

Brian Van Koten

Contact Information

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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

Assistant Professor, The University of Massachusetts, Amherst, Fall 2018-present

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 Statistics

Fall 2021: Stat 515, undergraduate probability

Summer 2020 and Summer 2021: Stat 190F, summer course in data science for high school students

Spring 2020 and Spring 2021: Math 652, graduate introduction to numerical analysis

Fall 2019 and Fall 2020: Math 651, graduate introduction to numerical analysis

Spring 2019: Math 697U, graduate stochastic processes

Fall 2018: Stat 605, graduate introduction to probability and measure theory

The University of Chicago, Department of Statistics

Winter 2014-present: Working in collaboration with graduate students in chemistry

Spring 2017: Taught Stat 23400, introduction to statistics

Winter 2017: With Prof. John Lafferty, developed and taught introductory course on numerical analysis for students in statistics and the sciences

Fall 2015: Developed and taught course on numerical integration of ordinary differential equations

University of California, Los Angeles, Department of Mathematics

Fall 2013: Math 31B, single variable calculus

Spring 2013: Math 133, undergraduate course in Fourier analysis

Winter 2013: Math 135, undergraduate course in ordinary differential equations

Fall 2012: Math 32A, multi-variable calculus

For each course, I wrote and delivered lectures, supervised teaching assistants, and wrote all exams.

University of Minnesota, Twin Cities, School of Mathematics

Summer 2011: With Prof. Mitchell Luskin, supervised undergraduate research project

Fall 2007-Spring 2009: Teaching assistant for calculus and for an introductory mathematics course for students in the humanities

Research Interests

Molecular simulation and applications in chemistry and materials science.

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

Markov chain Monte Carlo and applications in statistics and science.

Machine learning and applications to molecular simulation.

Sampling rare events.

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

Computer Skills

User of C, OpenMP, Julia, MATLAB, and Python

Have taught statistics courses using R

Invited Presentations

SIAM Annual Meeting

19 July 2021, Virtual

Organized minisymposium and delivered 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 probabilities 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

Academic Service and Organizations

Member of SIAM

Referee for journals in applied mathematics and engineering, including most recently 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

Organized minisymposium at SIAM AN21

Publications

In progress

- [1] G. Earle and B. Van Koten. Efficiency of iterative aggregation/disaggregation methods for computing nonequilibrium steady-states. *In progress*.
- [2] X. S. Li, B. Van Koten, A. R. Dinner, J. Weare, and E. H. Thiede. Asymptotic error analysis of the mbar equations. *In progress, draft available on request*.

Published

- [3] 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](https://arxiv.org/abs/1705.08445).
- [4] 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](https://arxiv.org/abs/1807.06094).

- [5] 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](#).
- [6] D. Olson, X. Li, C. Ortner, and B. Van Koten. Force-based atomistic/continuum blending for multi-lattices. *Numer. Math.*, 140(3):703–754, 2018. [arXiv:1611.05935](#).
- [7] 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](#).
- [8] 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](#).
- [9] 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](#).
- [10] 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](#).
- [11] 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](#).
- [12] 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](#).
- [13] 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](#).
- [14] 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](#).
- [15] 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.