

Nawaf Bou-Rabee

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Research Interests

My research lies at the intersection of probability theory and computational mathematics. I work on the mathematical foundations and algorithmic development of Markov Chain Monte Carlo (MCMC), focusing on spectral gaps, mixing times, convergence diagnostics and metastability in high-dimensional and geometrically complex settings. I also work on long-time-accurate numerical methods for stochastic differential equations (SDEs and SPDEs). A central theme of my current work is locally adaptive MCMC: its mathematical foundations and algorithmic architecture needed to make these methods reliable in challenging sampling problems arising in statistics and machine learning. Recent advances fundamentally extend and generalize the widely used No-U-Turn Sampler: such as WALNUTS, a step-size-adaptive extension for continuously differentiable targets; NURS, a gradient-free locally adaptive sampler; and new discrete-space variants of NURS.

Academic Appointments

- Adjunct Professor, Department of Statistics and Data Science, Wharton School, University of Pennsylvania (2026–present)
- Visiting Scholar, Center for Computational Mathematics, Flatiron Institute (2023–present)
- Professor, Department of Mathematical Sciences, Rutgers University–Camden (2023–present)
- Visiting Professor, Institute for Applied Mathematics, University of Bonn (2019–2021)
- Associate Professor of Mathematics, Rutgers University–Camden (2017–2023)
- Assistant Professor of Mathematics, Rutgers University–Camden (2011–2017)
- Courant Instructor and NSF Postdoctoral Fellow, New York University (2008–2011)
- Guest Scientist, Freie Universität Berlin (2008)
- Postdoctoral Scholar, California Institute of Technology (2007–2008)

Education

- Ph.D., Applied and Computational Mathematics, California Institute of Technology
- B.A., Computational and Applied Mathematics, Rice University
- B.S., Mechanical Engineering, Rice University

Third-Party Funding

- NSF DMS-2111224, *Collaborative Research: Numerical Methods for High-Dimensional Sticky Diffusions*, PI (2021–2024)
- Alexander von Humboldt Fellowship for Experienced Researchers (2019–2021)
- NSF DMS-1816378, *SPDEs and Their Numerical Solution*, PI (2018–2021)
- NSF DMS-1212058, *Schemes for Brownian Dynamics with Hydrodynamic Interactions*, PI (2012–2015)
- NSF DMS-0803095, *Mathematical Sciences Postdoctoral Research Fellowship*, PI (2008–2011)

Publications

1. Bou-Rabee, N., Mitra, S., Wibisono, A. (2026). Tail-Sensitive KL and Rényi Convergence of Unadjusted Hamiltonian Monte Carlo via One-Shot Couplings. In revision, *Ann. Appl. Probab.*
2. Bou-Rabee, N., Wang, Z. (2026). From Continuous to Discrete: A No-U-Turn Sampler for Permutations. *Quart. Appl. Math.* 84(4), 699–741.
3. Bou-Rabee, N., Schuh, K. (2026). Nonlinear Hamiltonian Monte Carlo & its Particle Approximation. In revision, *Stoch PDEs: Anal. Comp.*
4. Bou-Rabee, N., Carpenter, B., Kleppe, T. S., Liu, S. (2026). The Within-Orbit Adaptive Leapfrog No-U-Turn Sampler. *Journal of Machine Learning Research* 27, 1–64.
5. Bou-Rabee, N., Carpenter, B., Marsden, M. (2026). GIST: Gibbs self-tuning for locally adaptive Hamiltonian Monte Carlo. *Statist. Surv.* 20, 135–179.
6. Bou-Rabee, N., Eberle, A., Oberdörster, S. (2025). Accelerated Convergence in Hit-and-Run Monte Carlo and a Coordinate-free Randomized Kaczmarz Algorithm. *Electron. J. Probab.* 30, 1–28.
7. Bou-Rabee, N., Carpenter, B., Kleppe, T. S., Marsden, M. (2025). Incorporating Local Step-Size Adaptivity into the No-U-Turn Sampler using Gibbs Self Tuning. *J. Chem. Phys.* 163, 084119.
8. Bou-Rabee, N., Kleppe, T. S. (2025). Randomized Runge-Kutta-Nyström methods for unadjusted Hamiltonian and kinetic Langevin Monte Carlo. *Mathematics of Computation*, 94 (356), 2839–2865.
9. Bou-Rabee, N., Marsden, M. (2025). Unadjusted Hamiltonian MCMC with Stratified Monte Carlo Time Integration. *Ann. Appl. Probab.* 35(1), 360–392.
10. Bou-Rabee, N., Oberdörster, S. (2024). Mixing of Metropolis-Adjusted Markov Chains via Couplings: The High Acceptance Regime. *Electron. J. Probab.* 29, 1–27.

11. Bou-Rabee, N., Schuh, K. (2023). Convergence of Unadjusted Hamiltonian Monte Carlo for Mean-Field Models. *Electron. J. Probab.* 28, 1–40.
12. Bou-Rabee, N., Eberle, A. (2023). Mixing Time Guarantees for Unadjusted Hamiltonian Monte Carlo. *Bernoulli* 29(1), 75–104.
13. Bou-Rabee, N., Eberle, A. (2022). Couplings for Andersen Dynamics. *Ann. Inst. Henri Poincaré (B)* 58(2), 916–944.
14. Bou-Rabee, N., Eberle, A. (2021). Two-scale coupling for preconditioned Hamiltonian Monte Carlo in infinite dimensions. *Stoch PDEs: Anal. Comp.* 9, 207–242.
15. Rosa-Raíces, J. L., Sun, J., Bou-Rabee, N., Miller III, T. F. (2021). A generalized class of strongly stable and dimension-free T-RPMD integrators. *J. Chem. Phys.* 154, 024106.
16. Korol, R., Rosa-Raíces, J. L., Bou-Rabee, N., Miller III, T. F. (2020). Dimension-free path-integral molecular dynamics without preconditioning. *J. Chem. Phys.* 152, 104102.
17. Bou-Rabee, N., Holmes-Cerfon, M. (2020). Sticky Brownian Motion and its Numerical Solution. *SIAM Rev.* 62(1), 164–195.
18. Bou-Rabee, N., Eberle, A., Zimmer, R. (2020). Coupling and Convergence for Hamiltonian Monte Carlo. *Ann. Appl. Probab.* 30(3), 1209–1250.
19. Korol, R., Bou-Rabee, N., Miller III, T. F. (2019). Cayley modification for strongly stable path-integral and ring-polymer molecular dynamics. *J. Chem. Phys.* 151, 124103.
20. Bou-Rabee, N., Sanz-Serna, J. M. (2018). Geometric Integrators and the Hamiltonian Monte Carlo Method. *Acta Numerica* 27, 113–206.
21. Bou-Rabee, N. (2018). Spectrwm: Spectral Random Walk Method for the Numerical Solution of SPDEs. *SIAM Rev.* 60(2), 386–406.
22. Bou-Rabee, N., Vanden-Eijnden, E. (2018). Continuous-Time Random Walks for the Numerical Solution of SDEs. *Mem. Amer. Math. Soc.* 256(1228).
23. Bou-Rabee, N., Sanz-Serna, J. M. (2017). Randomized Hamiltonian Monte Carlo. *Ann. Appl. Probab.* 27, 2159–2194.
24. Bou-Rabee, N., Donev, A., Vanden-Eijnden, E. (2014). Metropolized Integration Schemes for Self-Adjoint Diffusions. *Multiscale Model. Simul.* 12, 781–831.
25. Bou-Rabee, N. (2014). Time Integrators for Molecular Dynamics. *Entropy* 16, 138–162.
26. Bou-Rabee, N., Hairer, M. (2012). Non-asymptotic mixing of the MALA algorithm. *IMA J. Numer. Anal.* 33, 80–110.
27. Bou-Rabee, N., Vanden-Eijnden, E. (2012). A patch that imparts unconditional stability to explicit integrators for Langevin-like equations. *J. Comput. Phys.* 231, 2565–2580.

28. Bou-Rabee, N., Vanden-Eijnden, E. (2010). Pathwise Accuracy and Ergodicity of Metropolized Integrators for SDEs. *Comm. Pure Appl. Math.* 63, 655–696.
29. Bou-Rabee, N., Owhadi, H. (2010). Long-Run Accuracy of Variational Integrators in the Stochastic Context. *SIAM J. Numer. Anal.* 48, 278–297.
30. Bou-Rabee, N., Owhadi, H. (2009). Stochastic Variational Integrators. *IMA J. Numer. Anal.* 29, 421–443.
31. Akhmatskaya, E., Bou-Rabee, N., Reich, S. (2009). A Comparison of GHMC with and without Momentum Flips. *J. Comput. Phys.* 228, 2256–2265.
32. Bou-Rabee, N., Marsden, J. E., Romero, L. A. (2008). Dissipation-Induced Heteroclinic Orbits in Tippe Tops. *SIAM Rev. (SIGEST)* 50, 325–344.
33. Bou-Rabee, N., Marsden, J. E. (2008). Hamilton-Pontryagin Integrators on Lie Groups: Introduction and Structure-Preserving Properties. *Found. Comput. Math.* 9, 197–219.
34. Bou-Rabee, N., Chossat, P. (2005). The Motion of the Spherical Pendulum Subjected to a $\mathbf{D}_n$ Symmetric Perturbation. *SIAM J. Appl. Dyn. Syst.* 4, 1140–1158.
35. Bou-Rabee, N., Marsden, J. E., Romero, L. A. (2005). A Geometric Treatment of Jellett’s Egg. *Z. Angew. Math. Mech.* 85, 618–642.
36. Bou-Rabee, N., Marsden, J. E., Romero, L. A. (2004). Tippe Top Inversion as a Dissipation-Induced Instability. *SIAM J. Appl. Dyn. Syst.* 3, 352–377.
37. Bou-Rabee, N., Romero, L. A., Salinger, A. G. (2002). A Multi-Parameter, Numerical Stability Analysis of a Tubular Cantilever Conveying Fluid. *SIAM J. Appl. Dyn. Syst.* 1, 190–214.

Invited Talks & Academic Activities

Plenary & Distinguished Lectures

- SIAM Conference on Uncertainty Quantification (Plenary Speaker), March 2026

Workshops, Conferences, & Seminar Invitations (Selected)

- University of Florida, *Fast and Curious III: Mixing in Gainesville*, January 2027
- University of Pennsylvania, *Wharton Statistics and Data Science Seminar*, October 2026
- FoCM 2026, *Workshop on Stochastic Computation*, Vienna, July 2026 (co-organizer)
- Bonn University, *CRC 1720 Colloquium*, June 2026
- ETH Zürich, *FIM Workshop on “Scalable MCMC Sampling”*, June 2026
- Columbia University, *Applied Probability Seminar*, October 2025
- University of Toronto, *Fast and Curious II: MCMC in Action*, September 2025

- Illinois Institute of Technology, *Monte Carlo Methods and Applications*, August 2025
- University of Nottingham, *Milstein's Method: 50 Years On*, July 2025
- Stanford University, *Applied Mathematics Seminar*, April 2025
- Courant Institute (NYU), *Computational Mathematics Seminar*, April 2025
- Temple University, *Penn/Temple Probability Seminar*, December 2024
- International Monte Carlo Seminar, October 2024
- Yale University, *Institute for Foundations of Data Science*, October 2024
- Bernoulli/IMS World Congress, Bochum, August 2024
- Sorbonne University, *Monte Carlo Methods and Applications*, June 2023
- University of Delaware, *Probability Seminar*, March 2023
- Flatiron Institute, *CCM Colloquium*, February 2023
- Maxwell Institute (Edinburgh), *Probability Seminar*, January 2022
- KTH Royal Institute of Technology, *Probability and Statistics Seminar*, December 2021
- SIAM Conference on Mathematical Aspects of Materials Science, May 2021
- Oberwolfach Workshop, *Geometric Numerical Integration*, March 2021
- RWTH Aachen, *Mathematics Colloquium*, March 2021
- Bonn University, *Hausdorff School on "MCMC: Recent developments and new connections"*, September 2020 (co-organizer)
- University of Oxford, *Computational Statistics & Machine Learning Seminar*, June 2020
- Caltech, *Workshop on Inverse Problems*, February 2020
- University of Florida, *Bayes Comp 2020*, January 2020 (organized both a contributed and an invited session)

Professional Service & Leadership

- Organizer, *Mathematics Seminar Series* at Rutgers University–Camden (2017–2019, 2022). Invited speakers included Yuansi Chen (Duke), Sonja Cox (Amsterdam), Andreas Eberle (Bonn), Murat Erdogdu (Toronto), Charles Epstein (Penn), Miranda Holmes-Cerfon (NYU), Lina Meinicke (UCI), Katherine Newhall (UNC), Qian Qin (Minnesota), Grant Rotskoff (Stanford), Jesús Sanz-Serna (UC3M), Aaron Smith (Ottawa), Thomas F. Miller III (Caltech), Santosh Vempala (Georgia Tech), Lihan Wang (CMU), and Guanyang Wang (Rutgers).

Mini-Courses & Summer Schools

- Co-organizer, Hausdorff School on MCMC (2020)
- Lecturer, SIAM Gene Golub Summer School, *Spectrum for SPDEs* (2016)
- Lecturer, Valladolid MCMC School, *MCMC-based Integrators for SDEs* (2015)

Honors and Awards

- Chancellor's Award for Outstanding Research, Rutgers University–Camden (2022)
- Editor's Pick, *Journal of Chemical Physics* (2019, 2020)
- Humboldt Fellowship for Experienced Researchers (2019–2021)
- Editor's Choice, *IMA J. Numer. Anal.* (2009)
- NSF Mathematical Sciences Postdoctoral Fellowship (2008–2011)
- SIGEST Reprint, *SIAM Review* (2008)
- ASCIT Teaching Award, Caltech (2007)
- Caltech GSC Teaching and Mentoring Award (2005)
- DOE Computational Science Graduate Fellowship (2002–2006)
- Outstanding Sandia Labs Student Intern (2001)
- Rice Engineering Alumni Award in CAAM (2001)

Mentoring & Supervision

- **Ph.D. Students:** Milo Marsden (Stanford), Jorge Rosa-Raíces (Caltech), Stefan Oberdörster (Bonn), Siddarth Mitra (Yale), Katharina Schuh (Bonn), Roy Schieven (Amsterdam), and Raphael Zimmer (Bonn).
- **M.S. Students:** Solomon Jacobs, Sebastian Jonas Schmidt, Zelin Ren, Stefan Oberdörster, Mike Schäfer (all University of Bonn).

Teaching (Selected)

- Rutgers–Camden: Probability & Stochastic Processes; Markov Chain Monte Carlo.
- Wharton School: Probability (STAT 4300), Mathematical Statistics (STAT 4320).

Editorial Activity

- Reviewer for: *QAM*, *EJP*, *PNAS*, *AAP*, *MOR*, *CMP*, *AIHP*, *ECP*, *Bernoulli*, *AOS*, *SS*, *JRSS-B*, *SPDE*, *JMLR*, *JUQ*, *FoCM*, *CPAM*, *SPA*, *JCGS*, *SJS*, *PRSA*, *MCOM*, *SISC*, *SINUM*, *SIAP*, *IMAJNA*, *JCP*, etc.

- Grant reviewer for the US National Science Foundation and the European Research Council

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