

Samuel A. Isaacson

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 molecular cell biology. I am especially interested in the numerical analysis of schemes for solving systems of partial differential, ordinary differential, and integral equations. Recently, my research has focused on the development, analysis, numerical approximation, and applications of stochastic as well as deterministic reaction-diffusion methods appropriate for modeling biochemical systems at the scale of a single biological cell.

APPOINTMENTS

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

Assistant Professor of Mathematics (Fall 2008 - Present)

- 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)

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

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 NSF - DMS, Computational Mathematics, 1255408, PI for Project: CAREER: *Numerical Methods for Stochastic Reaction-Diffusion Equations*, \$434,043 (2013–2018).
- 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 A. M. 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*, Available on webpage and at arXiv:1302.0793 (preprint is 39 pp), Submitted.
- 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*, In Press, Available as journal epub ahead of print publication (25 pp) (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).
- I. C. Agbanusi and S. A. Isaacson, *A Comparison of Bimolecular Reaction Models for Stochastic Reaction-Diffusion Systems*, *Bulletin of Mathematical Biology*, In press, Available as journal epub ahead of print publication (25 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).

INVITED TALKS

Stochastic Reaction-Diffusion Modeling in Cell Biology, Mathematical Sciences Colloquium, Rensselaer Polytechnic Institute, NY (May 2013).

A Convergent Reaction-Diffusion Master Equation, SIAM Conference on Computational Science and Engineering, Boston, MA (March 2013).

Biological Dynamics in Space and Time, Gordon Conference on Stochastic Physics in Biology, Ventura, CA (January 2013). Invited talk / discussion leader.

Influence of Subcellular Structure on Gene Expression and Regulation, Hariri Institute / Oral Cancer Research Initiative Workshop, Boston University, MA (September 2012)

Stochastic Simulation of Spatially-Distributed Models Arising in the Life Sciences, SIAM Conference on the Life Sciences, San Diego, CA (August 2012) - Invited minitutorial.

Stochastic Reaction-drift-diffusion Methods for Studying the Influence of Subcellular Structure on Biochemical Processes, SIAM Conference on the Life Sciences, San Diego, CA (August 2012)

Influence of Nuclear Substructure on Gene Regulation and Expression, Workshop on Stochastic Modelling of Reaction-Diffusion Processes in Biology, Oxford, UK (July 2012)

Relationships between Several Particle-Based Stochastic Reaction-Diffusion Models, OCCAM Seminar, Oxford Center for Collaborative Applied Mathematics (OCCAM), Oxford, UK (May 2012)

Relationships between Several Particle-Based Stochastic Reaction-Diffusion Models, Probability Seminar, University of Wisconsin, Madison, WI (May 2012)

Stochastic Reaction-drift-diffusion Methods for Studying the Influence of Subcellular Structure on Biochemical Processes, Engineering Science and Applied Mathematics Colloquia, Northwestern University, IL (February 2012).

Influence of Cellular Substructure on Gene Regulation and Expression, Systems and Integrative Biology Seminar, Boston University, Boston, MA (September 2011)

Stochastic Reaction and Stochastic Reaction-Transport Equations in Biology, Department of Information Technology, Division of Scientific Computing, Uppsala University, Sweden (June 2011)

Approximation of Smoluchowski Diffusion-Limited Reaction Models, New England Numerical Analysis Day, North Dartmouth, MA (April 2011)

Stochastic Reaction-Diffusion Evolution Equations in Biology, Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory, Athens, GA (April 2011)

Relationship between the Reaction-Diffusion Master Equation and Particle Tracking Models, SIAM Conference on the Life Sciences, Pittsburgh, PA (July 2010)

Influence of Cellular Substructure on Gene Expression and Regulation, SIAM Conference on the Life Sciences, Pittsburgh, PA (July 2010).

Influence of Cellular Substructure on the Dynamics of Gene Regulation, Systems Biology Center NY, Mount Sinai School of Medicine, NY, NY (June 2010).

Influence of Cellular Substructure on Gene Expression and Regulation, Department of Mathematics, Georgia Institute of Technology, Atlanta, GA (April 2010)

Influence of Cellular Substructure on Gene Expression and Regulation, Department of Mathematics, University of California, Santa Barbara, Santa Barbara, CA (March 2010)

Influence of Volume Exclusion due to Chromatin on Gene Expression and Regulation, Systems Biology Center New York Annual Symposium, Mount Sinai School of Medicine, NY, NY (December 2009)

Effects of cellular substructure on the dynamics of gene regulation, Society for Mathematical Biology Annual Meeting, Vancouver, Canada (July 2009)

Spatial Models of Transcription Factor-DNA Interactions, Annual Meeting of the National Centers for Systems Biology, National Institute of General Medical Sciences, NIH, Bethesda, MD (July 2009)

Effects of cellular substructure on the dynamics of gene regulation, Systems Biology Center New York, Mount Sinai School of Medicine, NY, NY (June 2009)

Effects of cellular substructure on the dynamics of gene regulation, Center for Biodynamics Annual Retreat, Boston University, Boston, MA (May 2009)

Stochastic Modeling in Cell Biology. Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden (2008)

Relationship between the Reaction-Diffusion Master Equation and Particle Tracking Models. Division of Scientific Computing, Uppsala University, Uppsala, Sweden (2008)

Spatial Stochastic Modeling in Cell Biology. Gordon Conference on Theoretical Biology & Biomathematics, Il Ciocco, Italy (2008)

Connections between the Reaction-Diffusion Master Equation, Quantum Field Theory, and Scattering. Applied Mathematics Seminar, University of Utah, Salt Lake City, UT (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, University of Utah, Salt Lake City, UT (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, University of Iowa, Iowa City, IA (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, Colorado State University - Fort Collins, Fort Collins, CO (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, University of Delaware, Newark, DE (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, Temple University, Philadelphia, PA (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, OSU, Columbus, OH (2008)

Mathematical Problems From Molecular Cell Biology. Department of Mathematics, MSU, East Lansing, MI (2008).

Mathematical Problems From Molecular Cell Biology. Dynamical Systems Seminar Boston University, Boston, MA (2008)

Connections between Several Stochastic Reaction-Diffusion Methods for Modeling Biochemical Systems. CRM/McGill Applied Mathematics Seminar, Montreal, Canada (2007)

The Reaction-Diffusion Master Equation is an Asymptotic Approximation of Diffusion to a Small Target. CAIMS 2007, Banff, Canada (2007)

The Reaction-Diffusion Master Equation is an Asymptotic Approximation of Diffusion to a Small Target. Applied Mathematics Seminar, MSU, East Lansing, MI (2007)

The Reaction-Diffusion Master Equation is an Asymptotic Approximation of Diffusion to a Small Target. Biosystems Modeling Workshop SAMSI, Research Triangle Park, NC (2007)

Stochastic Reaction-Diffusion Methods for Modeling Gene Expression and Regulation in Complex Geometries. University of British Columbia, Pacific Institute of Mathematics, MITACS Mathematical Biology Seminar, Vancouver, Canada, (March 2006).

The Reaction-Diffusion Master Equation and Spatially Continuous Stochastic Reaction-Diffusion Models. Applications of Mathematics in Biology, Physiology, and Medicine: Conference in honor of Charles S. Peskin's and David M. McQueen's 60th Birthdays, NY, NY (2006)

The Reaction-Diffusion Master Equation and Spatially Continuous Stochastic Reaction-Diffusion Models. University of Utah Biomathematics Seminar, Salt Lake City, UT (2006)

A Stochastic Reaction-Diffusion Method for Studying the Control of Gene Expression in Eukaryotic Cells. SIAM Conference on Applications of Dynamical Systems, Snowbird, UT (2005)

Incorporating Diffusion in Complex Geometries into Stochastic Chemical Kinetics Simulations. Mostly Biomathematics Lunchtime Seminar, Courant Institute of Mathematical Sciences, NY, NY (2003)

Comparison of an ODE and a Stochastic Model for Transcription and Translation in Prokaryotes. Applied Math Days, Rensselaer Polytechnic Institute, Troy, NY (2002)

Comparison of an ODE and a Stochastic Model for Transcription and Translation in Prokaryotes. Mostly Biomathematics Lunchtime Seminar, Courant Institute of Mathematical Sciences, NY, NY (2002)

OTHER RECENT
TALKS

The Reaction-Diffusion Master Equation is an Asymptotic Approximation of Diffusion to a Small Target. SIAM Dynamical Systems, Snowbird, UT (2007). (Mini-symposium Organizer)

The Reaction-Diffusion Master Equation and Spatially Continuous Stochastic Reaction-Diffusion Models. SIAM-SMB Conference on the Life Sciences (2006), Raleigh, NC. (Mini-symposium Organizer)

POSTER
PRESENTATIONS
(SINCE 2008)

"Effects of Cellular Substructure on the Dynamics of Gene Regulation and Expression." With D. M. McQueen and C. S. Peskin. Poster presented at the conference "Imaging Transcription in Living Cells" at Janelia Farms, Howard Hughes Medical Institute (March 2010).

CO-ORGANIZED CONFERENCES AND MINISYMPOSIUM *Conferences:* Particle-Based Stochastic Reaction-Diffusion Models in Biology, Banff International Research Station. To be held November 2014.

Minisymposia:

Intracellular Processes: Stochastic Modeling and Numerical Methods, SIAM Conference on Computational Science and Engineering, Boston, MA (2013)

Stochastic Dynamics of Cellular Processes, SIAM Dynamical Systems, Snowbird, UT (2007).

Modeling, Simulation, and Analysis of Cellular and Intracellular Processes, Joint SIAM Life Sciences and SMB Annual Meeting, Raleigh, NC (2006).

CONFERENCES ATTENDED (SINCE SUMMER 2008)

SIAM Conference on Computational Science and Engineering, Boston, MA (March 2013)
Gordon Conference on Stochastic Physics in Biology, Ventura, CA (January 2013)
SIAM Conference on the Life Sciences, San Diego, CA (August 2012).
Stochastic Modelling of Reaction-Diffusion Processes in Biology, Oxford, UK (July 2012)
Systems Biology Center New York Annual Symposium, NY, NY (December 2011)
Stochastic Processes in Cell and Population Biology, Mathematical Biosciences Institute, Columbus, OH (October 2011)
Multimodel and Multialgorithm Coupling for Multiscale Problems, 2011 AMS von Neumann Symposium, Snowbird, UT (July 2011)
New England Numerical Analysis Day, North Dartmouth, MA (April 2011)
Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory, Athens, GA (April 2011)
Toward an *in silico* Cell, New York Academy of Sciences, NY, NY (March 2011)
Gordon Research Conference on Stochastic Physics in Biology, Ventura, CA (January 2011)
Systems Biology Center New York Annual Symposium, NY, NY (December 2010)
SIAM Annual Meeting, Pittsburgh, PA (July 2010)
SIAM Conference on the Life Sciences, Pittsburgh, PA (July 2010)
Systems Biology of Human Disease, Boston, MA (June 2010)
Imaging Transcription in Living Cells, Janelia Farms, Howard Hughes Medical Institute, VI (March 2010)
Systems Biology Center New York Annual Symposium, NY, NY (December 2009)
Society for Mathematical Biology Annual Meeting, Vancouver, Canada (July 2009)
Annual Meeting of the National Centers for Systems Biology, NIH-NIGMS, MD (July 2009)
SIAM Conference on Applications of Dynamical Systems, Snowbird, UT (May 2009)
Center for Biodynamics Annual Retreat, Boston, MA (May 2009)
Biophysical Society Annual Meeting, Boston, MA (March 2009)
Systems Biology Center New York Annual Symposium, NY, NY (December 2008)
Gordon Research Conference on Theoretical Biology & Biomathematics, Il Cioccio, Italy (June 2008)

REVIEWER FOR

Applied Numerical Mathematics	Bulletin of Mathematical Biology
IET Systems Biology	IMA Journal of Applied Mathematics
Journal of Chemical Physics	Journal of Computational Physics
Journal of Differential Equations	Journal of Mathematical Biology
Multiscale Modeling and Simulation	Nature Biotechnology
Physica D	Physical Biology
PLOS Computational Biology	Proceedings of the National Academy of Sciences
SIAM Journal on Applied Mathematics	

COLLABORATORS: Paul J. Atzberger, UCSB
 Srinivas (Ravi) Iyengar, Mt. Sinai School of Medicine
 Carolyn Larabell, UCSF
 Jay Newby, MBI, OSU

David Isaacson, RPI
 Robert M. Kirby, University of Utah
 David M. McQueen, Courant Institute, NYU
 Charles S. Peskin, Courant Institute, NYU

STUDENTS SUPERVISED: *Ph.D. Advisees:*
 Ikemefuna Agbanusi, defended and submitted thesis: April 2013, graduation date: May 2013.
 Thesis title: *Modeling Stochastic Reaction-Diffusion via Boundary Conditions and Interaction Functions.*
 Has accepted a postdoctoral position in the University of Illinois at Urbana-Champaign mathematics department (2013-2016).

Ava Mauro, expected graduation May 2014.

Undergraduate Research Opportunity Projects:
 Jonathan Chamberlain, 2010-2012, *Volume Potential Methods for Solving the Fokker-Planck Equation.*
 Abriana Tasillo, Fall 2013, *A Convergent Reaction-Diffusion Master Equation for Unstructured Meshes.*

Undergraduate Work for Honors:
 Ben Vadala-Roth, Fall 2013, *The Immersed Boundary Method.*

COURSES TAUGHT AT BOSTON UNIVERSITY (FALL 2008 TO PRESENT)

Undergraduate Level:
 Calculus II
 Calculus for the Life and Social Sciences I

Undergraduate / Graduate Level:
 Methods of Applied Mathematics I (twice)
 Mathematical Methods in the Life Sciences (twice)

Graduate Level:
 Real Analysis (twice)
 Finite Element Methods (Reading Course)

Multivariable Calculus (twice)
 Linear Algebra
 Methods of Scientific Computing
 Numerical Methods in the Biological Sciences (twice)
 Complex Analysis (twice)
 Spectral and Perturbation Theory for Linear Operators (Reading Course)

COURSES TAUGHT AT THE UNIVERSITY OF UTAH (FALL 2005 TO SPRING 2008)

Undergraduate Level:
 Calculus I
 ODEs and Linear Algebra for Engineers

Undergraduate / Graduate Level:
 Survey of Numerical Analysis (three times)

PDEs for Engineers

COURSES TAUGHT AT NEW YORK UNIVERSITY (FALL 2000 TO SPRING 2005)

Undergraduate Level Courses Taught:
 Calculus I
 Linear Algebra

Also Served as Teaching Assistant for:
 Mathematics in Medicine and Biology
 Computational Methods for Finance (Graduate Course)

Calculus II
 Computers in Medicine and Biology

DEPARTMENTAL SERVICE	Mathematics and Statistics Department Computer Committee, 2008–Present (<i>Chair</i>). Mathematics and Statistics Department Reader for Graduate Applications in Applied Mathematics and Mathematical Biology, 2011-2013. Member of five oral qualifying exam committees. Member of two Ph.D. thesis defense committees.
OTHER SERVICE	Opponent for Ph.D. thesis defense of Andreas Hellander, Uppsala University, Sweden (June 2011) NSF grant reviewer
PROFESSIONAL MEMBERSHIPS	2001–present American Mathematical Society 2000–present Society for Industrial and Applied Mathematics 2008–present Mathematical Association of America 2008–2010 Biophysical Society 2004–2005 New York Academy of Sciences 2000–2002 Society for Mathematical Biology
CONSULTING	2004 Summer Consulting for Johnson and Johnson developing numerical methods and software for cardiac treatment system design. 1999 Summer Consulting for ABB Corp. developing numerical methods and software to determine the interior conductivity of solid objects based on boundary voltage measurements.
MEDIA	Effects of Cellular Substructure on the Dynamics of Gene Regulation, Talk from the National Centers for Systems Biology Annual Meeting 2009, Available on webpage. Protein Search Process for a DNA Binding Site within a Nonuniform Distribution of Chromatin, Supplemental material to PNAS paper, Movie available on Webpage. A 3D, stochastic reaction-diffusion model of transcription, mRNA export, translation, protein import, and gene regulation. Model from SISC paper and Ph.D. thesis, Movie available on Webpage.