the dynamin motor: a molecular python" SFB1035 seminar, TUM, Munich, Germany	Oct 2018
"Toward understanding the dynamin molecular motor: a molecular python" Centre of New Technologies Seminar, Warsaw, Poland	Mar 2018
"Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes" Neuroscience Dept, Okayama, Japan	Mar 2018
"Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes" NanoLSI Seminar, Kanazawa, Japan	Mar 2018
"The operation of the dynamin molecular motor" 9th International Conference Engineering of Chemical Complexity, Barcelona, Spain	Jun 2017
"How EF-Tu Can Contribute to Efficient Proofreading of aa-tRNA by the Ribosome" Huenfeld Theory 2017, Huenfeld, Germany	Mar 2017
"Connecting tRNA accommodation, EF-Tu dissociation, and kinetic proofreading in the ribosome." 6th Visegrad Symposium on Structural Systems Biology, Warsaw, Poland	Jun 2016
"Kinetic proofreading in the ribosome: Probing the free-energy landscape of fidelity" Kyoto University, Kyoto, Japan	Mar 2016
"Kinetic proofreading in the ribosome: Probing the free-energy landscape of fidelity" Hiroshima University, Hiroshima, Japan	Mar 2016
"Enriching structure-based models with coevolutionary information" New Frontiers in Nonlinear Sciences Workshop, Niseko, Japan	Mar 2016
"Energy Landscapes of Biomolecular Machines: Capturing Transition Paths for Conformational Rearrangements in the Ribosome" BCSCCS Seminar, Fritz-Haber Institute, Berlin	Nov 2015
"Enriching structure-based models with coevolutionary information" Protein Folding Consortium Meeting, Berkeley, CA	May 2015
"Free energy landscape of tRNA accommodation in the ribosome" Max Delbrück Center, Berlin, Germany	Jan 2015
"Understanding knotted protein folding by combining coarse-grained and explicit solvent simulations" Biophysical Society Meeting: The Significance of Knotted Structures for the Function of Proteins and Nucleic Acids, Warsaw, Poland	Sept 2014
"The Massive Functional Rearrangement of Influenza Hemagglutinin" ACS Fall Meeting, San Francisco	Aug 2014
"Characterizing the Energy Landscape of tRNA Accommodation in the Ribosome" 1st Symposium on Current Topics in Molecular Biophysics, University of Sao Paulo, Brazil	May 2014
"Structure-based models: Versatile models for studying protein folding and function through energy landscape theory" University of Chile, Santiago, Chile	May 2014
"How protein folding is teaching us about molecular machines" Frontiers in Science Seminar Series, University of Houston, Houston, TX	Mar 2014
"Folding of topologically complex proteins: slipknots and lassos" CIBR, Baylor College of Medicine, Houston, TX	Feb 2014
"Understanding knotted protein folding" Physics Seminar, Northeastern University, Boston, MA	Jul 2013

"Detailed simulations of protein slipknotting events during folding" Protein Folding Consortium Meeting, Berkeley, CA	May 2013
"Studying biomolecular dynamics using structure-based potentials with SMOG," SCC seminar, Karlsruhe Institute of Technology, Karlsruhe, Germany	Sep 2012
"Studying biomolecular dynamics using structure-based potentials with SMOG," TCB Seminar, Beckman Institute, Urbana, IL	Aug 2012
"Structure-based Models with SMOG@ctbp: From Protein Folding Landscapes to Structural Characterization of Complex Biomolecules," International Conference on Biological Physics, La Jolla, CA	Jun 2011
"Folding a Trefoil Knot Protein," Topological Problems in Molecular Biology, American Mathematical Society Meeting, Iowa City, Iowa	Mar 2011
"Entropy, Symbolic Dynamics, and Dynamical Systems," Chaos and Complex Systems Seminar, University of Wisconsin, Madison	Apr 2005