Markos A Katsoulakis

List of Publications by Year
in descending order

86 papers	2,476 citations	236833 25 h-index	206029 48 g-index
89 all docs	89 docs citations	89 times ranked	1860 citing authors

#	Article	IF	Citations
1	Cumulant GAN. IEEE Transactions on Neural Networks and Learning Systems, 2023, 34, 9439-9450.	7.2	3
2	Optimizing Variational Representations of Divergences and Accelerating their Statistical Estimation. IEEE Transactions on Information Theory, 2022, , 1-1.	1.5	0
3	Quantification of model uncertainty on path-space *via* goal-oriented relative entropy. ESAIM: Mathematical Modelling and Numerical Analysis, 2021, 55, 131-169.	0.8	1
4	GINNs: Graph-Informed Neural Networks for multiscale physics. Journal of Computational Physics, 2021, 433, 110192.	1.9	18
5	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
6	Mutual information for explainable deep learning of multiscale systems. Journal of Computational Physics, 2021, 444, 110551.	1.9	7
7	Variational Representations and Neural Network Estimation of Rényi Divergences. SIAM Journal on Mathematics of Data Science, 2021, 3, 1093-1116.	1.0	7
8	Uncertainty Quantification for Markov Random Fields. SIAM-ASA Journal on Uncertainty Quantification, 2021, 9, 1457-1498.	1.1	1
9	Data-driven, variational model reduction of high-dimensional reaction networks. Journal of Computational Physics, 2020, 401, 108997.	1.9	10
10	Explainable and trustworthy artificial intelligence for correctable modeling in chemical sciences. Science Advances, 2020, 6, .	4.7	26
11	Data-driven uncertainty quantification for systematic coarse-grained models. Soft Materials, 2020, 18, 348-368.	0.8	2
12	How Biased Is Your Model? Concentration Inequalities, Information and Model Bias. IEEE Transactions on Information Theory, 2020, 66, 3079-3097.	1.5	13
13	Systematic Coarse-Grained Models for Molecular Systems Using Entropy. Proceedings (mdpi), 2020, 46, 27.	0.2	0
14	Sensitivity analysis for rare events based on Rényi divergence. Annals of Applied Probability, 2020, 30, .	0.6	10
15	Causality and Bayesian Network PDEs for multiscale representations of porous media. Journal of Computational Physics, 2019, 394, 658-678.	1.9	13
16	Global sensitivity analysis of multiscale properties of porous materials. Journal of Applied Physics, 2018, 123, 075103.	1.1	9
17	Non-parametric correlative uncertainty quantification and sensitivity analysis: Application to a Langmuir bimolecular adsorption model. AIP Advances, 2018, 8, .	0.6	8
18	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

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19	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
20	ISAP-<i>MATLAB</i> Package for Sensitivity Analysis of High-Dimensional Stochastic Chemical Networks. Journal of Statistical Software, 2018, 85, .	1.8	1
21	Scalable information inequalities for uncertainty quantification. Journal of Computational Physics, 2017, 336, 513-545.	1.9	14
22	Information criteria for quantifying loss of reversibility in parallelized KMC. Journal of Computational Physics, 2017, 328, 438-454.	1.9	2
23	FROM ATOMISTIC TO SYSTEMATIC COARSE-GRAINED MODELS FOR MOLECULAR SYSTEMS. , 2017, , .		1
24	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
25	Efficient estimators for likelihood ratio sensitivity indices of complex stochastic dynamics. Journal of Chemical Physics, 2016, 144, 104107.	1.2	9
26	Uncertainty quantification for generalized Langevin dynamics. Journal of Chemical Physics, 2016, 145, 224108.	1.2	7
27	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
28	Path-space variational inference for non-equilibrium coarse-grained systems. Journal of Computational Physics, 2016, 314, 355-383.	1.9	32
29	Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling. Nature Chemistry, 2016, 8, 331-337.	6.6	131
30	Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics. Journal of Chemical Physics, 2015, 143, 014116.	1.2	13
31	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
32	Pathwise Sensitivity Analysis in Transient Regimes. Mathematical Engineering, 2015, , 105-124.	0.1	2
33	Accelerated Sensitivity Analysis in High-Dimensional Stochastic Reaction Networks. PLoS ONE, 2015, 10, e0130825.	1.1	11
34	Measuring the Irreversibility of Numerical Schemes for Reversible Stochastic Differential Equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2014, 48, 1351-1379.	0.8	5
35	Goal-oriented sensitivity analysis for lattice kinetic Monte Carlo simulations. Journal of Chemical Physics, 2014, 140, 124108.	1.2	12
36	Spatial Two-Level Interacting Particle Simulations and Information Theory–Based Error Quantification. SIAM Journal of Scientific Computing, 2014, 36, A634-A667.	1.3	5

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37	Parallelization, Processor Communication and Error Analysis in Lattice Kinetic Monte Carlo. SIAM Journal on Numerical Analysis, 2014, 52, 1156-1182.	1.1	8
38	Coarse-graining schemes for stochastic lattice systems with short and long-range interactions. Mathematics of Computation, 2014, 83, 1757-1793.	1.1	4
39	Parametric sensitivity analysis for biochemical reaction networks based on pathwise information theory. BMC Bioinformatics, 2013, 14, 311.	1.2	22
40	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
41	Information-theoretic tools for parametrized coarse-graining of non-equilibrium extended systems. Journal of Chemical Physics, 2013, 139, 074115.	1.2	36
42	Deterministic equations for stochastic spatial evolutionary games. Theoretical Economics, 2013, 8, 829-874.	0.5	12
43	Hierarchical fractional-step approximations and parallel kinetic Monte Carlo algorithms. Journal of Computational Physics, 2012, 231, 7795-7814.	1.9	18
44	Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems. Journal of Computational Physics, 2012, 231, 2599-2620.	1.9	9
45	Coupled Coarse Graining and Markov Chain Monte Carlo for Lattice Systems. Lecture Notes in Computational Science and Engineering, 2012, , 235-257.	0.1	1
46	A novel multi-layer framework for modeling the evolution of spectrum markets and cognitive-radio devices. , 2011, , .		3
47	Long-time integration methods for mesoscopic models of pattern-forming systems. Journal of Computational Physics, 2011, 230, 5704-5715.	1.9	9
48	Multibody Interactions in Coarse-Graining Schemes for Extended Systems. SIAM Journal of Scientific Computing, 2009, 31, 987-1015.	1.3	10
49	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
50	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
51	Numerical and Statistical Methods forÂtheÂCoarse-Graining ofÂMany-Particle Stochastic Systems. Journal of Scientific Computing, 2008, 37, 43-71.	1.1	14
52	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
53	Coarse-graining schemes and <i>a posteriori</i> error estimates for stochastic lattice systems. ESAIM: Mathematical Modelling and Numerical Analysis, 2007, 41, 627-660.	0.8	16
54	Noise regularization and computations for the 1-dimensional stochastic Allenâ€"Cahn problem. Interfaces and Free Boundaries, 2007, 9, 1-30.	0.2	26

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55	The role of multiple microscopic mechanisms in cluster interface evolution. Journal of Differential Equations, 2007, 235, 418-438.	1.1	20
56	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
57	Error Analysis of Coarse–Graining for Stochastic Lattice Dynamics. SIAM Journal on Numerical Analysis, 2006, 44, 2270-2296.	1.1	25
58	Mechanistic principles of nanoparticle evolution to zeolite crystals. Nature Materials, 2006, 5, 400-408.	13.3	416
59	Information Loss in Coarse-Graining of Stochastic Particle Dynamics. Journal of Statistical Physics, 2006, 122, 115-135.	0.5	25
60	Stochastic hydrodynamical limits of particle systems. Communications in Mathematical Sciences, 2006, 4, 513-549.	0.5	9
61	Mesoscopic Modeling for Continuous Spin Lattice Systems: Model Problems and Micromagnetics Applications. Journal of Statistical Physics, 2005, 119, 347-389.	0.5	4
62	A Mathematical Model for Crystal Growth by Aggregation of Precursor Metastable Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 23879-23887.	1.2	59
63	Binomial distribution based τ-leap accelerated stochastic simulation. Journal of Chemical Physics, 2005, 122, 024112.	1.2	184
64	Mathematical Strategies for the Coarse-Graining of Microscopic Models. , 2005, , 1477-1490.		1
65	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
66	Mathematical Strategies for the Coarse-Graining of Microscopic Models. , 2005, , 1477-1490.		0
67	Mesoscopic Modeling of Surface Processes. The IMA Volumes in Mathematics and Its Applications, 2004, , 179-198.	0.5	4
68	Spatially adaptive lattice coarse-grained Monte Carlo simulations for diffusion of interacting molecules. Journal of Chemical Physics, 2004, 121, 11420.	1.2	45
69	Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. Journal of Computational Physics, 2003, 186, 250-278.	1.9	107
70	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
71	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
72	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

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73	Spectral Methods for Mesoscopic Models of Pattern Formation. Journal of Computational Physics, 2001, 173, 364-390.	1.9	35
74	Stochastic curvature flows: asymptotic derivation, level set formulation and numerical experiments. Interfaces and Free Boundaries, 2001, 3, 265-290.	0.2	11
75	From Microscopic Interactions to Macroscopic Laws of Cluster Evolution. Physical Review Letters, 2000, 84, 1511-1514.	2.9	33
76	Derivation and Validation of Mesoscopic Theories for Diffusion of Interacting Molecules. Physical Review Letters, 2000, 85, 3898-3901.	2.9	63
77	Hyperbolic Systems with Supercharacteristic Relaxations and Roll Waves. SIAM Journal on Applied Mathematics, 2000, 61, 273-292.	0.8	19
78	Multiscale Analysis for Interacting Particles: Relaxation Systems and Scalar Conservation Laws. , 1999, 96, 715-763.		8
79	Relaxation schemes for curvature-dependent front propagation. , 1999, 52, 1587-1615.		8
80	Contractive relaxation systems and the scalar multidimensional conservation law. Communications in Partial Differential Equations, 1997, 22, 225-267.	1.0	73
81	Relaxation Approximations to Front Propagation. Journal of Differential Equations, 1997, 138, 380-387.	1.1	8
82	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
83	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
84	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
85	Interacting particle systems and generalized evolution of fronts. Archive for Rational Mechanics and Analysis, 1994, 127, 133-157.	1.1	38
86	Title is missing!. Indiana University Mathematics Journal, 1994, 43, 493.	0.4	49