Benedict Leimkuhler

List of Publications by Year
in descending order

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24 papers	1,022 citations	623574 14 h-index	642610 23 g-index
26 all docs	26 docs citations	26 times ranked	1083 citing authors

#	Article	IF	Citations
1	Symplectic splitting methods for rigid body molecular dynamics. Journal of Chemical Physics, 1997, 107, 5840-5851.	1.2	205
2	Algorithms for constrained molecular dynamics. Journal of Computational Chemistry, 1995, 16, 1192-1209.	1.5	149
3	Robust and efficient configurational molecular sampling via Langevin dynamics. Journal of Chemical Physics, 2013, 138, 174102.	1.2	127
4	A Stochastic Algorithm for the Isobaricâ€“Isothermal Ensemble with Ewald Summations for All Long Range Forces. Journal of Chemical Theory and Computation, 2015, 11, 5624-5637.	2.3	114
5	The Adaptive Verlet Method. SIAM Journal of Scientific Computing, 1997, 18, 239-256.	1.3	84
6	Efficient molecular dynamics using geodesic integration and solventâ€“solute splitting. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160138.	1.0	49
7	Geometric Integrators for Classical Spin Systems. Journal of Computational Physics, 1997, 133, 160-172.	1.9	48
8	On the numerical treatment of dissipative particle dynamics and related systems. Journal of Computational Physics, 2015, 280, 72-95.	1.9	38
9	Quantifying Configuration-Sampling Error in Langevin Simulations of Complex Molecular Systems. Entropy, 2018, 20, 318.	1.1	29
10	The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics. IMA Journal of Numerical Analysis, 0, , dru056.	1.5	27
11	Adaptive Thermostats for Noisy Gradient Systems. SIAM Journal of Scientific Computing, 2016, 38, A712-A736.	1.3	22
12	Ensemble preconditioning for Markov chain Monte Carlo simulation. Statistics and Computing, 2018, 28, 277-290.	0.8	20
13	Pairwise adaptive thermostats for improved accuracy and stability in dissipative particle dynamics. Journal of Computational Physics, 2016, 324, 174-193.	1.9	17
14	Langevin Dynamics with Variable Coefficients and Nonconservative Forces: From Stationary States to Numerical Methods. Entropy, 2017, 19, 647.	1.1	17
15	Asymptotic Error Analysis of the Adaptive Verlet Method. BIT Numerical Mathematics, 1999, 39, 25-33.	1.0	15
16	Assessing numerical methods for molecular and particle simulation. Soft Matter, 2017, 13, 8565-8578.	1.2	14
17	A Time-Reversible Variable-Stepsize Integrator for Constrained Dynamics. SIAM Journal of Scientific Computing, 1999, 21, 1027-1044.	1.3	12
18	Generalized Bulgac-Kusnezov methods for sampling of the Gibbs-Boltzmann measure. Physical Review E, 2010, 81, 026703.	0.8	12

#	Article	IF	Citations
19	Hypocoercivity Properties of Adaptive Langevin Dynamics. SIAM Journal on Applied Mathematics, 2020, 80, 1197-1222.	0.8	9
20	Efficient Numerical Algorithms for the Generalized Langevin Equation. SIAM Journal of Scientific Computing, 2022, 44, A364-A388.	1.3	5
21	Ergodic Properties of Quasi-Markovian Generalized Langevin Equations with Configuration Dependent Noise and Non-conservative Force. Springer Proceedings in Mathematics and Statistics, 2019, , 282-330.	0.1	4
22	Observation-based correction of dynamical models using thermostats. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2017, 473, 20160730.	1.0	2
23	Reversible adaptive regularization methods for atomic N-body problems in applied fields. Applied Numerical Mathematics, 1999, 29, 31-43.	1.2	1
24	Direct control of the small-scale energy balance in two-dimensional fluid dynamics. Journal of Fluid Mechanics, 2015, 782, 240-259.	1.4	1