

Christopher P. Calderon

Email: calderon.christopher@gmail.com

Cellular Phone: (201) 220-0227

Education

Ph.D., Chemical Engineering, Princeton University 2007

B.S., Chemical Engineering (summa cum laude), Purdue University 2001

Professional Positions

Research Scientist 2010- Present
Numerica Corporation

Computational Science Visiting Postdoctoral Fellow 2009- 2010
Lawrence Berkeley National Laboratory

Postdoctoral Fellow 2007-2009
Rice University

Refereed Publications & Submitted Manuscripts

C.P. CALDERON, Estimation and Inference of Diffusion Coefficients in Complex Biomolecular Environments, *submitted*, (2010).

C.P. CALDERON, J.G. MARTINEZ, R.J. CARROLL, AND D.C. SORENSEN, Penalized Splines Using Derivative Information, *Multiscale Modeling & Simulation (SIAM)*, **8** pg 1562 (2010).

C.P. CALDERON, Detection of Subtle Dynamical Changes Induced by Unresolved “Conformational Coordinates” in Single-Molecule Trajectories via Goodness-of-Fit Tests, *J. Phys. Chem. B* **114** pg. 3242 (2010).

C.P. CALDERON, A Data-driven Approach to Decomposing Complex Enzyme Kinetics with Surrogate Models *Phys. Rev. E* **80** pg. 061118 (2009) [**Also Selected for Dec 15, 2009 issue of Virtual Journal of Biological Physics Research**].

C.P. CALDERON, L. JANOSI, AND I. KOSZTIN, Using Stochastic Models Calibrated from Nanosecond Nonequilibrium Simulations to Approximate Mesoscale Information *J. Chem. Phys.*, **130**, pg. 144908 (2009) [**Also Selected for April 15, 2009 issue of Virtual J. Biological Physics Research and April 27, 2009 issue of Virtual J. of Nanoscale Science & Technology**].

C.P. CALDERON, N.C. HARRIS, C.-H. KIANG, AND D.D. COX, Quantifying Multiscale Noise Sources in Single-Molecule Experiments via Pathwise Statistical Inference Procedures *J. Phys. Chem. B*, **113**, pg.138 (2009).

C.P. CALDERON, W.-H CHEN, K.-J. LIN, N. C. HARRIS, AND C.-H. KIANG, Quantifying DNA Melting Transitions Using Single-Molecule Force Spectroscopy *J. Phys.: Condensed Matter*, **21**, pg. 034114 (2009).

C.P. CALDERON AND K. ARORA, Extracting Kinetic and Stationary Distribution Information from Short MD Trajectories via a Collection of Surrogate Diffusion Models *J. Chem. Theory & Comput.*, **5**, pg. 47 (2009).

C.P. CALDERON, N. C. HARRIS, C.-H. KIANG, AND D. D. COX, Analyzing Single-Molecule Manipulation Experiments *J. Mol. Recognit.*, **22**, pg. 356 (2009).

C.P. CALDERON AND R. CHELLI, Approximating Nonequilibrium Processes Using a Collection of Surrogate Diffusion Models *J. Chem. Phys.*, **128**, pg. 145103 (2008) [**Also Selected for April 15, 2008 issue of Virtual Journal of Biological Physics Research**].

C.P. CALDERON, Fitting Effective Diffusion Models to Data Associated with a “Glassy Potential”: Estimation, Classical Inference Procedures, and Some Heuristics, *Multiscale Modeling & Simulation (SIAM)*, **6**, pg. 656 (2007).

C.P. CALDERON, Local Diffusion Models for Stochastic Reacting Systems: Estimation Issues in Equation-free Numerics, *Mol. Sim.*, **33**, pg. 713 (2007).

C.P. CALDERON, On the Use of Local Diffusion Models in Path Ensemble Averaging in Potential of Mean Force Computations, *J. Chem. Phys.*, **126**, pg. 084106 (2007) [**Also Selected for March 1, 2007 issue of Virtual Journal of Biological Physics Research**].

C.P. CALDERON AND W.T. ASHURST, Comment on “Reversing the Perturbation in Nonequilibrium Molecular Dynamics: An Easy Way to Calculate the Shear Viscosity of Fluids”, *Phys. Rev. E*, **66**, pg. 013201 (2002).

Book Chapters, Technical Reports & Doctoral Thesis

C.P. CALDERON, G. A. TSEKOURAS, A. PROVATA, AND I.G. KEVREKIDIS, *Coarse-Graining the Cyclic Lotka-Volterra Model: SSA and local maximum likelihood estimation in Model Reduction and Coarse-Graining Approaches for Multiscale Phenomena*, A. Gorban, N. Kazantzis, Y. Kevrekidis, H.C. Ottinger, C. Theodoropoulos [Eds.], Springer, Berlin–Heidelberg–New York (2006).

C.P. CALDERON, J.G. MARTINEZ, R.J. CARROLL, AND D.C. SORENSEN, PSQR: A Stable and Efficient Penalized Spline Algorithm (http://www.caam.rice.edu/tech_reports/2009_abstracts.html#TR09-15).

C.P. CALDERON **On the Development of Numerical Methods Driven by Atomistic Phase Space Statistics**, Ph.D. Dissertation, Princeton University, Princeton, NJ, 2007. Academic Advisors: Prof. I. G. Kevrekidis and Prof. A. Z. Panagiotopoulos.

Awards

- NIH Nanobiology Training Grant Postdoctoral Fellowship 2008-2009
- Ford Foundation/ National Research Council Pre-doctoral Diversity Fellowship for Achieving Excellence in College and University Teaching 2001-2005
- Gordon Wu Fellowship in Engineering 2001-2005
- Lottes Memorial Award for Outstanding Chemical Engineering Senior 2001
- American Chemical Society Scholar 1997-2001
- Senator Richard G. Lugar Scholar 1997-2001

Invited Presentations

Pathwise Statistical Inference Methods for Continuous Time SDEs, Lecture Series for “Levy Processes in Finance” at CIMAT, Guanajuato, Mexico, June 2010.

Characterizing Nanoscale Dynamics via a Collection of Estimated Stochastic Differential Equations, Department of Applied Mathematics Colloquium, University of Colorado, Boulder, January 2010.

Functional Data Analysis Applications in Path Thermodynamics, Center for Statistical Bioinformatics Lecture Series, Texas A&M University, College Station, TX, October 2007.

Many Faces of Chemistry: ACS Scholars Contributions to the Chemical Sciences, American Chemical Society National Meeting, Boston, MA, August 2007.

Selected Presentations

Characterizing nanoscale dynamics: Pathwise approaches that avoid excessive coarse-graining, Spring ACS Meeting, San Francisco, March 2010.

Extracting multiscale information from time series characterizing nanoscale systems, Joint Mathematics Meetings, San Francisco, January 2010.

Extracting multiscale information from time series characterizing single-molecule systems, Annual ACS Meeting, Washington D.C., August 2009.

Multiscale Stochastic Dynamical Models Calibrated from AFM Single-Molecule Time Series and Computer Simulations, Annual AIChE Meeting, Philadelphia, PA, November 2008.

Multiscale Stochastic Dynamical Models Calibrated from Single-Molecule Force Spectroscopy Time Series, AFM BioMed Conference, Monterey, CA, October 2008.

Stochastic Process Approximations of Steered Molecular Dynamics Simulations, Annual AIChE Conference, Salt Lake City, UT, November 2007.

Multiscale Model Modeling?, Computational and Applied Mathematics Colloquium, Rice University, Houston, TX, March 2007.

Local Estimation and Coarse-Grained Numerics for Stochastic Reaction Models, Annual AIChE Conference, San Francisco, CA, November 2006.

Parametric Estimation Strategies in Molecular Simulation Using Ideas from Finance, Conference on Financial Mathematics, Boston, MA, July 2006.

Estimation Strategies for Stochastic Systems in Equation-free Methods, Biocomplexity Workshop, Notre Dame, October 2005.

Coarse-grained Micelle Computations, Annual AIChE Conference, Austin, TX, October 2004.

On the Development of Numerical Methods Driven by Atomistic Phase Space Statistics, Conference for Ford Fellows, San Juan, Puerto Rico, October 2003.

Teaching Experience

Instructor for Stochastic Differential Equations (Graduate Level) *Spring 2007*
Statistics Department, Rice University, Houston, TX

Instructor for Elementary Applied Statistics *Fall 2007*
Statistics Department, Rice University, Houston, TX

Instructor for Elementary Applied Statistics *Spring 2007*
Statistics Department, Rice University, Houston, TX

Teaching Assistant for Introduction to Chemical Engineering *Fall 2006*
Chemical Engineering Department, Princeton University, Princeton, NJ

Teaching Assistant for Chemical Engineering Senior Design *Fall 2002*
Chemical Engineering Department, Princeton University, Princeton, NJ

Teaching Assistant for Statistical Modeling and Quality Enhancement
Chemical Engineering Department, Purdue University, W. Lafayette, IN

Spring 2000

Work Experience

Internship with Sandia National Laboratory
Combustion Research Facility , Livermore, CA

Summer 2001

R&D Internship with DuPont
Sabine Riverworks, Orange, TX

Summer 2000

Process Engineering Internship with DuPont
Sabine Riverworks, Orange, TX

Summer 1999

References

Prof. Danny C. Sorensen
Dept. of Computational & Applied Mathematics
Rice University
Houston, TX 77251
(713) 348-5193
sorensen@rice.edu

Prof. Dennis D. Cox
Dept. of Statistics
Rice University
Houston, TX 77251
(713) 348-6007
dcox@stat.rice.edu

Prof. Raymond J. Carroll
Dept. of Statistics
Texas A & M University
College Station, TX 77843
(979) 845-3141
carroll@stat.tamu.edu

Prof. Javier Rojo
Dept. of Statistics
Rice University
Houston, TX 77251
(713) 348-2797
jrojo@rice.edu

Prof. Ioannis G. Kevrekidis
Dept. of Chemical Engineering
Princeton University
Princeton, NJ 08544
(609) 258-2818
yannis@arnold.Princeton.edu

Prof. Athanassios Z. Panagiotopoulos
Dept. of Chemical Engineering
Princeton University
Princeton, NJ 08544
(609) 258-4591
azp@Princeton.edu