Eric Vanden-Eijnden

List of Publications by Year
in descending order

71 papers	9,659 citations	57631 44 h-index	85405 71 g-index
71 all docs	71 docs citations	71 times ranked	5242 citing authors

#	Article	IF	Citations
1	String method for the study of rare events. Physical Review B, 2002, 66, .	1.1	843
2	Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 19011-19016.	3.3	730
3	String method in collective variables: Minimum free energy paths and isocommittor surfaces. Journal of Chemical Physics, 2006, 125, 024106.	1.2	600
4	Simplified and improved string method for computing the minimum energy paths in barrier-crossing events. Journal of Chemical Physics, 2007, 126, 164103.	1.2	516
5	Transition-Path Theory and Path-Finding Algorithms for the Study of Rare Events. Annual Review of Physical Chemistry, 2010, 61, 391-420.	4.8	481
6	A temperature accelerated method for sampling free energy and determining reaction pathways in rare events simulations. Chemical Physics Letters, 2006, 426, 168-175.	1.2	428
7	Finite Temperature String Method for the Study of Rare Events€. Journal of Physical Chemistry B, 2005, 109, 6688-6693.	1.2	397
8	Towards a Theory of Transition Paths. Journal of Statistical Physics, 2006, 123, 503-523.	0.5	375
9	Transition Path Theory for Markov Jump Processes. Multiscale Modeling and Simulation, 2009, 7, 1192-1219.	0.6	362
10	The heterogeneous multiscale method. Acta Numerica, 2012, 21, 1-87.	6.3	334
11	Mori–Zwanzig formalism as a practical computational tool. Faraday Discussions, 2010, 144, 301-322.	1.6	275
12	Transition pathways in complex systems: Reaction coordinates, isocommittor surfaces, and transition tubes. Chemical Physics Letters, 2005, 413, 242-247.	1.2	187
13	Markov state models based on milestoning. Journal of Chemical Physics, 2011, 134, 204105.	1.2	184
14	Systematic Strategies for Stochastic Mode Reduction in Climate. Journals of the Atmospheric Sciences, 2003, 60, 1705-1722.	0.6	183
15	Revisiting the finite temperature string method for the calculation of reaction tubes and free energies. Journal of Chemical Physics, 2009, 130, 194103.	1.2	181
16	Transition pathways in complex systems: Application of the finite-temperature string method to the alanine dipeptide. Journal of Chemical Physics, 2005, 123, 134109.	1.2	168
17	Markovian milestoning with Voronoi tessellations. Journal of Chemical Physics, 2009, 130, 194101.	1.2	167
18	Large-scale conformational sampling of proteins using temperature-accelerated molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 4961-4966.	3.3	165

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19	Illustration of transition path theory on a collection of simple examples. Journal of Chemical Physics, 2006, 125, 084110.	1.2	159
20	On-the-fly string method for minimum free energy paths calculation. Chemical Physics Letters, 2007, 446, 182-190.	1.2	159
21	On the assumptions underlying milestoning. Journal of Chemical Physics, 2008, 129, 174102.	1.2	158
22	Second-order integrators for Langevin equations with holonomic constraints. Chemical Physics Letters, 2006, 429, 310-316.	1.2	155
23	Solvent coarse-graining and the string method applied to the hydrophobic collapse of a hydrated chain. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14559-14564.	3.3	155
24	Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates. Journal of Chemical Physics, 2005, 123, 194107.	1.2	135
25	Analysis of multiscale methods for stochastic differential equations. Communications on Pure and Applied Mathematics, 2005, 58, 1544-1585.	1.2	129
26	Numerical Techniques for Multi-Scale Dynamical Systems with Stochastic Effects. Communications in Mathematical Sciences, 2003, 1, 385-391.	0.5	126
27	Single-sweep methods for free energy calculations. Journal of Chemical Physics, 2008, 128, 184110.	1.2	119
28	Free energy of conformational transition paths in biomolecules: The string method and its application to myosin VI. Journal of Chemical Physics, 2011, 134, 085103.	1.2	116
29	Low-Order Stochastic Mode Reduction for a Realistic Barotropic Model Climate. Journals of the Atmospheric Sciences, 2005, 62, 1722-1745.	0.6	114
30	Transition state theory: Variational formulation, dynamical corrections, and error estimates. Journal of Chemical Physics, 2005, 123, 184103.	1.2	112
31	Nested stochastic simulation algorithms for chemical kinetic systems with multiple time scales. Journal of Computational Physics, 2007, 221, 158-180.	1.9	101
32	Mapping the Network of Pathways of CO Diffusion in Myoglobin. Journal of the American Chemical Society, 2010, 132, 1010-1017.	6.6	96
33	Subgrid-Scale Parameterization with Conditional Markov Chains. Journals of the Atmospheric Sciences, 2008, 65, 2661-2675.	0.6	95
34	A computational strategy for multiscale systems with applications to Lorenz 96 model. Journal of Computational Physics, 2004, 200, 605-638.	1.9	87
35	Energy landscape and thermally activated switching of submicron-sized ferromagnetic elements. Journal of Applied Physics, 2003, 93, 2275-2282.	1.1	83
36	A general strategy for designing seamless multiscale methods. Journal of Computational Physics, 2009, 228, 5437-5453.	1.9	80

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37	Exact rate calculations by trajectory parallelization and tilting. Journal of Chemical Physics, 2009, 131, 044120.	1.2	74
38	The geometric minimum action method for computing minimum energy paths. Journal of Chemical Physics, 2008, 128, 061103.	1.2	70
39	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2589-2594.	2.3	62
40	Some recent techniques for free energy calculations. Journal of Computational Chemistry, 2009, 30, 1737-1747.	1.5	57
41	Dynamic density functional theory with hydrodynamic interactions and fluctuations. Journal of Chemical Physics, 2014, 140, 234115.	1.2	52
42	A reversible mesoscopic model of diffusion in liquids: from giant fluctuations to Fickâ€™s law. Journal of Statistical Mechanics: Theory and Experiment, 2014, 2014, P04004.	0.9	52
43	Order-parameter-aided temperature-accelerated sampling for the exploration of crystal polymorphism and solid-liquid phase transitions. Journal of Chemical Physics, 2014, 140, 214109.	1.2	47
44	Flows in Complex Networks: Theory, Algorithms, and Application to Lennardâ€"Jones Cluster Rearrangement. Journal of Statistical Physics, 2014, 156, 427-454.	0.5	47
45	Exact dynamical coarse-graining without time-scale separation. Journal of Chemical Physics, 2014, 141, 044109.	1.2	40
46	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. Journal of Chemical Theory and Computation, 2014, 10, 524-533.	2.3	38
47	Full Kinetics of CO Entry, Internal Diffusion, and Exit in Myoglobin from Transition-Path Theory Simulations. Journal of the American Chemical Society, 2015, 137, 3041-3050.	6.6	38
48	ON HMM-like integrators and projective integration methods for systems with multiple time scales. Communications in Mathematical Sciences, 2007, 5, 495-505.	0.5	33
49	Multiscale implementation of infinite-swap replica exchange molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11744-11749.	3.3	32
50	Transition Path Theory. Advances in Experimental Medicine and Biology, 2014, 797, 91-100.	0.8	30
51	Kinetics of phase transitions in two dimensional Ising models studied with the string method. Journal of Mathematical Chemistry, 2009, 45, 188-222.	0.7	28
52	Some Recent Progress in Multiscale Modeling. Lecture Notes in Computational Science and Engineering, 2004, , 3-21.	0.1	25
53	Metastability, conformation dynamics, and transition pathways in complex systems. Lecture Notes in Computational Science and Engineering, 2004, , 35-68.	0.1	24
54	On-the-fly free energy parameterization via temperature accelerated molecular dynamics. Chemical Physics Letters, 2012, 547, 114-119.	1.2	22

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55	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. Scientific Modeling and Simulation SMNS, 2008, 15, 187-206.	0.8	21
56	Rare Events in Stochastic Partial Differential Equations on Large Spatial Domains. Journal of Statistical Physics, 2008, 131, 1023-1038.	0.5	19
57	Optimized Markov state models for metastable systems. Journal of Chemical Physics, 2016, 145, 024102.	1.2	16
58	Metropolis Integration Schemes for Self-Adjoint Diffusions. Multiscale Modeling and Simulation, 2014, 12, 781-831.	0.6	12
59	Transition state theory and dynamical corrections in ergodic systems. Nonlinearity, 2006, 19, 501-509.	0.6	11
60	The simulated tempering method in the infinite switch limit with adaptive weight learning. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 013207.	0.9	10
61	Stochastic mode-reduction in models with conservative fast sub-systems. Communications in Mathematical Sciences, 2015, 13, 297-314.	0.5	6
62	Kinetics of O_2 Entry and Exit in Monomeric Sarcosine Oxidase via Markovian Milestoning Molecular Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 2964-2972.	2.3	6
63	Fluctuations in the heterogeneous multiscale methods for fast–slow systems. Research in Mathematical Sciences, 2017, 4, 1.	0.5	6
64	Response to "Comment on 'Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates'" [J. Chem. Phys. 123, 194107 (2005)]. Journal of Chemical Physics, 2007, 126, 137102.	1.2	4
65	Direct generation of loop-erased transition paths in non-equilibrium reactions. Faraday Discussions, 2016, 195, 443-468.	1.6	4
66	A Mathematical Theory of Optimal Milestoning (with a Detour via Exact Milestoning). Communications on Pure and Applied Mathematics, 2018, 71, 1149-1177.	1.2	4
67	Longtime convergence of the temperature-accelerated molecular dynamics method. Nonlinearity, 2018, 31, 3748-3769.	0.6	4
68	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. Lecture Notes in Computational Science and Engineering, 2008, , 187-206.	0.1	3
69	Mapping saddles and minima on free energy surfaces using multiple climbing strings. Journal of Chemical Physics, 2019, 151, 124112.	1.2	3
70	Methodological and Computational Aspects of Parallel Tempering Methods in the Infinite Swapping Limit. Journal of Statistical Physics, 2019, 174, 715-733.	0.5	3
71	Accelerated Simulation of a Heavy Particle in a Gas of Elastic Spheres. Multiscale Modeling and Simulation, 2008, 7, 349-361.	0.6	1