Megan C. Engel, D.Phil.

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EDUCATION

2018 D.Phil. in Theoretical Physics, Oxford University, Rhodes Scholar

Faculty Advisors: Ard Louis and Jonathan Doye.

<u>Thesis title</u>: Exploration of DNA systems under internal and external forcing using coarse-grained modelling.

2013 M.Sc. in Physics, University of Alberta, Canada

2012 B.Sc. in Honors Astrophysics, University of Alberta, Canada



PROFESSIONAL EXPERIENCE

2023 - Assistant Professor, Department of Biological Science, University of Calgary

2023 – Associate of the Harvard John A. Paulson School of Engineering and Applied Sciences,
Harvard University

2019 – 2023 Postdoctoral Fellow in Machine Learning, School of Engineering and Applied Science, Harvard University, Schmidt Science Fellow

Faculty Advisor: Michael Brenner.

<u>Project</u>: Using machine learning optimizers for nonequilibrium processes.

CAREER BREAKS

Maternity leave November 2023 – Maternity leave February 2021 – February 2022 Maternity leave June 2018 – October 2019

PUBLICATIONS

In Preparation

King, Ella M., *Engel, M. C., Schoenholz, S., Martin, C. S., Manoharan, V., and Brenner, M. Inferring interaction potentials from stochastic particle trajectories. (2023)

First Author Peer-Reviewed

- 1. *Engel, M. C., Smith, J., and Brenner, M. Optimal control of nonequilibrium systems through automatic differentiation. (2023) Physical Review X. 13:041032. https://doi.org/10.1103/PhysRevX.13.041032
- 2. *Engel, M.C., Romano F, Louis A.A., Doye JPK. Measuring Internal Forces in Single-Stranded DNA: Application to a DNA Force Clamp. (2020) J Chem Theory Comput. 16(12):7764-75. 10.1021/acs.jctc.0c00286 PMID: 33147408.
- 3. *Engel, M.C., Smith, D., Jobst, M., Sajfutdinow, M., Liedl, T., Romano, F., Rovigatti, L., Louis, A.A., and Doye, J.P.K. Force-induced Unravelling of DNA Origami. (2018) ACS Nano 12(7):6734-6747. pubs.acs.org/doi/abs/10.1021/acsnano.8b01844
- 4. *Engel, M.C., Ritchie, D.B., Foster, D.A.N., Beach, K.S.D., and Woodside, M.T. Reconstructing Folding Energy Landscape Profiles from Nonequilibrium Pulling Curves with an Inverse Weierstrass Integral Transforme. (2014) Physical Review Letters 113:238104-9, Editors' Suggestion. dx.doi.org/10.1103/PhysRevLett.113.238104
- 5. *Engel, M.C., Heinke, C. O., Sivakoff, G.R., Elshamouty, K. G., and Edmonds, P.D. A 2.15 Hour Orbital Period for the Low Mass X-Ray Binary XB 1832-330 in the Globular Cluster NGC 6652. (2012) The Astrophysical Journal 747(2):119-126. doi.org/10.1088/0004-637X/747/2/119

Additional Peer-Reviewed Publications

- 6. Doye, J.P.K, Fowler, H., Presern, D., Bohlin, J., Rovigatti, L., Romano, F., Sulc, P., Wong, C.K., Louis, A.A., Schreck, J.S., **Engel, M.C.**, Matthies, M., Benson, E., Poppleton, E., and Snodin, B.E.K., The oxDNA coarse-grained model as a tool to simulate DNA origami. (2023) Methods in Molecular Biology, in press. arxiv.org/abs/2004.05052
- 7. Doye, J.P.K., Louis, A.A., Schreck, J.S., Romano, F., Harrison, R.M., Mosayebi, M., **Engel, M.C.**, and Ouldridge, T.E., Free-energy landscapes of DNA and its assemblies: Perspectives from coarse-grained modelling. (2021) Book chapter, in press at Elsevier. arXiv:2111.10166v1
- 8. Rajpaul, V. M., Lindstrøm, C., **Engel, M.C.**, Brendehaug, M., and Allie, S. Cross-sectional study of students' knowledge of sizes and distances of astronomical objects. (2018) Physical Review Physics Education Research 14:020108. doi.org/10.1103/PhysRevPhysEducRes.14.020108. Featured in a Physics Focus story, "Astronomy Students Not Learning the Basics"
- 9. Khmelinskaia, A., **Engel, M.C.**, and Schwille, P. Design of a switchable DNA origami structure for shaping lipid membranes. (2017) European Biophysics Journal With Biophysics Letters 46:S122. (poster abstract). link.springer.com/content/pdf/10.1007%2Fs00249-017-1222-x.pdf

- 10. Lindstrøm, C., Rajpaul, V., Brendehaug, M., and **Engel, M.C.**, Perspectives on astronomy: probing Norwegian pre-service teachers and middle school students, 2015 PERC Proceedings [College Park, MD, July 29-30, 2015], edited by A. D. Churukian, D. L. Jones, and Lin Ding: pp. 195-198. dx.doi.org/10.1119/perc.2015.pr.044
- 11. Cartwright, T.F., **Engel, M.C.**, Heinke, C. O., Sivakoff, G.R., Berger, J.E., Gladstone, J.C., Ivanova, N., and Pavlovskiy, K.S. Galactic Ultracompact X-ray Binaries: Empirical Luminosities. (2012) The Astrophysical Journal 768(2):183-197. doi.org/10.1088/0004-637X/768/2/183
- 12. Heinke, C.O., Ivanova, N., **Engel, M.C.**, Pavlovskiy, K.S., Sivakoff, G.R., Cartwright, T.F., Gladstone, J.C. Galactic Ultracompact X-ray Binaries: Disk Stability and Evolution. (2012) The Astrophysical Journal 768(2):184-194. doi.org/10.1088/0004-637X/768/2/184

Books

*Engel, M.C. DNA Systems under Internal and External Forcing: An Exploration Using Coarse-Grained Modelling. Springer, 2019.

Conference Proceedings (<u>Underlined are my trainees</u>)

<u>Krueger, R.,</u> Brenner, M., and **Engel, M.C.** (2023 March 5-10) *A Differentiable Model of Nucleic Acid Dynamics*. American Physical Society March Meeting, Las Vegas, Nevada. https://meetings.aps.org/Meeting/MAR23/Session/M08.8

<u>King, Ella.,</u> **Engel, M.C.,** Schoenholz, S., Martin, C., Manoharan, V., and Brenner, M. (2023 March 5-10) *Inferring interaction potentials from particle trajectories*. American Physical Society March Meeting, Las Vegas, Nevada. https://meetings.aps.org/Meeting/MAR23/Session/F16

Science Book Reviews

- *Engel, M.C., Confronting age-old questions, big and small. (2022) Science 375(6576): 35. doi.org/10.1126/science.abn0901
- *Engel, M.C., Mysteries of the Mundane. (2017) Science 355(6320): 33. doi.org/10.1126/science.aak9964
- *Engel, M.C., The Unknown Universe. (2016) Science 352(6290): 1171. doi.org/10.1126/science.aaf6929
- *Engel, M.C., Picking Up Grand Vibrations. (2014) Science 645(6194): 261-262. doi.org/10.1126/science.1255862

SOFTWARE PROJECTS

Jax-MD | contributor

Github: https://github.com/jax-md/jax-md

Implemented improved Langevin integrators for rigid bodies; working on Virtual Move Monte Carlo functionality

Non-equilibrium optimal protocols | developer

Github: https://github.com/mc2engel/noneq_opt

PRESENTATIONS

Invited Talks

Optimizing non-equilibrium processes using differentiable simulation, MIT, 2023

Optimizing non-equilibrium processes using differentiable simulation, Physics Colloquium, University of Calgary, 2023

Al Institute in Dynamic Systems, University of Washington, 2022

Special Statistical Physics Seminar, Simon Fraser University, 2021

Nonequilibrium statistical mechanics through the lens of machine learning, Bustamante group, University of California, Berkeley, 2020

Optimizing nonequilibrium processes, the Kavli Institute at Harvard University, 2020

Simulation-aided de novo biomolecular design, Institute for Protein Design, University of Washington, 2020

Coarse-grained modelling of DNA under internal and external forcing, Harvard University, 2019 Coarse-grained modelling of DNA origami behaviour under tension, Multi-university 'DNA Node' seminar, Ludwig Maximilian University of Munich, 2016

Conference Talks

Machine learning for optimal control of nonequilibrium systems, Lightning talk, Workshop on Stochastic Thermodynamics II, Santa Fe Institute, 2021 *talk acceptance rate: 11%

Systematic investigation of bias in Jarzynski-derived free energy landscapes using coarse-grained simulations, Institute of Physics (IOP) 'Physics Meets Biology' conference, Cambridge University, 2016

Reconstructing folding energy landscape profiles from nonequilibrium pulling curves with an inverse Weierstrass integral transform, Open Statistical Physics Conference, Open University, 2016

Posters

Coarse-grained modelling of DNA Origami behavior under tension. DNATEC17 Conference, Dresden, Germany. 2017; Foundations of Nanoscience (FNANO) Conference in Salt Lake City, Utah. 2016

- Noise-assisted transport through complex quantum networks. EPSRC Quantum Information, Computing, and Control summer school, University of Exeter. 2015 *won poster prize
- Probing the Secrets of RNA Pseudoknots with Nonequilibrium Statistical Mechanics. Graduate Physics Research Symposium, University of Alberta. 2012
- A 2.15 Hour Orbital Period for the Low Mass X-Ray Binary XB 1832-330 in the Globular Cluster NGC 6652. Canadian Astronomical Society conference, University of Calgary. 2012 *won poster prize

TEACHING & ADVISING EXPERIENCE

University Lecturer

Responsibilities include designing and delivering lectures, assignments, and exams, meeting with students, and grading exams.

<u>Biochemistry 471: Thermodynamics Section</u>, 2023 Fall Semester, University of Calgary.
 Third-year course focusing on thermodynamics and biophysics. 19 students. 22 hours of lecturing.

Teaching Fellow

Responsibilities include developing class materials and problem sets, meeting with students and supervising student research projects, and grading

 Applied Math 216: Inverse Problems in Science and Engineering, 2022 Winter Semester, Harvard University. Graduate-level course focusing on applying machine learning to solve scientific inverse problems.

College Lecturer

Responsibilities included developing new class materials, leading class discussions, and grading all assignments and 'collections' (termly) exams.

- <u>Mathematics for Chemists</u>, 2015-18, Queen's College, Oxford. 19 total students over 3 years. 2 instructional hours per week for 24 weeks x 3 years = 144 instructional hours.
- <u>Mathematics for Chemists</u>, 2017-18, Merton College, Oxford. 6 students. 3 instructional per week for 24 weeks = 72 instructional hours.

Teaching Assistant/Tutor

Responsibilities included leading class discussions and grading assignments.

• <u>Third year biophysics</u>, Terms 2 & 3, 2017, St. Anne's College, Oxford. 6 students, 6 instructional hours

- Third year biophysics, Term 2, 2017, Jesus College, Oxford. 7 students, 3 instructional hours
- <u>Graduate nonequilibrium statistical mechanics</u>, Term 2, 2016, Oxford Department of Physics, 3 students, 3 instructional hours

Laboratory Demonstrator

<u>First-year computer programming</u>, 2014-6, Oxford Department of Physics, ~20 students over 3 years. 3 hours instruction per week for 15 weeks x 3 years = 135 instructional hours

Mentoring Experience

- 4 undergraduate students at University of Calgary, summer 2023
- 2 PhD candidates at Harvard University, 2022 –
- 2 undergraduate students at Harvard University, 2022 –
- 1 MSc student at Oxford University (remotely from Harvard) 2021
- 1 MSc student at Oxford University, 2017
- 1 undergraduate student at Oxford University, 2016

FUNDING & AWARDS

Funding

Start-up grant from University of Calgary, 2023 (C\$200,000)

Schmidt Futures Virtual Institute for Scientific Software support grant, 2023 (9 months of support from professional software engineers and HPC time)

Fellowships

Schmidt Science Fellowship Renewal, 2020 (\$100,000 USD)

Schmidt Science Fellowship, 2019 (\$100,000 USD)

Izaak Walton Killam Postdoctoral Fellowship, 2018 (C\$46,000 x 2 years) (declined)

Academic Awards

Springer Thesis Prize, 2019 (€500)

Canadian Centennial Scholarship, 2017 (£3,000)

Canadian Natural Sciences and Engineering Research Council (NSERC) Postgraduate Scholarship, Doctoral level, 2015 (C\$42,000 x 2 years)

Rhodes Scholarship, 2013 (£90,000)

Sir James Lougheed Award of Distinction, 2015 and 2014 (C\$20,000 x 2)

Gov't of Canada Persons Case Scholarship for the Advancement of Women, 2014 (C\$4,500)

University of Alberta Alumni Horizon Award, 2014

Alberta Science & Technology Leadership Foundation Leaders of Tomorrow Award, 2014 (C\$10,000)

NSERC André Hamer Postgraduate Prize M, 2012 (C\$10,000)

NSERC Julie Payette Research Scholarship, 2012 (C\$25,000)

Four graduate level academic excellence scholarships (totaling C\$12,600), 2012-14

NSERC Undergraduate student research awards, 2010, 2011, & 2012 (\$8,000 x 2) (declined)

Louis S. Crosby Memorial Gold Medal in Physics for highest grade in Honors Physics, 2012

Fourteen undergraduate academic excellence scholarships, 2007-12 (totaling C\$23,650)

Scholastic Distinction Chancellor's Entrance Citation & three renewals, 2007 (C\$15,000)

Selected Other Awards

Selected for the Recruitment of Policy Leaders (RPL) program with the Canadian government (declined a position), 2021

Winner, Audience Vote – Institute of Physics 3-Minute Wonder Competition, 2017

SERVICE & OUTREACH

To Profession

Co-Organizer, 2024 SIAM Conference on Materials Science Mini Symposium ("Programmable assembly: inverse design of materials from discrete components"), 2023–

Co-Organizer, 8th Annual Biophysical Society of Canada Meeting, 2022 – 2023

Referee for Physical Review E 2023 -

Referee for Physical Review Letters 2022 -

Referee for *Physical Review X* 2022 –

Mentor with Harvard Graduate Women in Science and Engineering, 2020-22

Peer mentor in the Schmidt Science Fellows peer support scheme, 2020-21

Co-organizer, UK Women in Physics Intercollegiate Conference, Oxford University, 2014, 15, 16 Career panelist, Biophysical Society Conference, Philadelphia, 2013

Outreach

Career panelist, Biological Sciences Graduate Symposium 2023

Lecturer, Institute of Physics London's 3-Minute Wonder competition, November 2017

Volunteer, Oxford 'Girls in Physics Day', July 2014

Volunteer, Oxford 'Physics Alumni Day', June 2014

Science Activity Leader, Women in Scholarship, Engineering, Science and Technology (WISEST) Choices 2013 Conference, University of Alberta, 2013

To Community

Accompanist for children's choir at St Bernard's Parish, Calgary, 2023 –

Soprano in the St. Joseph's Basilica choir, Edmonton, 2018-19

Pianist & vocalist, Isis long-term care home, St. John's Care Trust, and Grove House, Oxford, 2014-18

Pianist and vocalist, Catholic Chaplaincy in Oxford (2013-18) and Good Shepherd Parish in Edmonton (2009-13)

Volunteer, Companions of the Order of Malta, 2014-17

Events coordinator, Rhodes Scholars South African Forum, 2014-15.

Volunteer pianist & vocalist, Artists on the Wards program, University of Alberta Hospital, 2012-13

President and co-founder, The University of Alberta Tolkien Society, 2013 'Student Group of the Year', 2011-13

Piano teacher, Heart of the City Piano Program, 2011-12

ADDITIONAL EXPERIENCE

Admissions interviewer, Queen's College, Oxford University, 2015 & 2016 Professional musician at 50+ events, piano, vocals & guitar, 2005-