Brian Van Koten

Contact Information

The University of Massachusetts, Amherst
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Education

University of Minnesota, Twin Cities, Minneapolis, Minnesota, USA

Ph.D., Mathematics, 2012.

Advisor: Mitchell Luskin
Thesis Title: Development and analysis of the blended energy-based quasicontinuum method

M.S., Mathematics, 2011.

Lewis and Clark College, Portland, Oregon, USA

B.A., Mathematics and Physics, *summa cum laude*, 2007.

Employment

Associate Professor, The University of Massachusetts, Amherst, Fall 2025-present

Assistant Professor, The University of Massachusetts, Amherst, Fall 2018-Summer 2025

William H. Kruskal Instructor, The University of Chicago, Fall 2015-Summer 2018

Postdoctoral Scholar, The University of Chicago, Winter 2014-Summer 2015

RTG Assistant Professor, University of California, Los Angeles, Summer 2012-Fall 2013

Research Assistant, University of Minnesota, Twin Cities, Fall 2009-Spring 2012

Teaching Assistant, University of Minnesota, Twin Cities, Fall 2007-Spring 2009

External Funding

NSF DMS-2012207: Efficient Monte Carlo Methods for Nonequilibrium Statistical Physics, $200,000, 2020-2023, sole PI.

Teaching

The University of Massachusetts, Amherst, Department of Mathematics and Statistcs

Probability and Stochastic Processes

- Math 606/Stat 697U, graduate stochastic processes: Spring 2019, Spring 2026
- Math 605, graduate probability and measure theory: Fall 2018, Fall 2025
- Stat 315/515, undergraduate probability: Fall 2021, Spring 2022, Fall 2022, Spring 2022 (course chair)

Scientific Computing and Numerical Analysis

- Math 651, graduate numerical analysis: Fall 2019, Fall 2020, Fall 2023, Fall 2024
- Math 652, graduate numerical partial differential equations: Spring 2020, Spring 2021, Spring 2024, Spring 2025
- Math 551, undergraduate scientific computing: Spring 2023, Spring 2024, Fall 2025

Linear Algebra

- Math 545, second undergraduate course in linear algebra: Spring 2025

Data Science

- Taught summer course in data science for high school students during Summer 2020, 2021, and 2022. Students awarded credit at the University of Massachusetts, Amherst.

The University of Chicago, Department of Statistics

- Taught Stat 23400, introduction to statistics, Spring 2017
- Developed and taught introductory course on numerical analysis for students in statistics, with Prof. John Lafferty, Winter 2017
- Developed and taught course on numerical ordinary differential equations, Fall 2015

University of California, Los Angeles, Department of Mathematics

- Math 31B, single variable calculus: Fall 2013
- Math 32A, multi-variable calculus: Fall 2012
- Math 133, undergraduate Fourier analysis: Spring 2013
- Math 135, undergraduate ordinary differential equations: Winter 2013

Mentoring

Fall 2021-Spring 2025: Mentored Visiting Assistant Professor Gabriel Earle at University of Massachusetts, Amherst.

Winter 2014-Spring 2018: Mentored and worked in collaboration with graduate students in chemistry at The University of Chicago.

Have advised one undergraduate honors thesis and five independent study projects at University of Massachusetts, Amherst.

Research Interests

Molecular simulation and applications in chemistry and materials science.

Multiscale modeling, including methods for the simulation of defects in crystalline materials and the analysis and development of continuum models.

Variance reduction methods for Markov chain Monte Carlo with applications to Bayesian statistics and computational statistical physics.

Sampling and analysis of rare events in physical systems.

Scientific machine learning, including the development of efficient sampling methods based on neural surrogate models.

Multigrid methods and analogous sampling methods based on coarse-grained or multiscale surrogate models.

Numerical methods for finding saddle points and applications to computational statistical physics.

Computer Skills

User of C, Julia, and Python (PyTorch, NumPy, Numba)

Have taught statistics courses using R and Python

Invited Presentations

SIAM Conference on Uncertainty Quantification
23 - 26 March 2026, Minneapolis, MN
Delivered minisymposium lecture entitled *Relative Entropy Methods for the Approximation of Reactive Trajectories*.

The Third Joint SIAM/CAIMS Annual Meetings
28 July - 1 August 2025, Montreal, QC, Canada
Organized minisymposium and delivered minisymposium lecture entitled *Relative Entropy Methods for Computing Committor Functions*.

SIAM Conference on Materials Science
19-23 May 2024, Pittsburgh, PA
Organized minisymposium.

University of North Carolina Charlotte, Department of Mathematics, Colloquium
27 March 2024, Charlotte, NC
Delivered seminar lecture entitled *Importance Sampling of Transition Paths*

SIAM New York, New Jersey, and Pennsylvania Sectional Meeting
10-12 October 2023, Newark, NJ
Delivered minisymposium lecture entitled *Sampling Molecular Systems Using Multigrid*

17th U.S. National Congress on Computational Mechanics
23-27 July 2023, Albuquerque, NM
Delivered minisymposium lecture entitled *Sampling Molecular Systems Using Multigrid*

SIAM Mathematics of Data Science
20 September 2022, San Diego, CA
Delivered minisymposium lecture entitled *Sampling Molecular Systems Using Multigrid*

SIAM Annual Meeting
7 July 2022, Pittsburgh, PA
Organized minisymposium and delivered minisymposium lecture entitled *Error Bars for Free Energy Calculations*

Flatiron Institute CCM Colloquium
20 April 2021, New York City, NY
Delivered lecture entitled *Sampling Molecular Systems Using Multigrid*

SIAM Annual Meeting
19 July 2021, Virtual
Organized minisymposium and delivered minisymposium lecture entitled *Efficient Calculation of Nonequilibrium Steady-States*

IPAM: Complex High-Dimensional Energy Landscapes Reunion Conference II
6 June 2021, Lake Arrowhead, CA
Delivered invited lecture entitled *Efficient Calculation of Nonequilibrium Steady-States*

SIAM Conference on Computational Science and Engineering
1 March 2021, Virtual
Delivered minisymposium lecture entitled *Efficient Calculation of Nonequilibrium Steady-States*

Department Colloquium, Colorado State University
11 November 2019, Fort Collins, CO
Delivered lecture entitled *Efficient Monte Carlo for (Equilibrium and) Nonequilibrium Systems*

ICIAM 2019
15-19 July 2019, Valencia, Spain
Delivered lecture entitled *Stratified Markov chain Monte Carlo*

ICERM Workshop: Mathematical optimization of systems impacted by rare, high-impact random events
24-28 June 2019, Providence, RI
Delivered lecture entitled *Computing rare event probabilites by stratified Markov chain Monte Carlo*

CIB-CECAM Workshop: Computational mathematics for model reduction and predictive modelling in molecular and complex systems
21-29 May 2019, Lausanne, Switzerland
Delivered lecture entitled *Stratified Markov chain Monte Carlo*

RESIM 2018
29-31 August 2019, Stockholm, Sweden
Delivered presentation entitled *Stratification and Markov chain Monte Carlo*

SIAM Annual Meeting
9-13 July 2018, Portland, OR
Delivered minisymposium lecture entitled *Stability and convergence of the String Method*

Modeling Seminar, University of Arizona
30 November 2017, Tucson, AZ
Delivered lecture entitled *Stratification and Markov chain Monte Carlo*

IPAM Workshop: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces
19 October 2017, Los Angeles, CA
Delivered invited lecture entitled *Stability and convergence of the string method*

LANS Seminar, Argonne National Laboratory
17 May 2017, Lemont, IL
Delivered lecture entitled *Stratification of Markov chain Monte Carlo*

Mathematics Department Seminar, University of North Carolina, Charlotte
2 December 2016, Charlotte, NC
Delivered lecture entitled *Stratification of Markov chain Monte Carlo*

SIAM Conference on Mathematical Aspects of Materials Science
8-12 May 2016, Philadelphia, PA
Delivered minisymposium lecture entitled *Analysis and optimization of stratified sampling*

Applied Math Seminar, Colorado State University
5 May 2016, Fort Collins, CO
Delivered lecture entitled *Analysis of stratified Markov chain Monte Carlo*

SIAM Conference on Uncertainty Quantification
5-8 April 2016, Lausanne, Switzerland
Delivered minisymposium lecture entitled *Analysis and optimization of stratified sampling*

Séminaire de Mathématiques Appliquées et de Calcul Scientifique du CERMICS, École des Ponts ParisTech
27 January 2016, Champs-sur-Marne, France
Delivered lecture entitled *Analysis of stratified sampling*

Scientific and Statistical Computing Seminar, The University of Chicago
21 May 2015, Chicago, IL
Delivered lecture entitled *Stratified sampling in computational statistical mechanics*

BIRS Workshop: Multiscale Models of Crystal Defects
21-16 September 2014, Banff, Canada
Delivered lecture entitled *Analysis of an atomistic/continuum model of a screw dislocation*

SIAM Conference on Mathematical Aspects of Materials Science
9-13 June 2013, Philadelphia, PA
Delivered minisymposium lecture entitled *Numerical analysis of a method for the simulation of defects in crystalline materials*

M. Ortiz Group Meeting, CalTech
30 April 2013, Pasadena, CA
Delivered lecture entitled *Numerical analysis of a method for the simulation of defects in crystalline materials*

Applied Math/PDE Seminar, University of California, Santa Barbara
7 December 2012, Santa Barbara, CA
Delivered lecture entitled *The Blended Quasicontinuum Method for the simulation of defects in crystals*

Applied Math Colloquium, University of California, Los Angeles
7 November 2012, Los Angeles, CA
Delivered lecture entitled *Numerical analysis of a method for the simulation of defects in crystalline materials*

SIAM Annual Meeting
9-13 July 2012, Minneapolis, MN
Delivered minisymposium lecture entitled *Energy-based Blended Quasicontinuum Methods*

NSF PIRE Summer School: New Frontiers in Multiscale Analysis and Computing for Materials
21-29 June 2012, Minneapolis, MN
Delivered invited lecture entitled *New continuum models of multi-lattices and their application in atomistic-to-continuum coupling*

PIRE/OxMos Workshop on Pattern Formation and Multiscale Phenomena in Materials
26-28 September 2011, Oxford, UK
Delivered invited lecture entitled *Energy-based Blended Quasicontinuum Methods*

US National Congress on Computational Mechanics
25-28 July 2011, Minneapolis, MN
Delivered minisymposium lecture entitled *Energy-based Blended Quasicontinuum Methods*

ACMAC Workshop on Coarse-graining of Many-body Systems
27 June - 1 July 2011, Heraklion, Greece
Presented poster entitled *Blended Quasicontinuum Energies*

Invited Visit

Warwick Mathematics Institute
29 September - 22 October 2011, University of Warwick, UK
Visited Warwick to collaborate with Prof. Christoph Ortner

Conference Organization

Organized minisymposia at SIAM AN21, AN22, MS24, and AN25.

Academic Service and Organizations

Member of SIAM

Referee for various journals, including most recently Journal of Computational Physics, SIAM/ASA Journal on Uncertainty Quantification, SIAM Journal on Multiscale Modeling and Simulation, Multiscale Modelling and Simulation, IMA Journal of Numerical Analysis, Statistics and Probability Letters, and Chemical Physics Letters

Publications

[1] G. Earle and B. Van Koten. Relative entropy methods for the approximation of reactive trajectories. *accepted for publication in SIAM-ASA Journal On Uncertainty Quantification*, 2026. arXiv:2502.04605.

[2] G. Earle and B. Van Koten. Aggregation methods for computing steady-states in statistical physics. *Multiscale Model. Simul.*, 21(3):1170–1209, 2023. arXiv:2209.11164.

[3] X. S. Li, B. Van Koten, A. R. Dinner, and E. H. Thiede. Understanding the sources of error in mbar through asymptotic analysis. *The Journal of Chemical Physics*, 158(21):214107, June 2023. arXiv:2203.01227.

[4] A. R. Dinner, E. H. Thiede, B. Van Koten, and J. Weare. Stratification as a general variance reduction method for Markov chain Monte Carlo. *SIAM-ASA Journal On Uncertainty Quantification*, 8(3):1139–1188, 2020. ISSN: 2166-2525. arXiv:1705.08445.

[5] B. Van Koten and M. Luskin. Stability and convergence of the string method for computing minimum energy paths. *Multiscale Model. Simul.*, 17(2):873–898, 2019. arXiv:1807.06094.

[6] A. R. Dinner, J. C. Mattingly, J. O. B. Tempkin, B. Van Koten, and J. Weare. Trajectory stratification of stochastic dynamics. *SIAM Rev.*, 60(4):909–938, 2018. arXiv:1610.09426.

[7] D. Olson, X. Li, C. Ortner, and B. Van Koten. Force-based atomistic/continuum blending for multilattices. *Numer. Math.*, 140(3):703–754, 2018. arXiv:1611.05935.

[8] X. H. Li, C. Ortner, A. V. Shapeev, and B. Van Koten. Analysis of blended atomistic/continuum hybrid methods. *Numerische Mathematik*, 134(2):275–326, 2016. arXiv:1404.4878.

[9] E. H. Thiede, B. Van Koten, J. Weare, and A. R. Dinner. Eigenvector method for umbrella sampling enables error analysis. *The Journal of Chemical Physics*, 145(8), 084115, 2016. arXiv:1603.04505.

[10] E. Thiede, B. Van Koten, and J. Weare. Sharp entrywise perturbation bounds for Markov chains. *SIAM Journal on Matrix Analysis and Applications*, 36(3):917–941, 2015. arXiv:1410.1431.

[11] M. Luskin, C. Ortner, and B. Van Koten. Formulation and optimization of the energy-based blended quasicontinuum method. *Computer Methods in Applied Mechanics and Engineering*, 253:160–168, 2013. arXiv:1112.2377.

[12] B. Van Koten and C. Ortner. Symmetries of 2-lattices and second order accuracy of the Cauchy–Born model. *Multiscale Modeling & Simulation*, 11(2):615–634, 2013. arXiv:1012.6031.

[13] B. Van Koten, X. H. Li, M. Luskin, and C. Ortner. A computational and theoretical investigation of the accuracy of quasicontinuum methods. In I. Graham, T. Hou, O. Lakkis, and R. Scheichl, editors, *Numerical Analysis of Multiscale Problems*. Volume 83, Lect. Notes Comput. Sci. Eng. Springer, 2012. arXiv:1012.6031.

[14] B. Van Koten and M. Luskin. Analysis of energy-based blended quasi-continuum approximations. *SIAM Journal on Numerical Analysis*, 49(5):2182–2209, 2011. arXiv:1008.2138.

[15] R. Held, I. Stavrov, and B. VanKoten. (Semi-)Riemannian geometry of (para-)octonionic projective planes. *Differential Geometry and its Applications*, 27(4):464–481, 2009. arXiv:0702631.

[16] J. Hardin, A. Mitani, L. Hicks, and B. VanKoten. A robust measure of correlation between two genes on a microarray. *BMC Bioinformatics*, 8(1):220, 2007.