Markos A Katsoulakis

List of Publications by Year
in descending order

86	2,476	236833	206029
papers	citations	25 h-index	48 g-index

89	89	89	1860
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanistic principles of nanoparticle evolution to zeolite crystals. Nature Materials, 2006, 5, 400-408.	13.3	416
2	Binomial distribution based Ï„-leap accelerated stochastic simulation. Journal of Chemical Physics, 2005, 122, 024112.	1.2	184
3	Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling. Nature Chemistry, 2016, 8, 331-337.	6.6	131
4	Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. Journal of Computational Physics, 2003, 186, 250-278.	1.9	107
5	Coarse-grained stochastic processes for microscopic lattice systems. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 782-787.	3.3	106
6	Stochastic Modeling and Simulation of Traffic Flow: Asymmetric Single Exclusion Process with Arrhenius look-ahead dynamics. SIAM Journal on Applied Mathematics, 2006, 66, 921-944.	0.8	97
7	Coarse-grained stochastic models for tropical convection and climate. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11941-11946.	3.3	89
8	Coarse-grained stochastic processes and kinetic Monte Carlo simulators for the diffusion of interacting particles. Journal of Chemical Physics, 2003, 119, 9412-9427.	1.2	76
9	Contractive relaxation systems and the scalar multidimensional conservation law. Communications in Partial Differential Equations, 1997, 22, 225-267.	1.0	73
10	Derivation and Validation of Mesoscopic Theories for Diffusion of Interacting Molecules. Physical Review Letters, 2000, 85, 3898-3901.	2.9	63
11	A Mathematical Model for Crystal Growth by Aggregation of Precursor Metastable Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 23879-23887.	1.2	59
12	Generalized motion by mean curvature as a macroscopic limit of stochastic ising models with long range interactions and Glauber dynamics. Communications in Mathematical Physics, 1995, 169, 61-97.	1.0	54
13	Title is missing!. Indiana University Mathematics Journal, 1994, 43, 493.	0.4	49
14	Generalized motion by mean curvature with Neumann conditions and the Allen-Cahn model for phase transitions. Journal of Geometric Analysis, 1995, 5, 255.	0.5	47
15	Spatially adaptive lattice coarse-grained Monte Carlo simulations for diffusion of interacting molecules. Journal of Chemical Physics, 2004, 121, 11420.	1.2	45
16	Interacting particle systems and generalized evolution of fronts. Archive for Rational Mechanics and Analysis, 1994, 127, 133-157.	1.1	38
17	A relative entropy rate method for path space sensitivity analysis of stationary complex stochastic dynamics. Journal of Chemical Physics, 2013, 138, 054115.	1.2	37
18	A Comparison Principle for Hamiltonâ€“Jacobi Equations Related to Controlled Gradient Flows in Infinite Dimensions. Archive for Rational Mechanics and Analysis, 2009, 192, 275-310.	1.1	36

#	Article	IF	Citations
19	Information-theoretic tools for parametrized coarse-graining of non-equilibrium extended systems. Journal of Chemical Physics, 2013, 139, 074115.	1.2	36
20	Spectral Methods for Mesoscopic Models of Pattern Formation. Journal of Computational Physics, 2001, 173, 364-390.	1.9	35
21	Path-Space Information Bounds for Uncertainty Quantification and Sensitivity Analysis of Stochastic Dynamics. SIAM-ASA Journal on Uncertainty Quantification, 2016, 4, 80-111.	1.1	34
22	From Microscopic Interactions to Macroscopic Laws of Cluster Evolution. Physical Review Letters, 2000, 84, 1511-1514.	2.9	33
23	The geometry of generalized force matching and related information metrics in coarse-graining of molecular systems. Journal of Chemical Physics, 2015, 143, 084105.	1.2	32
24	Path-space variational inference for non-equilibrium coarse-grained systems. Journal of Computational Physics, 2016, 314, 355-383.	1.9	32
25	Noise regularization and computations for the 1-dimensional stochastic Allenâ€“Cahn problem. Interfaces and Free Boundaries, 2007, 9, 1-30.	0.2	26
26	Explainable and trustworthy artificial intelligence for correctable modeling in chemical sciences. Science Advances, 2020, 6, .	4.7	26
27	Error Analysis of Coarseâ€Graining for Stochastic Lattice Dynamics. SIAM Journal on Numerical Analysis, 2006, 44, 2270-2296.	1.1	25
28	Information Loss in Coarse-Graining of Stochastic Particle Dynamics. Journal of Statistical Physics, 2006, 122, 115-135.	0.5	25
29	A representation formula and regularizing properties for viscosity solutions of second-order fully nonlinear degenerate parabolic equations. Nonlinear Analysis: Theory, Methods & Applications, 1995, 24, 147-158.	0.6	23
30	Parametric sensitivity analysis for biochemical reaction networks based on pathwise information theory. BMC Bioinformatics, 2013, 14, 311.	1.2	22
31	The role of multiple microscopic mechanisms in cluster interface evolution. Journal of Differential Equations, 2007, 235, 418-438.	1.1	20
32	Hyperbolic Systems with Supercharacteristic Relaxations and Roll Waves. SIAM Journal on Applied Mathematics, 2000, 61, 273-292.	0.8	19
33	Hierarchical fractional-step approximations and parallel kinetic Monte Carlo algorithms. Journal of Computational Physics, 2012, 231, 7795-7814.	1.9	18
34	GINNs: Graph-Informed Neural Networks for multiscale physics. Journal of Computational Physics, 2021, 433, 110192.	1.9	18
35	Coarse-graining schemes anda posteriorierror estimates for stochastic lattice systems. ESAIM: Mathematical Modelling and Numerical Analysis, 2007, 41, 627-660.	0.8	16
36	Numerical and Statistical Methods forÂtheÂCoarse-Graining ofÂMany-Particle Stochastic Systems. Journal of Scientific Computing, 2008, 37, 43-71.	1.1	14

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37	Scalable information inequalities for uncertainty quantification. Journal of Computational Physics, 2017, 336, 513-545.	1.9	14
38	Mathematical strategies in the coarse-graining of extensive systems: Error quantification and adaptivity. Journal of Non-Newtonian Fluid Mechanics, 2008, 152, 101-112.	1.0	13
39	Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics. Journal of Chemical Physics, 2015, 143, 014116.	1.2	13
40	Causality and Bayesian Network PDEs for multiscale representations of porous media. Journal of Computational Physics, 2019, 394, 658-678.	1.9	13
41	How Biased Is Your Model? Concentration Inequalities, Information and Model Bias. IEEE Transactions on Information Theory, 2020, 66, 3079-3097.	1.5	13
42	Deterministic equations for stochastic spatial evolutionary games. Theoretical Economics, 2013, 8, 829-874.	0.5	12
43	Goal-oriented sensitivity analysis for lattice kinetic Monte Carlo simulations. Journal of Chemical Physics, 2014, 140, 124108.	1.2	12
44	Accelerated Sensitivity Analysis in High-Dimensional Stochastic Reaction Networks. PLoS ONE, 2015, 10, e0130825.	1.1	11
45	Stochastic curvature flows: asymptotic derivation, level set formulation and numerical experiments. Interfaces and Free Boundaries, 2001, 3, 265-290.	0.2	11
46	Multibody Interactions in Coarse-Graining Schemes for Extended Systems. SIAM Journal of Scientific Computing, 2009, 31, 987-1015.	1.3	10
47	Data-driven, variational model reduction of high-dimensional reaction networks. Journal of Computational Physics, 2020, 401, 108997.	1.9	10
48	Sensitivity analysis for rare events based on RÃ©nyi divergence. Annals of Applied Probability, 2020, 30, .	0.6	10
49	Long-time integration methods for mesoscopic models of pattern-forming systems. Journal of Computational Physics, 2011, 230, 5704-5715.	1.9	9
50	Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems. Journal of Computational Physics, 2012, 231, 2599-2620.	1.9	9
51	Efficient estimators for likelihood ratio sensitivity indices of complex stochastic dynamics. Journal of Chemical Physics, 2016, 144, 104107.	1.2	9
52	Global sensitivity analysis of multiscale properties of porous materials. Journal of Applied Physics, 2018, 123, 075103.	1.1	9
53	Stochastic hydrodynamical limits of particle systems. Communications in Mathematical Sciences, 2006, 4, 513-549.	0.5	9
54	Relaxation Approximations to Front Propagation. Journal of Differential Equations, 1997, 138, 380-387.	1.1	8

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55	Multiscale Analysis for Interacting Particles: Relaxation Systems and Scalar Conservation Laws. , 1999, 96, 715-763.		8
56	Relaxation schemes for curvature-dependent front propagation. , 1999, 52, 1587-1615.		8
57	Parallelization, Processor Communication and Error Analysis in Lattice Kinetic Monte Carlo. SIAM Journal on Numerical Analysis, 2014, 52, 1156-1182.	1.1	8
58	Non-parametric correlative uncertainty quantification and sensitivity analysis: Application to a Langmuir bimolecular adsorption model. AIP Advances, 2018, 8, .	0.6	8
59	Uncertainty Quantification and Error Propagation in the Enthalpy and Entropy of Surface Reactions Arising from a Single DFT Functional. Journal of Physical Chemistry C, 2021, 125, 18187-18196.	1.5	8
60	Uncertainty quantification for generalized Langevin dynamics. Journal of Chemical Physics, 2016, 145, 224108.	1.2	7
61	Mutual information for explainable deep learning of multiscale systems. Journal of Computational Physics, 2021, 444, 110551.	1.9	7
62	Numerical Assessment of Theoretical Error Estimates in Coarse-Grained Kinetic Monte Carlo Simulations: Application to Surface Diffusion. International Journal for Multiscale Computational Engineering, 2005, 3, 59-70.	0.8	7
63	Variational Representations and Neural Network Estimation of RÃ©nyi Divergences. SIAM Journal on Mathematics of Data Science, 2021, 3, 1093-1116.	1.0	7
64	Measuring the Irreversibility of Numerical Schemes for Reversible Stochastic Differential Equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2014, 48, 1351-1379.	0.8	5
65	Spatial Two-Level Interacting Particle Simulations and Information Theory–Based Error Quantification. SIAM Journal of Scientific Computing, 2014, 36, A634-A667.	1.3	5
66	Mesoscopic Modeling of Surface Processes. The IMA Volumes in Mathematics and Its Applications, 2004, , 179-198.	0.5	4
67	Mesoscopic Modeling for Continuous Spin Lattice Systems: Model Problems and Micromagnetics Applications. Journal of Statistical Physics, 2005, 119, 347-389.	0.5	4
68	Coarse-graining schemes for stochastic lattice systems with short and long-range interactions. Mathematics of Computation, 2014, 83, 1757-1793.	1.1	4
69	Information Metrics For Long-Time Errors in Splitting Schemes For Stochastic Dynamics and Parallel Kinetic Monte Carlo. SIAM Journal of Scientific Computing, 2016, 38, A3808-A3832.	1.3	4
70	Robust Information Divergences for Model-Form Uncertainty Arising from Sparse Data in Random PDE. SIAM-ASA Journal on Uncertainty Quantification, 2018, 6, 1364-1394.	1.1	4
71	A novel multi-layer framework for modeling the evolution of spectrum markets and cognitive-radio devices. , 2011, , .		3
72	Cumulant GAN. IEEE Transactions on Neural Networks and Learning Systems, 2023, 34, 9439-9450.	7.2	3

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73	Coarse-grained Langevin approximations and spatiotemporal acceleration for kinetic Monte Carlo simulations of diffusion of interacting particles. Chinese Annals of Mathematics Series B, 2009, 30, 653-682.	0.2	2
74	Information criteria for quantifying loss of reversibility in parallelized KMC. Journal of Computational Physics, 2017, 328, 438-454.	1.9	2
75	Path space force matching and relative entropy methods for coarse-graining molecular systems at transient regimes. Procedia Computer Science, 2018, 136, 331-340.	1.2	2
76	Data-driven uncertainty quantification for systematic coarse-grained models. Soft Materials, 2020, 18, 348-368.	0.8	2
77	Pathwise Sensitivity Analysis in Transient Regimes. Mathematical Engineering, 2015, , 105-124.	0.1	2
78	Quantification of model uncertainty on path-spaceviagoal-oriented relative entropy. ESAIM: Mathematical Modelling and Numerical Analysis, 2021, 55, 131-169.	0.8	1
79	Mathematical Strategies for the Coarse-Graining of Microscopic Models. , 2005, , 1477-1490.		1
80	ISAP-MATLAB Package for Sensitivity Analysis of High-Dimensional Stochastic Chemical Networks. Journal of Statistical Software, 2018, 85, .	1.8	1
81	Uncertainty Quantification for Markov Random Fields. SIAM-ASA Journal on Uncertainty Quantification, 2021, 9, 1457-1498.	1.1	1
82	Coupled Coarse Graining and Markov Chain Monte Carlo for Lattice Systems. Lecture Notes in Computational Science and Engineering, 2012, , 235-257.	0.1	1
83	FROM ATOMISTIC TO SYSTEMATIC COARSE-GRAINED MODELS FOR MOLECULAR SYSTEMS. , 2017, , .		1
84	Systematic Coarse-Grained Models for Molecular Systems Using Entropy. Proceedings (mdpi), 2020, 46, 27.	0.2	0
85	Mathematical Strategies for the Coarse-Graining of Microscopic Models. , 2005, , 1477-1490.		0
86	Optimizing Variational Representations of Divergences and Accelerating their Statistical Estimation. IEEE Transactions on Information Theory, 2022, , 1-1.	1.5	0