Xiantao Li

List of Publications by Year
in descending order

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57	790	687363 13	526287 27
papers	citations	h-index	g-index

57	57	57	507
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Projectionâ€based model reduction for the immersed boundary method. International Journal for Numerical Methods in Biomedical Engineering, 2022, 38, e3558.	2.1	1
2	Some error analysis for the quantum phase estimation algorithms. Journal of Physics A: Mathematical and Theoretical, 2022, 55, 325303.	2.1	1
3	Markovian embedding procedures for non-Markovian stochastic SchrÃ¶dinger equations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 387, 127036.	2.1	3
4	Nonlinear Constitutive Models for Nano-Scale Heat Conduction. Multiscale Modeling and Simulation, 2021, 19, 533-549.	1.6	0
5	Linear response based parameter estimation in the presence of model error. Journal of Computational Physics, 2021, 430, 110112.	3.8	1
6	Petrovâ€“Galerkin methods for the construction of non-Markovian dynamics preserving nonlocal statistics. Journal of Chemical Physics, 2021, 154, 184108.	3.0	2
7	A projection-based reduced-order method for electron transport problems with long-range interactions. Journal of Chemical Physics, 2021, 155, 114105.	3.0	1
8	Error bounds of the invariant statistics in machine learning of ergodic ItÃ´ diffusions. Physica D: Nonlinear Phenomena, 2021, 427, 133022.	2.8	4
9	Absorbing boundary conditions for the time-dependent SchrÃ¶dinger-type equations in R3. Physical Review E, 2020, 101, 013304.	2.1	4
10	Data-driven molecular modeling with the generalized Langevin equation. Journal of Computational Physics, 2020, 418, 109633.	3.8	21
11	Exponential integrators for stochastic SchrÃ¶dinger equations. Physical Review E, 2020, 101, 013312.	2.1	5
12	Reduced-Order Modeling Approach for Electron Transport in Molecular Junctions. Journal of Chemical Theory and Computation, 2020, 16, 3746-3756.	5.3	2
13	Estimating linear response statistics using orthogonal polynomials: An rkhs formulation. , 2020, 2, 443-485.		7
14	The computation of local stress in ab initio molecular simulations. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 065016.	2.0	0
15	Absorbing boundary conditions for time-dependent SchrÃ¶dinger equations: A density-matrix formulation. Journal of Chemical Physics, 2019, 150, 114111.	3.0	7
16	A parameter estimation method using linear response statistics: Numerical scheme. Chaos, 2019, 29, 033101.	2.5	5
17	Coarse-graining Langevin dynamics using reduced-order techniques. Journal of Computational Physics, 2019, 380, 170-190.	3.8	13
18	The Moriâ€“Zwanzig formalism for the derivation of a fluctuating heat conduction model from molecular dynamics. Communications in Mathematical Sciences, 2019, 17, 539-563.	1.0	9

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19	On the Asymptotic Behavior of the Kernel Function in the Generalized Langevin Equation: A One-Dimensional Lattice Model. Journal of Statistical Physics, 2018, 170, 378-398.	1.2	3
20	Stable absorbing boundary conditions for molecular dynamics in general domains. Computational Mechanics, 2018, 62, 1259-1272.	4.0	5
21	PEXSI-$Sigma$: a Greenâ€™s function embedding method for Kohnâ€“Sham density functional theory. Annals of Mathematical Sciences and Applications, 2018, 3, 441-472.	0.4	4
22	Simulations of micron-scale fracture using atomistic-based boundary element method. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085008.	2.0	1
23	A Parameter Estimation Method Using Linear Response Statistics. Journal of Statistical Physics, 2017, 168, 146-170.	1.2	4
24	Fluctuation-dissipation theorem consistent approximation of the Langevin dynamics model. Communications in Mathematical Sciences, 2017, 15, 1171-1181.	1.0	2
25	Data-driven parameterization of the generalized Langevin equation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14183-14188.	7.1	103
26	The derivation and approximation of coarse-grained dynamics from Langevin dynamics. Journal of Chemical Physics, 2016, 145, 204117.	3.0	26
27	From generalized Langevin equations to Brownian dynamics and embedded Brownian dynamics. Journal of Chemical Physics, 2016, 145, 114102.	3.0	5
28	Traction boundary conditions for molecular static simulations. Computer Methods in Applied Mechanics and Engineering, 2016, 308, 310-329.	6.6	3
29	Parametric reduced models for the nonlinear SchrÃ¶dinger equation. Physical Review E, 2015, 91, 053306.	2.1	12
30	Incorporation of memory effects in coarse-grained modeling via the Mori-Zwanzig formalism. Journal of Chemical Physics, 2015, 143, 243128.	3.0	107
31	An Atomistic/Continuum Coupling Method Using Enriched Bases. Multiscale Modeling and Simulation, 2015, 13, 766-789.	1.6	3
32	On consistent definitions of momentum and energy fluxes for molecular dynamics models with multi-body interatomic potentials. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 015003.	2.0	6
33	On the Cauchyâ€“Born approximation at finite temperature. Computational Materials Science, 2015, 99, 21-28.	3.0	3
34	Coarseâ€graining molecular dynamics models using an extended Galerkin projection method. International Journal for Numerical Methods in Engineering, 2014, 99, 157-182.	2.8	13
35	A numerical study of crack initiation in a bcc iron system based on dynamic bifurcation theory. Journal of Applied Physics, 2014, 116, 164314.	2.5	5
36	Computation of the memory functions in the generalized Langevin models for collective dynamics of macromolecules. Journal of Chemical Physics, 2014, 141, 064112.	3.0	31

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37	A Study on the Quasi-continuum Approximations of a One-Dimensional Fracture Model. Multiscale Modeling and Simulation, 2014, 12, 1379-1400.	1.6	3
38	Heat conduction in nanoscale materials: A statistical-mechanics derivation of the local heat flux. Physical Review E, 2014, 90, 032112.	2.1	5
39	On the Effect of Ghost Force in the Quasicontinuum Method: Dynamic Problems in One Dimension. Communications in Computational Physics, 2014, 15, 647-676.	1.7	9
40	A bifurcation study of crack initiation and kinking. European Physical Journal B, 2013, 86, 1.	1.5	8
41	A generalized Irvingâ€“Kirkwood formula for the calculation of stress in molecular dynamics models. Journal of Chemical Physics, 2012, 137, 134104.	3.0	37
42	An atomistic-based boundary element method for the reduction of molecular statics models. Computer Methods in Applied Mechanics and Engineering, 2012, 225-228, 1-13.	6.6	7
43	INTRODUCTION TO MOLECULAR DYNAMICS SIMULATIONS. Lecture Notes Series, Institute for Mathematical Sciences, 2011, , 95-146.	0.2	2
44	A coarseâ€grained molecular dynamics model for crystalline solids. International Journal for Numerical Methods in Engineering, 2010, 83, 986-997.	2.8	38
45	A multiscale coupling method for the modeling of dynamics of solids with application to brittle cracks. Journal of Computational Physics, 2010, 229, 3970-3987.	3.8	27
46	Efficient boundary conditions for molecular statics models of solids. Physical Review B, 2009, 80, .	3.2	12
47	The Heterogeneous Multiscale Method for Dynamics of Solids with Applications to Brittle Cracks. Materials Research Society Symposia Proceedings, 2009, 1229, 10201.	0.1	0
48	On the stability of boundary conditions for molecular dynamics. Journal of Computational and Applied Mathematics, 2009, 231, 493-505.	2.0	11
49	Variational boundary conditions for molecular dynamics simulations: Treatment of the loading condition. Journal of Computational Physics, 2008, 227, 10078-10093.	3.8	12
50	The Discontinuous Galerkin Method for the Multiscale Modeling of Dynamics of Crystalline Solids. Multiscale Modeling and Simulation, 2008, 7, 294-320.	1.6	7
51	Variational boundary conditions for molecular dynamics simulations of crystalline solids at finite temperature: Treatment of the thermal bath. Physical Review B, 2007, 76, .	3.2	44
52	Interface Conditions for Coupled Atomistic and Continuum Models of Solids for Dynamics Problems at Finite Temperature. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
53	Comparative study of boundary conditions for molecular dynamics simulations of solids at low temperature. Physical Review B, 2006, 73, .	3.2	15
54	Multiscale modeling of the dynamics of solids at finite temperature. Journal of the Mechanics and Physics of Solids, 2005, 53, 1650-1685.	4.8	96

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55	Multiscale Modeling Of Crystalline Solids. , 2005, , 1491-1506.		5
56	Some Recent Progress in Multiscale Modeling. Lecture Notes in Computational Science and Engineering, 2004, , 3-21.	0.3	25
57	Quantum simulation in the semi-classical regime. Quantum - the Open Journal for Quantum Science, 0, 6, 739.	0.0	5