Tony LeliÃ"vre

List of Publications by Year in descending order

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TONY LELIÃ"VRE

#	Article	IF	CITATIONS
1	Quasi-stationary distribution for the Langevin process in cylindrical domains, Part I: Existence, uniqueness and long-time convergence. Stochastic Processes and Their Applications, 2022, 144, 173-201.	0.9	5
2	An Adaptive Parareal Algorithm: Application to the Simulation of Molecular Dynamics Trajectories. SIAM Journal of Scientific Computing, 2022, 44, B146-B176.	2.8	3
3	Chasing Collective Variables Using Autoencoders and Biased Trajectories. Journal of Chemical Theory and Computation, 2022, 18, 59-78.	5.3	39
4	A probabilistic study of the kinetic Fokker–Planck equation in cylindrical domains. Journal of Evolution Equations, 2022, 22, 1.	1.1	3
5	Convergence of metadynamics: Discussion of the adiabatic hypothesis. Annals of Applied Probability, 2021, 31, .	1.3	1
6	The exit from a metastable state: Concentration of the exit point distribution on the low energy saddle points, part 1. Journal Des Mathematiques Pures Et Appliquees, 2020, 138, 242-306.	1.6	11
7	Analysis of a micro–macro acceleration method with minimum relative entropy moment matching. Stochastic Processes and Their Applications, 2020, 130, 3753-3801.	0.9	1
8	Parareal computation of stochastic differential equations with time-scale separation: a numerical convergence study. Computing and Visualization in Science, 2020, 23, 1.	1.2	5
9	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775.	5.3	120
10	Stochastic homogenization of a scalar viscoelastic model exhibiting stress–strain hysteresis. ESAIM: Mathematical Modelling and Numerical Analysis, 2020, 54, 879-928.	1.9	1
11	Mathematical Foundations of Accelerated Molecular Dynamics Methods. , 2020, , 773-803.		1
12	Hybrid Monte Carlo methods for sampling probability measures on submanifolds. Numerische Mathematik, 2019, 143, 379-421.	1.9	19
13	Preface: Special Issue on Model Reduction. Journal of Scientific Computing, 2019, 81, 1-2.	2.3	3
14	gen.parRep: A first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems. Computer Physics Communications, 2019, 239, 311-324.	7.5	5
15	Sharp Asymptotics of the First Exit Point Density. Annals of PDE, 2019, 5, 1.	1.8	13
16	Analysis of the adaptive multilevel splitting method on the isomerization of alanine dipeptide. Journal of Computational Chemistry, 2019, 40, 1198-1208.	3.3	11
17	On a new class of score functions to estimate tail probabilities of some stochastic processes with adaptive multilevel splitting. Chaos, 2019, 29, 033126.	2.5	11
18	Pathwise Estimates for Effective Dynamics: The Case of Nonlinear Vectorial Reaction Coordinates. Multiscale Modeling and Simulation, 2019, 17, 1019-1051.	1.6	8

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19	Effective dynamics for non-reversible stochastic differential equations: a quantitative study. Nonlinearity, 2019, 32, 4779-4816.	1.4	7
20	Exit Event from a Metastable State and Eyring-Kramers Law for the Overdamped Langevin Dynamics. Springer Proceedings in Mathematics and Statistics, 2019, , 331-363.	0.2	6
21	Convergence and Efficiency of Adaptive Importance Sampling Techniques with Partial Biasing. Journal of Statistical Physics, 2018, 171, 220-268.	1.2	4
22	A non linear approximation method for solving high dimensional partial differential equations: Application in finance. Mathematics and Computers in Simulation, 2018, 143, 14-34.	4.4	0
23	Computation of sensitivities for the invariant measure of a parameter dependent diffusion. Stochastics and Partial Differential Equations: Analysis and Computations, 2018, 6, 125-183.	0.9	3
24	Mathematical Foundations of Accelerated Molecular Dynamics Methods. , 2018, , 1-32.		3
25	Central Limit Theorem for stationary Fleming-Viot particle systems in finite spaces. Alea, 2018, 15, 1163.	0.7	5
26	Self-healing umbrella sampling: convergence and efficiency. Statistics and Computing, 2017, 27, 147-168.	1.5	9
27	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1566-1576.	5.3	44
28	Smoothed Biasing Forces Yield Unbiased Free Energies with the Extended-System Adaptive Biasing Force Method. Journal of Physical Chemistry B, 2017, 121, 3676-3685.	2.6	113
29	Pathwise estimates for an effective dynamics. Stochastic Processes and Their Applications, 2017, 127, 2841-2863.	0.9	13
30	Adaptive multilevel splitting for Monte Carlo particle transport. EPJ Nuclear Sciences & Technologies, 2017, 3, 29.	0.7	8
31	Adaptive Multilevel Splitting for Monte Carlo particle transport. EPJ Web of Conferences, 2017, 153, 06006.	0.3	3
32	Partial differential equations and stochastic methods in molecular dynamics. Acta Numerica, 2016, 25, 681-880.	10.7	98
33	New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.	3.2	2
34	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	3.2	4
35	Adaptive Multilevel Splitting Method for Molecular Dynamics Calculation of Benzamidine-Trypsin Dissociation Time. Journal of Chemical Theory and Computation, 2016, 12, 2983-2989.	5.3	80
36	Jump Markov models and transition state theory: the quasi-stationary distribution approach. Faraday Discussions, 2016, 195, 469-495.	3.2	34

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37	Unbiasedness of some generalized adaptive multilevel splitting algorithms. Annals of Applied Probability, 2016, 26, .	1.3	35
38	Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure. Computer Methods in Applied Mechanics and Engineering, 2016, 305, 422-440.	6.6	1
39	Variance Reduction Using Nonreversible Langevin Samplers. Journal of Statistical Physics, 2016, 163, 457-491.	1.2	70
40	Local and global solution for a nonlocal Fokker–Planck equation related to the adaptive biasing force process. Journal of Differential Equations, 2016, 260, 7032-7058.	2.2	1
41	Variants of the Empirical Interpolation Method: Symmetric formulation, choice of norms and rectangular extension. Applied Mathematics Letters, 2016, 56, 23-28.	2.7	3
42	Optimal scaling for the transient phase of the random walk Metropolis algorithm: The mean-field limit. Annals of Applied Probability, 2015, 25, .	1.3	15
43	Convergence of the Wang-Landau algorithm. Mathematics of Computation, 2015, 84, 2297-2327.	2.1	14
44	Combining a reactive potential with a harmonic approximation for molecular dynamics simulation of failure: construction of a reduced potential. Journal of Physics: Conference Series, 2015, 574, 012041.	0.4	3
45	Adaptive Multilevel Splitting in Molecular Dynamics Simulations. ESAIM Proceedings and Surveys, 2015, 48, 215-225.	0.4	8
46	Low temperature asymptotics for quasistationary distributions in a bounded domain. Analysis and PDE, 2015, 8, 561-628.	1.4	16
47	A generalized parallel replica dynamics. Journal of Computational Physics, 2015, 284, 595-616.	3.8	23
48	Accelerated dynamics: Mathematical foundations and algorithmic improvements. European Physical Journal: Special Topics, 2015, 224, 2429-2444.	2.6	15
49	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. Journal of Physical Chemistry B, 2015, 119, 1129-1151.	2.6	351
50	A nonintrusive reduced basis method applied to aeroacoustic simulations. Advances in Computational Mathematics, 2015, 41, 961-986.	1.6	32
51	Analysis of adaptive multilevel splitting algorithms in an idealized case. ESAIM - Probability and Statistics, 2015, 19, 361-394.	0.5	17
52	Macroscopic Limit of a One-Dimensional Model for Aging Fluids. Multiscale Modeling and Simulation, 2014, 12, 1335-1378.	1.6	0
53	Efficiency of the Wang-Landau Algorithm: A Simple Test Case. Applied Mathematics Research EXpress, 2014, , .	1.0	2
54	Free energy calculations from adaptive molecular dynamics simulations with adiabatic reweighting. Journal of Chemical Physics, 2014, 140, 104108.	3.0	13

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55	Greedy Algorithms for High-Dimensional Eigenvalue Problems. Constructive Approximation, 2014, 40, 387-423.	3.0	13
56	Accurate and online-efficient evaluation of the <i>a posteriori</i> error bound in the reduced basis method. ESAIM: Mathematical Modelling and Numerical Analysis, 2014, 48, 207-229.	1.9	21
57	Mathematical Analysis of Temperature Accelerated Dynamics. Multiscale Modeling and Simulation, 2014, 12, 290-317.	1.6	16
58	Optimal scaling for the transient phase of Metropolis Hastings algorithms: The longtime behavior. Bernoulli, 2014, 20, .	1.3	15
59	Optimal Non-reversible Linear Drift for the Convergence to Equilibrium of a Diffusion. Journal of Statistical Physics, 2013, 152, 237-274.	1.2	77
60	MATHEMATICAL ANALYSIS OF A ONE-DIMENSIONAL MODEL FOR AN AGING FLUID. Mathematical Models and Methods in Applied Sciences, 2013, 23, 1561-1602.	3.3	0
61	Derivation of Langevin dynamics in a nonzero background flow field. ESAIM: Mathematical Modelling and Numerical Analysis, 2013, 47, 1583-1626.	1.9	10
62	A Micro-Macro Parareal Algorithm: Application to Singularly Perturbed Ordinary Differential Equations. SIAM Journal of Scientific Computing, 2013, 35, A1951-A1986.	2.8	33
63	Mathematical study of non-ideal electrostatic correlations in equilibrium electrolytes. Nonlinearity, 2012, 25, 1635-1652.	1.4	19
64	A mathematical formalization of the parallel replica dynamics. Monte Carlo Methods and Applications, 2012, 18, .	0.8	70
65	Langevin dynamics with constraints and computation of free energy differences. Mathematics of Computation, 2012, 81, 2071-2125.	2.1	50
66	Free energy methods for Bayesian inference: efficient exploration of univariate Gaussian mixture posteriors. Statistics and Computing, 2012, 22, 897-916.	1.5	28
67	Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics. Science China Mathematics, 2012, 55, 353-384.	1.7	29
68	Some Remarks on Free Energy and Coarse-Graining. Lecture Notes in Computational Science and Engineering, 2012, , 279-329.	0.3	7
69	Periodic long-time behaviour for an approximate model of nematic polymers. Kinetic and Related Models, 2012, 5, 357-382.	0.9	2
70	CONVERGENCE OF A GREEDY ALGORITHM FOR HIGH-DIMENSIONAL CONVEX NONLINEAR PROBLEMS. Mathematical Models and Methods in Applied Sciences, 2011, 21, 2433-2467.	3.3	51
71	Enhanced Sampling of Multidimensional Free-Energy Landscapes Using Adaptive Biasing Forces. SIAM Journal on Applied Mathematics, 2011, 71, 1673-1695.	1.8	31
72	Numerical study of a thin liquid film flowing down an inclined wavy plane. Physica D: Nonlinear Phenomena, 2011, 240, 1714-1723.	2.8	8

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73	Long-Time Convergence of an Adaptive Biasing Force Method: The Bi-Channel Case. Archive for Rational Mechanics and Analysis, 2011, 202, 1-34.	2.4	12
74	A numerical closure approach for kinetic models of polymeric fluids: Exploring closure relations for FENE dumbbells. Computers and Fluids, 2011, 43, 119-133.	2.5	13
75	A multiple replica approach to simulate reactive trajectories. Journal of Chemical Physics, 2011, 134, 054108.	3.0	52
76	Reduced Basis Techniques for Stochastic Problems. Archives of Computational Methods in Engineering, 2010, 17, 435-454.	10.2	81
77	Effective dynamics using conditional expectations. Nonlinearity, 2010, 23, 2131-2163.	1.4	74
78	Free Energy Calculations: An Efficient Adaptive Biasing Potential Method. Journal of Physical Chemistry B, 2010, 114, 5823-5830.	2.6	54
79	Potential of Mean Force Calculations: A Multiple-Walker Adaptive Biasing Force Approach. Journal of Chemical Theory and Computation, 2010, 6, 1008-1017.	5.3	69
80	Existence, uniqueness and convergence of a particle approximation for the Adaptive Biasing Force process. ESAIM: Mathematical Modelling and Numerical Analysis, 2010, 44, 831-865.	1.9	13
81	Beyond multiscale and multiphysics: Multimaths for model coupling. Networks and Heterogeneous Media, 2010, 5, 423-460.	1.1	2
82	A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm. Communications in Mathematical Sciences, 2010, 8, 735-762.	1.0	20
83	Results and Questions on a Nonlinear Approximation Approach for Solving High-dimensional Partial Differential Equations. Constructive Approximation, 2009, 30, 621-651.	3.0	63
84	A general two-scale criteria for logarithmic Sobolev inequalities. Journal of Functional Analysis, 2009, 256, 2211-2221.	1.4	11
85	Generalized Navier boundary condition and geometric conservation law for surface tension. Computer Methods in Applied Mechanics and Engineering, 2009, 198, 644-656.	6.6	65
86	Free-energy-dissipative schemes for the Oldroyd-B model. ESAIM: Mathematical Modelling and Numerical Analysis, 2009, 43, 523-561.	1.9	33
87	Conservative stochastic differential equations: Mathematical and numerical analysis. Mathematics of Computation, 2009, 78, 2047-2074.	2.1	13
88	Multiscale Modelling of Complex Fluids: A Mathematical Initiation. Lecture Notes in Computational Science and Engineering, 2009, , 49-137.	0.3	23
89	Projection of diffusions on submanifolds: Application to mean force computation. Communications on Pure and Applied Mathematics, 2008, 61, 371-408.	3.1	69
90	Analyse de certains schémas de discrétisation pour des équations différentielles stochastiques contraintes. Comptes Rendus Mathematique, 2008, 346, 471-476.	0.3	13

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91	Long-time convergence of an adaptive biasing force method. Nonlinearity, 2008, 21, 1155-1181.	1.4	62
92	Computation of free energy profiles with parallel adaptive dynamics. Journal of Chemical Physics, 2007, 126, 134111.	3.0	101
93	Diffusion Monte Carlo method: Numerical Analysis in a Simple Case. ESAIM: Mathematical Modelling and Numerical Analysis, 2007, 41, 189-213.	1.9	17
94	Adaptive models for polymeric fluid flow simulation. Comptes Rendus Mathematique, 2007, 344, 473-476.	0.3	4
95	Computation of free energy differences through nonequilibrium stochastic dynamics: The reaction coordinate case. Journal of Computational Physics, 2007, 222, 624-643.	3.8	21
96	An efficient sampling algorithm for variational Monte Carlo. Journal of Chemical Physics, 2006, 125, 114105.	3.0	26
97	Long-Time Asymptotics of a Multiscale Model for Polymeric Fluid Flows. Archive for Rational Mechanics and Analysis, 2006, 181, 97-148.	2.4	75
98	QUANTUM MONTE CARLO SIMULATIONS OF FERMIONS: A MATHEMATICAL ANALYSIS OF THE FIXED-NODE APPROXIMATION. Mathematical Models and Methods in Applied Sciences, 2006, 16, 1403-1440.	3.3	19
99	Coupling PDEs and SDEs: The Illustrative Example of the Multiscale Simulation of Viscoelastic Flows. Lecture Notes in Computational Science and Engineering, 2005, , 149-168.	0.3	2
100	Optimal error estimate for the CONNFFESSIT approach in a simple case. Computers and Fluids, 2004, 33, 815-820.	2.5	7
101	Modeling and simulation of the industrial production of aluminium: the nonlinear approach. Computers and Fluids, 2004, 33, 801-814.	2.5	3
102	Existence of solution for a micro–macro model of polymeric fluid: the FENE model. Journal of Functional Analysis, 2004, 209, 162-193.	1.4	103
103	On a variance reduction technique for micro–macro simulations of polymeric fluids. Journal of Non-Newtonian Fluid Mechanics, 2004, 122, 91-106.	2.4	30
104	Simulations of MHD flows with moving interfaces. Journal of Computational Physics, 2003, 184, 163-191.	3.8	33
105	MATHEMATICAL ANALYSIS OF A STOCHASTIC DIFFERENTIAL EQUATION ARISING IN THE MICRO-MACRO MODELLING OF POLYMERIC FLUIDS. , 2003, , .		13
106	NUMERICAL ANALYSIS OF MICRO–MACRO SIMULATIONS OF POLYMERIC FLUID FLOWS: A SIMPLE CASE. Mathematical Models and Methods in Applied Sciences, 2002, 12, 1205-1243.	3.3	42
107	The Parallel Replica Method for Simulating Long Trajectories of Markov Chains. Applied Mathematics Research EXpress, 0, , .	1.0	2
108	The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 2. Stochastics and Partial Differential Equations: Analysis and Computations, 0, , 1.	0.9	1

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109	Long-time convergence of an adaptive biasing force method: Variance reduction by Helmholtz projection. SMAI Journal of Computational Mathematics, 0, 1, 55-82.	0.0	14
110	The Adaptive Biasing Force algorithm with non-conservative forces and related topics. ESAIM: Mathematical Modelling and Numerical Analysis, 0, , .	1.9	0