

Tony Lelièvre

List of Publications by Year in descending order

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110
papers

3,452
citations

182225

30
h-index

206121

51
g-index

116
all docs

116
docs citations

116
times ranked

2551
citing authors

#	ARTICLE	IF	CITATIONS
1	Quasi-stationary distribution for the Langevin process in cylindrical domains, Part I: Existence, uniqueness and long-time convergence. <i>Stochastic Processes and Their Applications</i> , 2022, 144, 173-201.	0.4	5
2	An Adaptive Parareal Algorithm: Application to the Simulation of Molecular Dynamics Trajectories. <i>SIAM Journal of Scientific Computing</i> , 2022, 44, B146-B176.	1.3	3
3	Chasing Collective Variables Using Autoencoders and Biased Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 59-78.	2.3	39
4	A probabilistic study of the kinetic Fokker-Planck equation in cylindrical domains. <i>Journal of Evolution Equations</i> , 2022, 22, 1.	0.6	3
5	Convergence of metadynamics: Discussion of the adiabatic hypothesis. <i>Annals of Applied Probability</i> , 2021, 31, .	0.6	1
6	The exit from a metastable state: Concentration of the exit point distribution on the low energy saddle points, part 1. <i>Journal Des Mathematiques Pures Et Appliquees</i> , 2020, 138, 242-306.	0.8	11
7	Analysis of a micro-macro acceleration method with minimum relative entropy moment matching. <i>Stochastic Processes and Their Applications</i> , 2020, 130, 3753-3801.	0.4	1
8	Parareal computation of stochastic differential equations with time-scale separation: a numerical convergence study. <i>Computing and Visualization in Science</i> , 2020, 23, 1.	1.2	5
9	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4757-4775.	2.3	120
10	Stochastic homogenization of a scalar viscoelastic model exhibiting stress-strain hysteresis. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2020, 54, 879-928.	0.8	1
11	Mathematical Foundations of Accelerated Molecular Dynamics Methods. , 2020, , 773-803.		1
12	Hybrid Monte Carlo methods for sampling probability measures on submanifolds. <i>Numerische Mathematik</i> , 2019, 143, 379-421.	0.9	19
13	Preface: Special Issue on Model Reduction. <i>Journal of Scientific Computing</i> , 2019, 81, 1-2.	1.1	3
14	gen.parRep: A first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems. <i>Computer Physics Communications</i> , 2019, 239, 311-324.	3.0	5
15	Sharp Asymptotics of the First Exit Point Density. <i>Annals of PDE</i> , 2019, 5, 1.	0.8	13
16	Analysis of the adaptive multilevel splitting method on the isomerization of alanine dipeptide. <i>Journal of Computational Chemistry</i> , 2019, 40, 1198-1208.	1.5	11
17	On a new class of score functions to estimate tail probabilities of some stochastic processes with adaptive multilevel splitting. <i>Chaos</i> , 2019, 29, 033126.	1.0	11
18	Pathwise Estimates for Effective Dynamics: The Case of Nonlinear Vectorial Reaction Coordinates. <i>Multiscale Modeling and Simulation</i> , 2019, 17, 1019-1051.	0.6	8

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19	Effective dynamics for non-reversible stochastic differential equations: a quantitative study. <i>Nonlinearity</i> , 2019, 32, 4779-4816.	0.6	7
20	Exit Event from a Metastable State and Eyring-Kramers Law for the Overdamped Langevin Dynamics. <i>Springer Proceedings in Mathematics and Statistics</i> , 2019, , 331-363.	0.1	6
21	Convergence and Efficiency of Adaptive Importance Sampling Techniques with Partial Biasing. <i>Journal of Statistical Physics</i> , 2018, 171, 220-268.	0.5	4
22	A non linear approximation method for solving high dimensional partial differential equations: Application in finance. <i>Mathematics and Computers in Simulation</i> , 2018, 143, 14-34.	2.4	0
23	Computation of sensitivities for the invariant measure of a parameter dependent diffusion. <i>Stochastics and Partial Differential Equations: Analysis and Computations</i> , 2018, 6, 125-183.	0.5	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. <i>Alea</i> , 2018, 15, 1163.	0.3	5
26	Self-healing umbrella sampling: convergence and efficiency. <i>Statistics and Computing</i> , 2017, 27, 147-168.	0.8	9
27	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1566-1576.	2.3	44
28	Smoothed Biasing Forces Yield Unbiased Free Energies with the Extended-System Adaptive Biasing Force Method. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3676-3685.	1.2	113
29	Pathwise estimates for an effective dynamics. <i>Stochastic Processes and Their Applications</i> , 2017, 127, 2841-2863.	0.4	13
30	Adaptive multilevel splitting for Monte Carlo particle transport. <i>EPJ Nuclear Sciences & Technologies</i> , 2017, 3, 29.	0.3	8
31	Adaptive Multilevel Splitting for Monte Carlo particle transport. <i>EPJ Web of Conferences</i> , 2017, 153, 06006.	0.1	3
32	Partial differential equations and stochastic methods in molecular dynamics. <i>Acta Numerica</i> , 2016, 25, 681-880.	6.3	98
33	New methods: general discussion. <i>Faraday Discussions</i> , 2016, 195, 521-556.	1.6	2
34	Application to large systems: general discussion. <i>Faraday Discussions</i> , 2016, 195, 671-698.	1.6	4
35	Adaptive Multilevel Splitting Method for Molecular Dynamics Calculation of Benzamidine-Trypsin Dissociation Time. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2983-2989.	2.3	80
36	Jump Markov models and transition state theory: the quasi-stationary distribution approach. <i>Faraday Discussions</i> , 2016, 195, 469-495.	1.6	34

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37	Unbiasedness of some generalized adaptive multilevel splitting algorithms. <i>Annals of Applied Probability</i> , 2016, 26, .	0.6	35
38	Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2016, 305, 422-440.	3.4	1
39	Variance Reduction Using Nonreversible Langevin Samplers. <i>Journal of Statistical Physics</i> , 2016, 163, 457-491.	0.5	70
40	Local and global solution for a nonlocal Fokker-Planck equation related to the adaptive biasing force process. <i>Journal of Differential Equations</i> , 2016, 260, 7032-7058.	1.1	1
41	Variants of the Empirical Interpolation Method: Symmetric formulation, choice of norms and rectangular extension. <i>Applied Mathematics Letters</i> , 2016, 56, 23-28.	1.5	3
42	Optimal scaling for the transient phase of the random walk Metropolis algorithm: The mean-field limit. <i>Annals of Applied Probability</i> , 2015, 25, .	0.6	15
43	Convergence of the Wang-Landau algorithm. <i>Mathematics of Computation</i> , 2015, 84, 2297-2327.	1.1	14
44	Combining a reactive potential with a harmonic approximation for molecular dynamics simulation of failure: construction of a reduced potential. <i>Journal of Physics: Conference Series</i> , 2015, 574, 012041.	0.3	3
45	Adaptive Multilevel Splitting in Molecular Dynamics Simulations. <i>ESAIM Proceedings and Surveys</i> , 2015, 48, 215-225.	0.5	8
46	Low temperature asymptotics for quasistationary distributions in a bounded domain. <i>Analysis and PDE</i> , 2015, 8, 561-628.	0.6	16
47	A generalized parallel replica dynamics. <i>Journal of Computational Physics</i> , 2015, 284, 595-616.	1.9	23
48	Accelerated dynamics: Mathematical foundations and algorithmic improvements. <i>European Physical Journal: Special Topics</i> , 2015, 224, 2429-2444.	1.2	15
49	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1129-1151.	1.2	351
50	A nonintrusive reduced basis method applied to aeroacoustic simulations. <i>Advances in Computational Mathematics</i> , 2015, 41, 961-986.	0.8	32
51	Analysis of adaptive multilevel splitting algorithms in an idealized case. <i>ESAIM - Probability and Statistics</i> , 2015, 19, 361-394.	0.2	17
52	Macroscopic Limit of a One-Dimensional Model for Aging Fluids. <i>Multiscale Modeling and Simulation</i> , 2014, 12, 1335-1378.	0.6	0
53	Efficiency of the Wang-Landau Algorithm: A Simple Test Case. <i>Applied Mathematics Research Express</i> , 2014, , .	1.0	2
54	Free energy calculations from adaptive molecular dynamics simulations with adiabatic reweighting. <i>Journal of Chemical Physics</i> , 2014, 140, 104108.	1.2	13

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55	Greedy Algorithms for High-Dimensional Eigenvalue Problems. <i>Constructive Approximation</i> , 2014, 40, 387-423.	1.8	13
56	Accurate and online-efficient evaluation of the <i>a posteriori</i> error bound in the reduced basis method. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2014, 48, 207-229.	0.8	21
57	Mathematical Analysis of Temperature Accelerated Dynamics. <i>Multiscale Modeling and Simulation</i> , 2014, 12, 290-317.	0.6	16
58	Optimal scaling for the transient phase of Metropolis Hastings algorithms: The longtime behavior. <i>Bernoulli</i> , 2014, 20, .	0.7	15
59	Optimal Non-reversible Linear Drift for the Convergence to Equilibrium of a Diffusion. <i>Journal of Statistical Physics</i> , 2013, 152, 237-274.	0.5	77
60	MATHEMATICAL ANALYSIS OF A ONE-DIMENSIONAL MODEL FOR AN AGING FLUID. <i>Mathematical Models and Methods in Applied Sciences</i> , 2013, 23, 1561-1602.	1.7	0
61	Derivation of Langevin dynamics in a nonzero background flow field. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2013, 47, 1583-1626.	0.8	10
62	A Micro-Macro Parareal Algorithm: Application to Singularly Perturbed Ordinary Differential Equations. <i>SIAM Journal of Scientific Computing</i> , 2013, 35, A1951-A1986.	1.3	33
63	Mathematical study of non-ideal electrostatic correlations in equilibrium electrolytes. <i>Nonlinearity</i> , 2012, 25, 1635-1652.	0.6	19
64	A mathematical formalization of the parallel replica dynamics. <i>Monte Carlo Methods and Applications</i> , 2012, 18, .	0.3	70
65	Langevin dynamics with constraints and computation of free energy differences. <i>Mathematics of Computation</i> , 2012, 81, 2071-2125.	1.1	50
66	Free energy methods for Bayesian inference: efficient exploration of univariate Gaussian mixture posteriors. <i>Statistics and Computing</i> , 2012, 22, 897-916.	0.8	28
67	Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics. <i>Science China Mathematics</i> , 2012, 55, 353-384.	0.8	29
68	Some Remarks on Free Energy and Coarse-Graining. <i>Lecture Notes in Computational Science and Engineering</i> , 2012, , 279-329.	0.1	7
69	Periodic long-time behaviour for an approximate model of nematic polymers. <i>Kinetic and Related Models</i> , 2012, 5, 357-382.	0.5	2
70	CONVERGENCE OF A GREEDY ALGORITHM FOR HIGH-DIMENSIONAL CONVEX NONLINEAR PROBLEMS. <i>Mathematical Models and Methods in Applied Sciences</i> , 2011, 21, 2433-2467.	1.7	51
71	Enhanced Sampling of Multidimensional Free-Energy Landscapes Using Adaptive Biasing Forces. <i>SIAM Journal on Applied Mathematics</i> , 2011, 71, 1673-1695.	0.8	31
72	Numerical study of a thin liquid film flowing down an inclined wavy plane. <i>Physica D: Nonlinear Phenomena</i> , 2011, 240, 1714-1723.	1.3	8

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73	Long-Time Convergence of an Adaptive Biasing Force Method: The Bi-Channel Case. <i>Archive for Rational Mechanics and Analysis</i> , 2011, 202, 1-34.	1.1	12
74	A numerical closure approach for kinetic models of polymeric fluids: Exploring closure relations for FENE dumbbells. <i>Computers and Fluids</i> , 2011, 43, 119-133.	1.3	13
75	A multiple replica approach to simulate reactive trajectories. <i>Journal of Chemical Physics</i> , 2011, 134, 054108.	1.2	52
76	Reduced Basis Techniques for Stochastic Problems. <i>Archives of Computational Methods in Engineering</i> , 2010, 17, 435-454.	6.0	81
77	Effective dynamics using conditional expectations. <i>Nonlinearity</i> , 2010, 23, 2131-2163.	0.6	74
78	Free Energy Calculations: An Efficient Adaptive Biasing Potential Method. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5823-5830.	1.2	54
79	Potential of Mean Force Calculations: A Multiple-Walker Adaptive Biasing Force Approach. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1008-1017.	2.3	69
80	Existence, uniqueness and convergence of a particle approximation for the Adaptive Biasing Force process. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2010, 44, 831-865.	0.8	13
81	Beyond multiscale and multiphysics: Multimaths for model coupling. <i>Networks and Heterogeneous Media</i> , 2010, 5, 423-460.	0.5	2
82	A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm. <i>Communications in Mathematical Sciences</i> , 2010, 8, 735-762.	0.5	20
83	Results and Questions on a Nonlinear Approximation Approach for Solving High-dimensional Partial Differential Equations. <i>Constructive Approximation</i> , 2009, 30, 621-651.	1.8	63
84	A general two-scale criteria for logarithmic Sobolev inequalities. <i>Journal of Functional Analysis</i> , 2009, 256, 2211-2221.	0.7	11
85	Generalized Navier boundary condition and geometric conservation law for surface tension. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2009, 198, 644-656.	3.4	65
86	Free-energy-dissipative schemes for the Oldroyd-B model. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2009, 43, 523-561.	0.8	33
87	Conservative stochastic differential equations: Mathematical and numerical analysis. <i>Mathematics of Computation</i> , 2009, 78, 2047-2074.	1.1	13
88	Multiscale Modelling of Complex Fluids: A Mathematical Initiation. <i>Lecture Notes in Computational Science and Engineering</i> , 2009, , 49-137.	0.1	23
89	Projection of diffusions on submanifolds: Application to mean force computation. <i>Communications on Pure and Applied Mathematics</i> , 2008, 61, 371-408.	1.2	69
90	Analyse de certains schémas de discrétisation pour des équations différentielles stochastiques contraintes. <i>Comptes Rendus Mathématique</i> , 2008, 346, 471-476.	0.1	13

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91	Long-time convergence of an adaptive biasing force method. <i>Nonlinearity</i> , 2008, 21, 1155-1181.	0.6	62
92	Computation of free energy profiles with parallel adaptive dynamics. <i>Journal of Chemical Physics</i> , 2007, 126, 134111.	1.2	101
93	Diffusion Monte Carlo method: Numerical Analysis in a Simple Case. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2007, 41, 189-213.	0.8	17
94	Adaptive models for polymeric fluid flow simulation. <i>Comptes Rendus Mathematique</i> , 2007, 344, 473-476.	0.1	4
95	Computation of free energy differences through nonequilibrium stochastic dynamics: The reaction coordinate case. <i>Journal of Computational Physics</i> , 2007, 222, 624-643.	1.9	21
96	An efficient sampling algorithm for variational Monte Carlo. <i>Journal of Chemical Physics</i> , 2006, 125, 114105.	1.2	26
97	Long-Time Asymptotics of a Multiscale Model for Polymeric Fluid Flows. <i>Archive for Rational Mechanics and Analysis</i> , 2006, 181, 97-148.	1.1	75
98	QUANTUM MONTE CARLO SIMULATIONS OF FERMIONS: A MATHEMATICAL ANALYSIS OF THE FIXED-NODE APPROXIMATION. <i>Mathematical Models and Methods in Applied Sciences</i> , 2006, 16, 1403-1440.	1.7	19
99	Coupling PDEs and SDEs: The Illustrative Example of the Multiscale Simulation of Viscoelastic Flows. <i>Lecture Notes in Computational Science and Engineering</i> , 2005, , 149-168.	0.1	2
100	Optimal error estimate for the CONNFESSIT approach in a simple case. <i>Computers and Fluids</i> , 2004, 33, 815-820.	1.3	7
101	Modeling and simulation of the industrial production of aluminium: the nonlinear approach. <i>Computers and Fluids</i> , 2004, 33, 801-814.	1.3	3
102	Existence of solution for a micro-macro model of polymeric fluid: the FENE model. <i>Journal of Functional Analysis</i> , 2004, 209, 162-193.	0.7	103
103	On a variance reduction technique for micro-macro simulations of polymeric fluids. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2004, 122, 91-106.	1.0	30
104	Simulations of MHD flows with moving interfaces. <i>Journal of Computational Physics</i> , 2003, 184, 163-191.	1.9	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. <i>Mathematical Models and Methods in Applied Sciences</i> , 2002, 12, 1205-1243.	1.7	42
107	The Parallel Replica Method for Simulating Long Trajectories of Markov Chains. <i>Applied Mathematics Research EXpress</i> , 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. <i>Stochastics and Partial Differential Equations: Analysis and Computations</i> , 0, , 1.	0.5	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, , .	0.8	0