Tony LeliÃ¨vre

List of Publications by Year
in descending order

110 papers	3,452 citations	159585 30 h-index	182427 51 g-index
116 all docs	116 docs citations	116 times ranked	2242 citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	Existence of solution for a microâ€“macro model of polymeric fluid: the FENE model. Journal of Functional Analysis, 2004, 209, 162-193.	1.4	103
5	Computation of free energy profiles with parallel adaptive dynamics. Journal of Chemical Physics, 2007, 126, 134111.	3.0	101
6	Partial differential equations and stochastic methods in molecular dynamics. Acta Numerica, 2016, 25, 681-880.	10.7	98
7	Reduced Basis Techniques for Stochastic Problems. Archives of Computational Methods in Engineering, 2010, 17, 435-454.	10.2	81
8	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
9	Optimal Non-reversible Linear Drift for the Convergence to Equilibrium of a Diffusion. Journal of Statistical Physics, 2013, 152, 237-274.	1.2	77
10	Long-Time Asymptotics of a Multiscale Model for Polymeric Fluid Flows. Archive for Rational Mechanics and Analysis, 2006, 181, 97-148.	2.4	75
11	Effective dynamics using conditional expectations. Nonlinearity, 2010, 23, 2131-2163.	1.4	74
12	A mathematical formalization of the parallel replica dynamics. Monte Carlo Methods and Applications, 2012, 18, .	0.8	70
13	Variance Reduction Using Nonreversible Langevin Samplers. Journal of Statistical Physics, 2016, 163, 457-491.	1.2	70
14	Projection of diffusions on submanifolds: Application to mean force computation. Communications on Pure and Applied Mathematics, 2008, 61, 371-408.	3.1	69
15	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
16	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
17	Results and Questions on a Nonlinear Approximation Approach for Solving High-dimensional Partial Differential Equations. Constructive Approximation, 2009, 30, 621-651.	3.0	63
18	Long-time convergence of an adaptive biasing force method. Nonlinearity, 2008, 21, 1155-1181.	1.4	62

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19	Free Energy Calculations: An Efficient Adaptive Biasing Potential Method. Journal of Physical Chemistry B, 2010, 114, 5823-5830.	2.6	54
20	A multiple replica approach to simulate reactive trajectories. Journal of Chemical Physics, 2011, 134, 054108.	3.0	52
21	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
22	Langevin dynamics with constraints and computation of free energy differences. Mathematics of Computation, 2012, 81, 2071-2125.	2.1	50
23	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
24	NUMERICAL ANALYSIS OF MICROâ€“MACRO SIMULATIONS OF POLYMERIC FLUID FLOWS: A SIMPLE CASE. Mathematical Models and Methods in Applied Sciences, 2002, 12, 1205-1243.	3.3	42
25	Chasing Collective Variables Using Autoencoders and Biased Trajectories. Journal of Chemical Theory and Computation, 2022, 18, 59-78.	5.3	39
26	Unbiasedness of some generalized adaptive multilevel splitting algorithms. Annals of Applied Probability, 2016, 26, .	1.3	35
27	Jump Markov models and transition state theory: the quasi-stationary distribution approach. Faraday Discussions, 2016, 195, 469-495.	3.2	34
28	Simulations of MHD flows with moving interfaces. Journal of Computational Physics, 2003, 184, 163-191.	3.8	33
29	Free-energy-dissipative schemes for the Oldroyd-B model. ESAIM: Mathematical Modelling and Numerical Analysis, 2009, 43, 523-561.	1.9	33
30	A Micro-Macro Parareal Algorithm: Application to Singularly Perturbed Ordinary Differential Equations. SIAM Journal of Scientific Computing, 2013, 35, A1951-A1986.	2.8	33
31	A nonintrusive reduced basis method applied to aeroacoustic simulations. Advances in Computational Mathematics, 2015, 41, 961-986.	1.6	32
32	Enhanced Sampling of Multidimensional Free-Energy Landscapes Using Adaptive Biasing Forces. SIAM Journal on Applied Mathematics, 2011, 71, 1673-1695.	1.8	31
33	On a variance reduction technique for microâ€“macro simulations of polymeric fluids. Journal of Non-Newtonian Fluid Mechanics, 2004, 122, 91-106.	2.4	30
34	Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics. Science China Mathematics, 2012, 55, 353-384.	1.7	29
35	Free energy methods for Bayesian inference: efficient exploration of univariate Gaussian mixture posteriors. Statistics and Computing, 2012, 22, 897-916.	1.5	28
36	An efficient sampling algorithm for variational Monte Carlo. Journal of Chemical Physics, 2006, 125, 114105.	3.0	26

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37	A generalized parallel replica dynamics. Journal of Computational Physics, 2015, 284, 595-616.	3.8	23
38	Multiscale Modelling of Complex Fluids: A Mathematical Initiation. Lecture Notes in Computational Science and Engineering, 2009, , 49-137.	0.3	23
39	Computation of free energy differences through nonequilibrium stochastic dynamics: The reaction coordinate case. Journal of Computational Physics, 2007, 222, 624-643.	3.8	21
40	Accurate and online-efficient evaluation of thea posteriorierror bound in the reduced basis method. ESAIM: Mathematical Modelling and Numerical Analysis, 2014, 48, 207-229.	1.9	21
41	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
42	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
43	Mathematical study of non-ideal electrostatic correlations in equilibrium electrolytes. Nonlinearity, 2012, 25, 1635-1652.	1.4	19
44	Hybrid Monte Carlo methods for sampling probability measures on submanifolds. Numerische Mathematik, 2019, 143, 379-421.	1.9	19
45	Diffusion Monte Carlo method: Numerical Analysis in a Simple Case. ESAIM: Mathematical Modelling and Numerical Analysis, 2007, 41, 189-213.	1.9	17
46	Analysis of adaptive multilevel splitting algorithms in an idealized case. ESAIM - Probability and Statistics, 2015, 19, 361-394.	0.5	17
47	Mathematical Analysis of Temperature Accelerated Dynamics. Multiscale Modeling and Simulation, 2014, 12, 290-317.	1.6	16
48	Low temperature asymptotics for quasistationary distributions in a bounded domain. Analysis and PDE, 2015, 8, 561-628.	1.4	16
49	Optimal scaling for the transient phase of Metropolis Hastings algorithms: The longtime behavior. Bernoulli, 2014, 20, .	1.3	15
50	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
51	Accelerated dynamics: Mathematical foundations and algorithmic improvements. European Physical Journal: Special Topics, 2015, 224, 2429-2444.	2.6	15
52	Convergence of the Wang-Landau algorithm. Mathematics of Computation, 2015, 84, 2297-2327.	2.1	14
53	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
54	Analyse de certains schÃ©mas de discrÃ©tisation pour des Ã©quations diffÃ©rentielles stochastiques contraintes. Comptes Rendus Mathematique, 2008, 346, 471-476.	0.3	13

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55	Conservative stochastic differential equations: Mathematical and numerical analysis. Mathematics of Computation, 2009, 78, 2047-2074.	2.1	13
56	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
57	Free energy calculations from adaptive molecular dynamics simulations with adiabatic reweighting. Journal of Chemical Physics, 2014, 140, 104108.	3.0	13
58	Greedy Algorithms for High-Dimensional Eigenvalue Problems. Constructive Approximation, 2014, 40, 387-423.	3.0	13
59	Pathwise estimates for an effective dynamics. Stochastic Processes and Their Applications, 2017, 127, 2841-2863.	0.9	13
60	Sharp Asymptotics of the First Exit Point Density. Annals of PDE, 2019, 5, 1.	1.8	13
61	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
62	MATHEMATICAL ANALYSIS OF A STOCHASTIC DIFFERENTIAL EQUATION ARISING IN THE MICRO-MACRO MODELLING OF POLYMERIC FLUIDS. , 2003, , .		13
63	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
64	A general two-scale criteria for logarithmic Sobolev inequalities. Journal of Functional Analysis, 2009, 256, 2211-2221.	1.4	11
65	Analysis of the adaptive multilevel splitting method on the isomerization of alanine dipeptide. Journal of Computational Chemistry, 2019, 40, 1198-1208.	3.3	11
66	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
67	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
68	Derivation of Langevin dynamics in a nonzero background flow field. ESAIM: Mathematical Modelling and Numerical Analysis, 2013, 47, 1583-1626.	1.9	10
69	Self-healing umbrella sampling: convergence and efficiency. Statistics and Computing, 2017, 27, 147-168.	1.5	9
70	Numerical study of a thin liquid film flowing down an inclined wavy plane. Physica D: Nonlinear Phenomena, 2011, 240, 1714-1723.	2.8	8
71	Adaptive Multilevel Splitting in Molecular Dynamics Simulations. ESAIM Proceedings and Surveys, 2015, 48, 215-225.	0.4	8
72	Adaptive multilevel splitting for Monte Carlo particle transport. EPJ Nuclear Sciences & Technologies, 2017, 3, 29.	0.7	8

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73	Pathwise Estimates for Effective Dynamics: The Case of Nonlinear Vectorial Reaction Coordinates. Multiscale Modeling and Simulation, 2019, 17, 1019-1051.	1.6	8
74	Optimal error estimate for the CONNFFESSIT approach in a simple case. Computers and Fluids, 2004, 33, 815-820.	2.5	7
75	Effective dynamics for non-reversible stochastic differential equations: a quantitative study. Nonlinearity, 2019, 32, 4779-4816.	1.4	7
76	Some Remarks on Free Energy and Coarse-Graining. Lecture Notes in Computational Science and Engineering, 2012, , 279-329.	0.3	7
77	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
78	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
79	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
80	Central Limit Theorem for stationary Fleming-Viot particle systems in finite spaces. Alea, 2018, 15, 1163.	0.7	5
81	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
82	Adaptive models for polymeric fluid flow simulation. Comptes Rendus Mathematique, 2007, 344, 473-476.	0.3	4
83	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	3.2	4
84	Convergence and Efficiency of Adaptive Importance Sampling Techniques with Partial Biasing. Journal of Statistical Physics, 2018, 171, 220-268.	1.2	4
85	Modeling and simulation of the industrial production of aluminium: the nonlinear approach. Computers and Fluids, 2004, 33, 801-814.	2.5	3
86	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
87	Variants of the Empirical Interpolation Method: Symmetric formulation, choice of norms and rectangular extension. Applied Mathematics Letters, 2016, 56, 23-28.	2.7	3
88	Adaptive Multilevel Splitting for Monte Carlo particle transport. EPJ Web of Conferences, 2017, 153, 06006.	0.3	3
89	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
90	Mathematical Foundations of Accelerated Molecular Dynamics Methods. , 2018, , 1-32.		3

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91	Preface: Special Issue on Model Reduction. Journal of Scientific Computing, 2019, 81, 1-2.	2.3	3
92	An Adaptive Parareal Algorithm: Application to the Simulation of Molecular Dynamics Trajectories. SIAM Journal of Scientific Computing, 2022, 44, B146-B176.	2.8	3
93	A probabilistic study of the kinetic Fokkerâ€“Planck equation in cylindrical domains. Journal of Evolution Equations, 2022, 22, 1.	1.1	3
94	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
95	Efficiency of the Wang-Landau Algorithm: A Simple Test Case. Applied Mathematics Research EXpress, 2014, , .	1.0	2
96	The Parallel Replica Method for Simulating Long Trajectories of Markov Chains. Applied Mathematics Research EXpress, 0, , .	1.0	2
97	New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.	3.2	2
98	Periodic long-time behaviour for an approximate model of nematic polymers. Kinetic and Related Models, 2012, 5, 357-382.	0.9	2
99	Beyond multiscale and multiphysics: Multimaths for model coupling. Networks and Heterogeneous Media, 2010, 5, 423-460.	1.1	2
100	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
101	Local and global solution for a nonlocal Fokkerâ€“Planck equation related to the adaptive biasing force process. Journal of Differential Equations, 2016, 260, 7032-7058.	2.2	1
102	Analysis of a microâ€“macro acceleration method with minimum relative entropy moment matching. Stochastic Processes and Their Applications, 2020, 130, 3753-3801.	0.9	1
103	Stochastic homogenization of a scalar viscoelastic model exhibiting stressâ€“strain hysteresis. ESAIM: Mathematical Modelling and Numerical Analysis, 2020, 54, 879-928.	1.9	1
104	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
105	Convergence of metadynamics: Discussion of the adiabatic hypothesis. Annals of Applied Probability, 2021, 31, .	1.3	1
106	Mathematical Foundations of Accelerated Molecular Dynamics Methods. , 2020, , 773-803.		1
107	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
108	Macroscopic Limit of a One-Dimensional Model for Aging Fluids. Multiscale Modeling and Simulation, 2014, 12, 1335-1378.	1.6	0

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109	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
110	The Adaptive Biasing Force algorithm with non-conservative forces and related topics. ESAIM: Mathematical Modelling and Numerical Analysis, 0, , .	1.9	0