Samuel A. Isaacson - Short CV

CONTACT INFORMATION

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CURRENT RESEARCH INTERESTS

My research interests are in the areas of numerical analysis, mathematical biology, and mathematical physics, with an emphasis on the development and the numerical analysis of methods for studying problems in cell biology. Recent research areas have included understanding the rigorous coarse-grained limits of particle stochastic reaction-diffusion models, developing accurate and efficient numerical methods for the simulation of such models within realistic cellular geometries, and the application of particle reactive transport models to the study of cell signaling, T cell signaling, and antibody-antigen interactions. For the latter I have helped to develop new combined experimental, modeling, and inference approaches to better estimate from experimental data the biophysical parameters that drive antibody-antigen and ligand-receptor interactions.

APPOINTMENTS

Department of Mathematics and Statistics, Boston University
Boston, MA USA

Professor of Mathematics (March 2021 - Present)
Associate Professor of Mathematics (May 2014 - February 2021)
Assistant Professor of Mathematics (Fall 2008 - May 2014)

- Member, Graduate Program in Bioinformatics (December 2011 - Present)
- Faculty Affiliate, Hariri Institute for Computing and Computational Science & Engineering (September 2011 - Present)
- Member, Center for Biodynamics (Spring 2009 - Summer 2011)

Isaac Newton Institute for Mathematical Sciences, University of Cambridge
Cambridge, UK

Simons Foundation Fellow of the Isaac Newton Institute (January 2016 - June 2016)

Oxford University, Mathematical Institute
Oxford, UK

Academic Visitor (February 2015 - March 2015)

Department of Anatomy, University of California, San Francisco
San Francisco, CA USA

Visiting Associate Professor (September 2014 - January 2015)

National Center for X-ray Tomography, Lawrence Berkeley National Laboratory
Berkeley, CA USA

Visiting Affiliate (September 2014 - January 2015)

Biomathematics Research Group, Department of Mathematics, University of Utah
Salt Lake City, Utah USA

Postdoctoral Fellow (Fall 2005 - Summer 2008)

EDUCATION

Courant Institute of Mathematical Sciences, New York University
New York, New York USA

Ph.D. in Mathematics (September 2005)

- Dissertation Topic: "A Stochastic Reaction–Diffusion Method for Studying the Control of Gene Expression in Eukaryotic Cells"

- Adviser: Charles S. Peskin

MS Mathematics, 2001

Brown University
Providence, Rhode Island USA

BS Applied Mathematics–Computer Science, May 2000
Graduated *Magna Cum Laude* with 4.0 GPA

HONORS AND AWARDS

2025	Nature Communications paper selected as an Editor's Highlight
2016	Simons Foundation Fellowship of the Isaac Newton Institute for Mathematical Sciences
2013–2018	NSF CAREER Award Recipient, DMS, Computational Mathematics
2005	Moses A Greenfield Research Award for Outstanding Interdisciplinary Studies, Courant Institute of Mathematical Sciences
2000–2005	MacCracken Fellow, Courant Institute of Mathematical Sciences
2000	Rohn Truell Premium Award in Applied Mathematics, Division of Applied Mathematics, Brown University
2000	*Magna Cum Laude*, Brown University
2000	College Honors, Brown University
2000	Sigma Xi
1996–2000	Theodore Jaffe' 32 I/II/III National Scholarships, Brown University

FUNDED GRANTS

Army Research Office, W911NF2510078, PI for: *Coarse-grained Limits for Agent-Based and Particle Models of Interacting Populations*, $578,638 (total award for both PIs) (2025-2029).

NSF - DMS, Emerging Mathematics in Biology, 2325185, PI for: *Collaborative Research: Discovery and calibration of stochastic chemical reaction network models*, SAI award: $119,728 (total award for both PIs: $494,728) (2023–2026).

Chan Zuckerberg Initiative, 2021-237457 (5022), PI for: *Enhancing the open source SciML stack for clinical trial simulations (EOSS4)*, $286,000.00 (total award for both PIs) (2021-2024).

Wellcome Trust, 223770/Z/21/Z, PI for: *Accelerating Drug Discovery with Symbolic-Numerics in SciML*, $140,453 (total award for both PIs) (2021-2022).

Army Research Office, W911NF2010244, PI for: *Coarse-Grained Limits of Particle-Based Stochastic Reaction-Diffusion Models*, $480,318.00 (total award for both PIs) (2020-2024).

NSF - DMS, DMS/NIGMS Initiative, 1902854, PI for: *Collaborative Research: Computational Methods for Understanding the Influence of Cellular Geometry and Substructure on Signaling*, SAI award: $699,929 (total award for both PIs: $1,149,929) (2019-2023).

NSF - DMS, Mathematical Biology, 1548520, PI for: *U.S. Participation in Newton Institute Program on Stochastic Dynamical Systems in Biology: Numerical Methods and Applications*, $23,530.00 (2016).

NSF - DMS, Computational Mathematics, 1255408, PI for Project: *CAREER: Numerical Methods for Stochastic Reaction-Diffusion Equations*, $434,043 (2013–2019).

NSF - DMS, Mathematical Biology, 0920886, PI for Project: *Multiscale Modeling of Subcellular Structure and its Effects on Gene Expression and Regulation*, $272,515 (2009–2013).

NIH - NIGMS, P50GM071558, Systems Biology Center New York, Center Member and Consultant for Subproject: *Explicit 3D Models of the Spatiotemporal Effects of the Regulatory Loops in cAMP Dependent Heart Failure*. Mount Sinai School of Medicine, NY, NY. Approximate Center Funding: $13,000,000, Approximate Project Funding: $1,000,000 (2007–2012).

PUBLICATIONS IN REVIEW

S. A. Isaacson, Q. Liu, K. Spiliopoulos, and C. Yao, *A Macroscopically Consistent Reactive Langevin Dynamics Model*, Submitted (2025).

PEER-REVIEWED PUBLICATIONS

A. Huhn, D. Nissley, D. B. Wilson, M. Kutuzov, R. Donat, T. K. Tan, Y. Zhang, M. I. Barton, C. Liu, W. Dejnirattisai, P. Supasa, J. Mongkolsapaya, A. Townsend, W. James, G. Screaton, P. Anton van der Merwe, C. M. Deane, S. A. Isaacson, and O. Dushek, *The molecular reach of antibodies crucially underpins their viral neutralisation capacity*, Nature Communications, 16(338), 18pp (2025).

M. Heldman, S. A. Isaacson, Q. Liu, and K. Spiliopoulos, *Mean field limits of particle-based stochastic reaction-drift-diffusion models*, Nonlinearity, 38(2), 55pp (2025).

S. A. Isaacson and Y. Zhang, *An Unstructured Mesh Reaction-Drift-Diffusion Master Equation with Reversible Reactions*, Bull Math Biol, 87(13), 41pp (2025).

G. Zagatti, S. A. Isaacson, C. Rackauckas, V. Ilin, S.K. Ng, and S. Bressan, *Extending JumpProcess.jl for fast point process simulation with time-varying intensities*, The Proceedings of the JuliaCon Conferences, 6 (58), 13 pp (2024).

M. Heldman, S. A. Isaacson, J. Ma, and K. Spiliopoulos, *Fluctuation analysis for particle-based stochastic reaction-diffusion models*, Stochastic Process. Appl., 167 (104234), 61 pp (2024).

T. Loman, Y. Ma, V. Ilin, S. Gowda, N. Korsbo, N. Yewale, C. V. Rackauckas, and S. A. Isaacson, *Catalyst: Fast and flexible modeling of reaction networks*, PLOS Computational Biology 19(10): e1011530 (2023).

S. A. Isaacson and Y. Zhang, *Detailed Balance for Particle Models of Reversible Reactions in Bounded Domains*, J. Chem. Phys., 156, 204105 (19 pp) (2022).

J. Goyette, D. Depoil, Z. Yang, S. A. Isaacson, J. Allard, P. Anton van der Merwe, K. Gaus, M. L. Dustin, and O. Dushek, *Dephosphorylation accelerates the dissociation of ZAP70 from the T cell receptor*, PNAS, 119(9), e2116815119 (2022).

S. A. Isaacson, J. Ma, and K. Spiliopoulos, *Mean-field Limits of Particle-Based Stochastic Reaction-Diffusion Models*, SIAM J. Math. Anal., 54(1), 453511 (2022).

S. A. Isaacson, J. Ma, and K. Spiliopoulos, *How reaction-diffusion PDEs approximate the large-population limit of stochastic particle models*, SIAM J. Applied Math, 81(6), 2622–2657 (2021).

J. Wang, C. Belta, S. A. Isaacson, *How Retroactivity Affects the Behavior of Incoherent Feed-Forward Loops*, iScience, Vol. 23, No. 12, 101779 (16pp) (2020).

J. Ma, M. Do, M. A. Le Gros, C. S. Peskin, C. A. Larabell, Y. Mori, and S A. Isaacson, *Strong Intracellular Signal Inactivation Produces Sharper and more Robust Signaling from Cell Membrane to Nucleus*, PLOS Comp. Bio., Vol. 16, No. 11, 19 pp (2020).

Y. Zhang, L. Clemens, J. Goyette, J. Allard, O. Dushek and S. A. Isaacson, *The Influence of Molecular Reach and Diffusivity on the Efficacy of Membrane-Confined Reactions*, Biophysical Journal, Vol. 117, No. 7, pp 1189-1201 (2019).

J. Wang, S. A. Isaacson and C. Belta, *Modeling Genetic Circuit Behavior in Transiently Transfected Mammalian Cells*, ACS Synthetic Biology, Vol. 8, No. 4, pp 697-707 (2019).

J. Wang, S. A. Isaacson and C. Belta, *Predictions of Genetic Circuit Behavior Based on Modular Composition in Transiently Transfected Mammalian Cells*, Proceedings of the IEEE Life Sciences Conference,

Montreal, Canada, 10.1109/LSC.2018.8572174 (4 pp) (2018).

S. A. Isaacson and Y. Zhang, *An Unstructured Mesh Convergent Reaction-Diffusion Master Equation for Reversible Reactions*, J. Comp. Phys., Vol. 374, pp 954-983 (2018).

J. Goyette, C. S. Salas, N. Coker-Gordon, M. Bridge, S. A. Isaacson, J. Allard, and O. Dushek, *Biophysical assay for tethered signaling reactions reveals tether-controlled activity for the phosphatase SHP-1*, Science Advances, Vol 3, No. 3, e1601692 (14 pp) (2017).

S. A. Isaacson, A. J. Mauro, and J. Newby, *Uniform Asymptotic Approximation of Diffusion to a Small Target: Generalized Reaction Models*, Phys. Rev. E, Vol. 94, No. 4, 042414 (17 pp) (2016).

S. J. Chapman, R. Erban, and S. A. Isaacson, *Reactive Boundary Conditions as Limits of Interaction Potentials for Brownian and Langevin Dynamics*, SIAM Journal on Applied Mathematics, Vol. 76, No. 1, pp 368-390 (2016).

M. Do, S. A. Isaacson, G. McDermott, M. A. Le Gros, and C. A. Larabell, *Imaging and Characterizing Cells using Tomography*, Arch. Biochem. and Biophys., Vol. 581, pp 111-121 (2015).

I. C. Agbanusi and S. A. Isaacson, *A Comparison of Bimolecular Reaction Models for Stochastic Reaction-Diffusion Systems*, Bulletin of Mathematical Biology, Vol. 76. No. 4, pp 922-946 (2014).

A. J. Mauro, J. K. Sigurdsson, J. Shrake, P. J. Atzberger, and S. A. Isaacson, *A First-Passage Kinetic Monte Carlo Method for Reaction-Drift-Diffusion Processes*, J. Computational Physics, Vol. 259, pp 536-567 (2014).

S. A. Isaacson, C. A. Larabell, M. A. Le Gros, D. M. McQueen, and C. S. Peskin, *The Influence of Spatial Variation in Chromatin Density Determined by X-ray Tomograms on the Time to Find DNA Binding Sites*, Bulletin of Mathematical Biology, Vol. 75, No. 11, pp 2093-2117 (2013).

S. A. Isaacson, *A Convergent Reaction-Diffusion Master Equation*, J. Chem. Phys., Vol. 139, No. 5, 054101 (12 pp) (2013).

S. A. Isaacson and J. Newby, *Uniform Asymptotic Approximation of Diffusion to a Small Target*, Phys. Rev. E, Vol. 88, No. 1, 012820 (13 pp) (2013).

S. A. Isaacson and R. M. Kirby, *Numerical Solution of Linear Volterra Integral Equations of the Second Kind with Sharp Gradients*, J. Comput. Appl. Math., Vol. 235, No. 14, pp 4283-4301 (2011).

S. A. Isaacson, D. M. McQueen, and C. S. Peskin, *The Influence of Volume Exclusion by Chromatin on the Time Required to Find Specific DNA Binding Sites by Diffusion*, Proceedings of the National Academy of Sciences, Vol. 108, No. 9, pp 3815-3820 (2011).

S. A. Isaacson and D. Isaacson, *Reaction-Diffusion Master Equation, Diffusion-Limited Reactions, and Singular Potentials*, Phys. Rev. E, Vol. 80, No. 6, 066106 (9 pp) (2009).

S. A. Isaacson, *The Reaction-Diffusion Master Equation as an Asymptotic Approximation of Diffusion to a Small Target*, SIAM J. Appl. Math., Vol. 70, No. 1, pp 77-111 (2009).

P. J. Atzberger, S. A. Isaacson, and C. S. Peskin, *A Microfluidic Pumping Mechanism Driven by Non-Equilibrium Osmotic Effects*, Physica D, Vol. 238, No. 14, pp 1168-1179 (2009).

S. A. Isaacson, *Relationship Between the Reaction-Diffusion Master Equation and Particle Tracking Models*, J. Phys. A: Math. Theor., Vol. 41, No. 6, 065003 (15 pp) (2008).

S. A. Isaacson and C. S. Peskin, *Incorporating Diffusion in Complex Geometries into Stochastic Chemical Kinetics Simulations*, SIAM J. Sci. Comput., Vol. 28, No. 1, pp 47-74 (2006).

S. A. Isaacson, *Stochastic Reaction-Diffusion Methods for Modeling Gene Expression and Spatially Distributed Chemical Kinetics*, Ph.D. dissertation, New York University, United States – New York (2005).

CONTRIBUTED PUBLICATIONS

S. T. Johnston, C. N. Angstmann, S. N.V. Arjunan, C. H. L. Beentjes, A. Coulier, S. A. Isaacson, A. A. Khan, K. L Lipkow, and S. S. Andrews, *Accurate particle-based reaction algorithms for fixed timestep simulators*, 2018 MATRIX Annals (16 pp) (2018).

SOFTWARE AND LIBRARIES:

SPRFitting.jl, `https://github.com/isaacsas/SPRFittingPaper2023.jl`,
Lead contributor (2024–present).

CatalystNetworkAnalysis.jl, `https://github.com/SciML/CatalystNetworkAnalysis.jl`,
Contributor to library and algorithm design (2024–present).

JumpProcesses.jl, `https://github.com/SciML/JumpProcesses.jl`,
Lead Contributor (2018–present).

Catalyst.jl, `https://github.com/SciML/Catalyst.jl`,
Co-lead Contributor (2018–present).

ModelingToolkit, `https://github.com/SciML/ModelingToolkit.jl`,
Contributor (2020–present).

Other open source mathematical software at: `https://github.com/isaacsas`.