Jianfeng Lu

List of Publications by Year in descending order

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		136950	91884
176	5,503	32	69
papers	citations	h-index	g-index

178	178	178	5503
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Defect Resonances of Truncated Crystal Structures. SIAM Journal on Applied Mathematics, 2022, 82, 49-74.	1.8	2
2	Existence and Computation of Generalized Wannier Functions for Non-Periodic Systems in Two Dimensions and Higher. Archive for Rational Mechanics and Analysis, 2022, 243, 1269-1323.	2.4	4
3	Neural collapse under cross-entropy loss. Applied and Computational Harmonic Analysis, 2022, 59, 224-241.	2.2	8
4	A priori generalization error analysis of two-layer neural networks for solving high dimensional SchrÃ¶dinger eigenvalue problems. Communications of the American Mathematical Society, 2022, 2, 1-21.	2.2	6
5	Self-Enhancement of Efficiency and Self-Attenuation of Hysteretic Behavior of Perovskite Solar Cells with Aging. Journal of Physical Chemistry Letters, 2022, 13, 2792-2799.	4.6	16
6	Fast Localization of Eigenfunctions via Smoothed Potentials. Journal of Scientific Computing, 2022, 90, 1.	2.3	2
7	On explicit L2-convergence rate estimate for piecewise deterministic Markov processes in MCMC algorithms. Annals of Applied Probability, 2022, 32, .	1.3	1
8	Universal approximation of symmetric and anti-symmetric functions. Communications in Mathematical Sciences, 2022, 20, 1397-1408.	1.0	4
9	Fast algorithms of bath calculations in simulations of quantum system-bath dynamics. Computer Physics Communications, 2022, 278, 108417.	7.5	4
10	Complexity of zigzag sampling algorithm for strongly log-concave distributions. Statistics and Computing, 2022, 32, .	1.5	1
11	Neural-network quantum states for periodic systems in continuous space. Physical Review Research, 2022, 4, .	3.6	18
12	Optimal Trapping for Brownian Motion: a Nonlinear Analogue of the Torsion Function. Potential Analysis, 2021, 54, 687-698.	0.9	1
13	Solving parametric PDE problems with artificial neural networks. European Journal of Applied Mathematics, 2021, 32, 421-435.	2.9	109
14	The impact of spiro-OMeTAD photodoping on the reversible light-induced transients of perovskite solar cells. Nano Energy, 2021, 82, 105658.	16.0	28
15	A Low-Rank Schwarz Method for Radiative Transfer Equation With Heterogeneous Scattering Coefficient. Multiscale Modeling and Simulation, 2021, 19, 775-801.	1.6	5
16	Computing Edge States without Hard Truncation. SIAM Journal of Scientific Computing, 2021, 43, B323-B353.	2.8	5
17	Numerical methods for stochastic differential equations based on Gaussian mixture. Communications in Mathematical Sciences, 2021, 19, 1549-1577.	1.0	1
18	Efficient Construction of Tensor Ring Representations from Sampling. Multiscale Modeling and Simulation, 2021, 19, 1261-1284.	1.6	7

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19	Deep Network Approximation for Smooth Functions. SIAM Journal on Mathematical Analysis, 2021, 53, 5465-5506.	1.9	45
20	Iterated projected position algorithm for constructing exponentially localized generalized Wannier functions for periodic and nonperiodic insulators in two dimensions and higher. Physical Review B, 2021, 103, .	3.2	5
21	Optimal Artificial Boundary Condition for Random Elliptic Media. Foundations of Computational Mathematics, 2021, 21, 1643-1702.	2.5	1
22	Printing strategies for scaling-up perovskite solar cells. National Science Review, 2021, 8, nwab075.	9.5	48
23	A grid-free approach for simulating sweep and cyclic voltammetry. Journal of Chemical Physics, 2021, 154, 161101.	3.0	1
24	Inclusionâ€“exclusion principle for open quantum systems with bosonic bath. New Journal of Physics, 2021, 23, 063049.	2.9	7
25	Microscopic origins of the crystallographically preferred growth in evaporation-induced colloidal crystals. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	17
26	Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation. Journal of Computational Physics, 2021, 438, 110338.	3.8	3
27	Stable phase retrieval from locally stable and conditionally connected measurements. Applied and Computational Harmonic Analysis, 2021, 55, 440-465.	2.2	5
28	Complexity of randomized algorithms for underdamped Langevin dynamics. Communications in Mathematical Sciences, 2021, 19, 1827-1853.	1.0	4
29	Actor-Critic Method for High Dimensional Static Hamilton–Jacobi–Bellman Partial Differential Equations based on Neural Networks. SIAM Journal of Scientific Computing, 2021, 43, A4043-A4066.	2.8	14
30	Analysis of a fourth-order exponential PDE arising from a crystal surface jump process with Metropolis-type transition rates. Pure and Applied Analysis, 2021, 3, 595-612.	1.1	3
31	A dimension-free Hermiteâ€“Hadamard inequality via gradient estimates for the torsion function. Proceedings of the American Mathematical Society, 2020, 148, 673-679.	0.8	7
32	Quadrature Points via Heat Kernel Repulsion. Constructive Approximation, 2020, 51, 27-48.	3.0	4
33	Stochastic modified equations for the asynchronous stochastic gradient descent. Information and Inference, 2020, 9, 851-873.	1.6	4
34	The Full Configuration Interaction Quantum Monte Carlo Method through the Lens of Inexact Power Iteration. SIAM Journal of Scientific Computing, 2020, 42, B1-B29.	2.8	5
35	Tensor Ring Decomposition: Optimization Landscape and One-loop Convergence of Alternating Least Squares. SIAM Journal on Matrix Analysis and Applications, 2020, 41, 1416-1442.	1.4	6
36	Efficient posterior sampling for high-dimensional imbalanced logistic regression. Biometrika, 2020, 107, 1005-1012.	2.4	7

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37	Continuum limit and preconditioned Langevin sampling of the path integral molecular dynamics. Journal of Computational Physics, 2020, 423, 109788.	3.8	1
38	Random Sampling and Efficient Algorithms for Multiscale PDEs. SIAM Journal of Scientific Computing, 2020, 42, A2974-A3005.	2.8	10
39	Optimal Orbital Selection for Full Configuration Interaction (OptOrbFCI): Pursuing the Basis Set Limit under a Budget. Journal of Chemical Theory and Computation, 2020, 16, 6207-6221.	5.3	8
40	Dirac Operators and Domain Walls. SIAM Journal on Mathematical Analysis, 2020, 52, 1115-1145.	1.9	4
41	Fisher information regularization schemes for Wasserstein gradient flows. Journal of Computational Physics, 2020, 416, 109449.	3.8	19
42	Inchworm Monte Carlo Method for Open Quantum Systems. Communications on Pure and Applied Mathematics, 2020, 73, 2430-2472.	3.1	11
43	Discontinuous Hamiltonian Monte Carlo for discrete parameters and discontinuous likelihoods. Biometrika, 2020, 107, 365-380.	2.4	21
44	ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	7.5	27
45	A stochastic version of Stein variational gradient descent for efficient sampling. Communications in Applied Mathematics and Computational Science, 2020, 15, 37-63.	1.8	14
46	Variational training of neural network approximations of solution maps for physical models. Journal of Computational Physics, 2020, 409, 109338.	3.8	20
47	Solvent Engineering of a Dopant-Free Spiro-OMeTAD Hole-Transport Layer for Centimeter-Scale Perovskite Solar Cells with High Efficiency and Thermal Stability. ACS Applied Materials & Interfaces, 2020, 12, 8260-8270.	8.0	42
48	Solving high-dimensional eigenvalue problems using deep neural networks: A diffusion Monte Carlo like approach. Journal of Computational Physics, 2020, 423, 109792.	3.8	40
49	Synchronization of Kuramoto oscillators in dense networks. Nonlinearity, 2020, 33, 5905-5918.	1.4	8
50	Randomized Sampling for Basis Function Construction in Generalized Finite Element Methods. Multiscale Modeling and Simulation, 2020, 18, 1153-1177.	1.6	11
51	Butterfly-Net: Optimal Function Representation Based on Convolutional Neural Networks. Communications in Computational Physics, 2020, 28, 1838-1885.	1.7	2
52	Estimating normalizing constants for log-concave distributions: algorithms and lower bounds. , 2020, , .		2
53	Analysis of a continuum theory for broken bond crystal surface models with evaporation and deposition effects. Nonlinearity, 2020, 33, 3816-3845.	1.4	7
54	Light induced degradation in mixed-halide perovskites. Journal of Materials Chemistry C, 2019, 7, 9326-9334.	5.5	67

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55	Oriented Attachment as the Mechanism for Microstructure Evolution in Chloride-Derived Hybrid Perovskite Thin Films. ACS Applied Materials & Interfaces, 2019, 11, 39930-39939.	8.0	26
56	A numerical method for coupling the BGK model and Euler equations through the linearized Knudsen layer. Journal of Computational Physics, 2019, 398, 108893.	3.8	2
57	Methodological and Computational Aspects of Parallel Tempering Methods in the Infinite Swapping Limit. Journal of Statistical Physics, 2019, 174, 715-733.	1.2	3
58	Fatigue stability of CH3NH3PbI3 based perovskite solar cells in day/night cycling. Nano Energy, 2019, 58, 687-694.	16.0	46
59	Exponential Decay of RÃ©nyi Divergence Under Fokkerâ€“Planck Equations. Journal of Statistical Physics, 2019, 176, 1172-1184.	1.2	8
60	Approximating pointwise products of Laplacian eigenfunctions. Journal of Functional Analysis, 2019, 277, 3271-3282.	1.4	8
61	Gradient flow structure and exponential decay of the sandwiched RÃ©nyi divergence for primitive Lindblad equations with GNS-detailed balance. Journal of Mathematical Physics, 2019, 60, .	1.1	4
62	Numerical methods for Kohnâ€“Sham density functional theory. Acta Numerica, 2019, 28, 405-539.	10.7	23
63	Scaling Limit of the Stein Variational Gradient Descent: The Mean Field Regime. SIAM Journal on Mathematical Analysis, 2019, 51, 648-671.	1.9	25
64	Coordinate Descent Full Configuration Interaction. Journal of Chemical Theory and Computation, 2019, 15, 3558-3569.	5.3	31
65	Bold diagrammatic Monte Carlo in the lens of stochastic iterative methods. Transactions of Mathematics and Its Applications, 2019, 3, .	3.3	1
66	Asymmetry in crystal facet dynamics of homoepitaxy by a continuum model. Physica D: Nonlinear Phenomena, 2019, 393, 54-67.	2.8	9
67	The simulated tempering method in the infinite switch limit with adaptive weight learning. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 013207.	2.3	10
68	Stop Memorizing: A Data-Dependent Regularization Framework for Intrinsic Pattern Learning. SIAM Journal on Mathematics of Data Science, 2019, 1, 476-496.	1.8	2
69	CoordinateWise Descent Methods for Leading Eigenvalue Problem. SIAM Journal of Scientific Computing, 2019, 41, A2681-A2716.	2.8	16
70	Learning interacting particle systems: Diffusion parameter estimation for aggregation equations. Mathematical Models and Methods in Applied Sciences, 2019, 29, 1-29.	3.3	9
71	Solving for high-dimensional committor functions using artificial neural networks. Research in Mathematical Sciences, 2019, 6, 1.	1.0	76
72	Interfacial benzenethiol modification facilitates charge transfer and improves stability of cm-sized metal halide perovskite solar cells with up to 20% efficiency. Energy and Environmental Science, 2018, 11, 1880-1889.	30.8	148

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73	Convergence of Phase-Field Free Energy and Boundary Force for Molecular Solvation. Archive for Rational Mechanics and Analysis, 2018, 227, 105-147.	2.4	14
74	A Quantum Kinetic Monte Carlo Method for Quantum Many-Body Spin Dynamics. SIAM Journal of Scientific Computing, 2018, 40, B706-B722.	2.8	2
75	A Mathematical Theory of Optimal Milestoning (with a Detour via Exact Milestoning). Communications on Pure and Applied Mathematics, 2018, 71, 1149-1177.	3.1	4
76	ELSI: A unified software interface for Kohnâ€“Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	7.5	78
77	Analysis of Multiscale Integrators for Multiple Attractors and Irreversible Langevin Samplers. Multiscale Modeling and Simulation, 2018, 16, 1859-1883.	1.6	3
78	A Diabatic Surface Hopping Algorithm Based on Time Dependent Perturbation Theory and Semiclassical Analysis. Multiscale Modeling and Simulation, 2018, 16, 1603-1622.	1.6	3
79	A Surface Hopping Gaussian Beam Method for High-Dimensional Transport Systems. SIAM Journal of Scientific Computing, 2018, 40, B1277-B1301.	2.8	1
80	Trigonometric integrators for quasilinear wave equations. Mathematics of Computation, 2018, 88, 717-749.	2.1	13
81	Detecting localized eigenstates of linear operators. Research in Mathematical Sciences, 2018, 5, 1.	1.0	11
82	Frozen Gaussian approximation for high frequency wave propagation in periodic media. Asymptotic Analysis, 2018, 110, 113-135.	0.5	1
83	Integrated tempering enhanced sampling method as the infinite switching limit of simulated tempering. Journal of Chemical Physics, 2018, 149, 084114.	3.0	7
84	Phase-Space Sketching for Crystal Image Analysis Based on Synchrosqueezed Transforms. SIAM Journal on Imaging Sciences, 2018, 11, 1954-1978.	2.2	5
85	Moderate deviation for random elliptic PDE with small noise. Annals of Applied Probability, 2018, 28, .	1.3	2
86	A Quasi-nonlocal Coupling Method for Nonlocal and Local Diffusion Models. SIAM Journal on Numerical Analysis, 2018, 56, 1386-1404.	2.3	25
87	Accelerated sampling by infinite swapping of path integral molecular dynamics with surface hopping. Journal of Chemical Physics, 2018, 148, 064110.	3.0	5
88	Stochastic dynamical low-rank approximation method. Journal of Computational Physics, 2018, 372, 564-586.	3.8	3
89	Thermodynamic Limit of Crystal Defects with Finite Temperature Tight Binding. Archive for Rational Mechanics and Analysis, 2018, 230, 701-733.	2.4	15
90	Point Cloud Discretization of Fokker--Planck Operators for Committor Functions. Multiscale Modeling and Simulation, 2018, 16, 710-726.	1.6	13

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91	A Concurrent Globalâ€“Local Numerical Method for Multiscale PDEs. Journal of Scientific Computing, 2018, 76, 1188-1215.	2.3	3
92	Fundamental Limitations for Measurements in Quantum Many-Body Systems. Physical Review Letters, 2018, 121, 080406.	7.8	5
93	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
94	Wavepackets in inhomogeneous periodic media: Effective particle-field dynamics and Berry curvature. Journal of Mathematical Physics, 2017, 58, 021503.	1.1	10
95	Orbital minimization method with â„“1 regularization. Journal of Computational Physics, 2017, 336, 87-103.	3.8	8
96	Path integral molecular dynamics with surface hopping for thermal equilibrium sampling of nonadiabatic systems. Journal of Chemical Physics, 2017, 146, 154110.	3.0	18
97	Continuum Limit of a Mesoscopic Model with Elasticity of Step Motion on Vicinal Surfaces. Journal of Nonlinear Science, 2017, 27, 873-926.	2.1	10
98	Weak Solution of a Continuum Model For Vicinal Surface in The Attachment-Detachment-Limited Regime. SIAM Journal on Mathematical Analysis, 2017, 49, 1705-1731.	1.9	12
99	Preconditioning Orbital Minimization Method for Planewave Discretization. Multiscale Modeling and Simulation, 2017, 15, 254-273.	1.6	8
100	Diammonium and Monoammonium Mixedâ€Organicâ€Cation Perovskites for High Performance Solar Cells with Improved Stability. Advanced Energy Materials, 2017, 7, 1700444.	19.5	121
101	On extending Kohn-Sham density functionals to systems with fractional number of electrons. Journal of Chemical Physics, 2017, 146, 214109.	3.0	5
102	Cubic scaling algorithms for RPA correlation using interpolative separable density fitting. Journal of Computational Physics, 2017, 351, 187-202.	3.8	36
103	Quasi-nonlocal Coupling of Nonlocal Diffusions. SIAM Journal on Numerical Analysis, 2017, 55, 2394-2415.	2.3	7
104	A variation on the Donskerâ€“Varadhan inequality for the principal eigenvalue. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2017, 473, 20160877.	2.1	1
105	Fractional Stochastic Differential Equations Satisfying Fluctuation-Dissipation Theorem. Journal of Statistical Physics, 2017, 169, 316-339.	1.2	21
106	A cubic scaling algorithm for excited states calculations in particleâ€“particle random phase approximation. Journal of Computational Physics, 2017, 340, 297-308.	3.8	5
107	Phase Segregation Enhanced Ion Movement in Efficient Inorganic CsPbIBr₂ Solar Cells. Advanced Energy Materials, 2017, 7, 1700946.	19.5	318
108	Validity and Regularization of Classical Half-Space Equations. Journal of Statistical Physics, 2017, 166, 398-433.	1.2	13

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109	Removal of Canvas Patterns in Digital Acquisitions of Paintings. IEEE Transactions on Image Processing, 2017, 26, 160-171.	9.8	19
110	Dislocation climb models from atomistic scheme to dislocation dynamics. Journal of the Mechanics and Physics of Solids, 2017, 99, 242-258.	4.8	29
111	Lindblad equation and its semiclassical limit of the Anderson-Holstein model. Journal of Mathematical Physics, 2017, 58, .	1.1	5
112	An Asymptotic Preserving Method for Transport Equations with Oscillatory Scattering Coefficients. Multiscale Modeling and Simulation, 2017, 15, 1694-1718.	1.6	3
113	A convergent method for linear half-space kinetic equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2017, 51, 1583-1615.	1.9	10
114	Frozen Gaussian approximation with surface hopping for mixed quantum-classical dynamics: A mathematical justification of fewest switches surface hopping algorithms. Mathematics of Computation, 2017, 87, 2189-2232.	2.1	12
115	Half-space kinetic equations with general boundary conditions. Mathematics of Computation, 2016, 86, 1269-1301.	2.1	12
116	Thermalization of oscillator chains with onsite anharmonicity and comparison with kinetic theory. Physical Review E, 2016, 94, 062104.	2.1	5
117	Improved sampling and validation of frozen Gaussian approximation with surface hopping algorithm for nonadiabatic dynamics. Journal of Chemical Physics, 2016, 145, 124109.	3.0	11
118	Localized density matrix minimization and linear-scaling algorithms. Journal of Computational Physics, 2016, 315, 194-210.	3.8	5
119	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.	7.1	32
120	Decay estimates of discretized Greenâ€™s functions for SchrÃ¶dinger type operators. Science China Mathematics, 2016, 59, 1561-1578.	1.7	5
121	Gauge-Invariant Frozen Gaussian Approximation Method for the SchrÃ¶dinger Equation with Periodic Potentials. SIAM Journal of Scientific Computing, 2016, 38, A2440-A2463.	2.8	7
122	Sparsifying preconditioner for soliton calculations. Journal of Computational Physics, 2016, 315, 458-466.	3.8	2
123	Combining 2D synchrosqueezed wave packet transform with optimization for crystal image analysis. Journal of the Mechanics and Physics of Solids, 2016, 89, 194-210.	4.8	12
124	Traction boundary conditions for molecular static simulations. Computer Methods in Applied Mechanics and Engineering, 2016, 308, 310-329.	6.6	3
125	Analysis of the divide-and-conquer method for electronic structure calculations. Mathematics of Computation, 2016, 85, 2919-2938.	2.1	5
126	Fast algorithm for periodic density fitting for Bloch waves. Annals of Mathematical Sciences and Applications, 2016, 1, 321-339.	0.4	13

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127	Crystal Image Analysis Using 2D Synchrosqueezed Transforms. Multiscale Modeling and Simulation, 2015, 13, 1542-1572.	1.6	24
128	Gentlest ascent dynamics for calculating first excited state and exploring energy landscape of Kohn-Sham density functionals. Journal of Chemical Physics, 2015, 143, 224110.	3.0	7
129	Classification of whale vocalizations using the Weyl transform. , 2015, , .		4
130	Efficient Rare Event Simulation for Failure Problems in Random Media. SIAM Journal of Scientific Computing, 2015, 37, A609-A624.	2.8	7
131	Orbital-Free Density Functional Theory of Out-of-Plane Charge Screening in Graphene. Journal of Nonlinear Science, 2015, 25, 1391-1430.	2.1	12
132	Emergence of step flow from an atomistic scheme of epitaxial growth in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mo>+</mml:mo 2.4 mml:mn>1</mml:m Physical Review E, 2015, 91, 032403.		7
133	Diffusion approximations and domain decomposition method of linear transport equations: Asymptotics and numerics. Journal of Computational Physics, 2015, 292, 141-167.	3.8	16
134	Numerical scheme for a spatially inhomogeneous matrix-valued quantum Boltzmann equation. Journal of Computational Physics, 2015, 291, 303-316.	3.8	1
135	Quantitative Canvas Weave Analysis Using 2-D Synchrosqueezed Transforms: Application of time-frequency analysis to art investigation. IEEE Signal Processing Magazine, 2015, 32, 55-63.	5.6	36
136	Compression of the electron repulsion integral tensor in tensor hypercontraction format with cubic scaling cost. Journal of Computational Physics, 2015, 302, 329-335.	3.8	68
137	Reactive trajectories and the transition path process. Probability Theory and Related Fields, 2015, 161, 195-244.	1.8	33
138	Strang splitting methods for a quasilinear SchrÃ¶dinger equation: convergence, instability, and dynamics. Communications in Mathematical Sciences, 2015, 13, 1051-1074.	1.0	7
139	Density matrix minimization with ${ell}_1$ regularization. Communications in Mathematical Sciences, 2015, 13, 2097-2117.	1.0	9
140	Analysis of Time Reversible Born-Oppenheimer Molecular Dynamics. Entropy, 2014, 16, 110-137.	2.2	24
141	Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies. Journal of Chemical Physics, 2014, 141, 124104.	3.0	40
142	Stability Of A Force-Based Hybrid Method With Planar Sharp Interface. SIAM Journal on Numerical Analysis, 2014, 52, 2005-2026.	2.3	7
143	Exact dynamical coarse-graining without time-scale separation. Journal of Chemical Physics, 2014, 141, 044109.	3.0	40
144	Nonexistence of a Minimizer for Thomasâ€“Fermiâ€“Diracâ€“von WeizsÃcker Model. Communications on Pure and Applied Mathematics, 2014, 67, 1605-1617.	3.1	57

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145	A Variational Perspective on Cloaking by Anomalous Localized Resonance. Communications in Mathematical Physics, 2014, 328, 1-27.	2.2	55
146	Mathematical theory of solids: From quantum mechanics to continuum models. Discrete and Continuous Dynamical Systems, 2014, 34, 5085-5097.	0.9	0
147	Convergence of a Forceâ€Based Hybrid Method in Three Dimensions. Communications on Pure and Applied Mathematics, 2013, 66, 83-108.	3.1	26
148	Infinite swapping replica exchange molecular dynamics leads to a simple simulation patch using mixture potentials. Journal of Chemical Physics, 2013, 138, 084105.	3.0	17
149	Seismic modeling using the frozen Gaussian approximation. , 2013, , .		5
150	Frozen Gaussian Approximation for General Linear Strictly Hyperbolic Systems: Formulation and Eulerian Methods. Multiscale Modeling and Simulation, 2012, 10, 451-472.	1.6	18
151	Stability and the continuum limit of the spin-polarized Thomas-Fermi-Dirac-von WeizsÃcker model. Journal of Mathematical Physics, 2012, 53, .	1.1	2
152	Convergence of frozen Gaussian approximation for highâ€frequency wave propagation. Communications on Pure and Applied Mathematics, 2012, 65, 759-789.	3.1	29
153	Adaptive local basis set for Kohnâ€“Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation. Journal of Computational Physics, 2012, 231, 2140-2154.	3.8	162
154	Optimized local basis set for Kohnâ€“Sham density functional theory. Journal of Computational Physics, 2012, 231, 4515-4529.	3.8	9
155	The Kohn-Sham equation for deformed crystals. Memoirs of the American Mathematical Society, 2012, 221, 1.	0.9	13
156	Markov state models based on milestoning. Journal of Chemical Physics, 2011, 134, 204105.	3.0	184
157	Effective Maxwell equations from time-dependent density functional theory. Acta Mathematica Sinica, English Series, 2011, 27, 339-368.	0.6	6
158	The Electronic Structure of Smoothly Deformed Crystals: Wannier Functions and the Cauchyâ€“Born Rule. Archive for Rational Mechanics and Analysis, 2011, 199, 407-433.	2.4	26
159	Fast construction of hierarchical matrix representation from matrixâ€“vector multiplication. Journal of Computational Physics, 2011, 230, 4071-4087.	3.8	72
160	Synchrosqueezed wavelet transforms: An empirical mode decomposition-like tool. Applied and Computational Harmonic Analysis, 2011, 30, 243-261.	2.2	1,698
161	A Fast Parallel Algorithm for Selected Inversion of Structured Sparse Matrices with Application to 2D Electronic Structure Calculations. SIAM Journal of Scientific Computing, 2011, 33, 1329-1351.	2.8	35
162	SelInv--An Algorithm for Selected Inversion of a Sparse Symmetric Matrix. ACM Transactions on Mathematical Software, 2011, 37, 1-19.	2.9	167

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163	Multiscale modeling. Scholarpedia Journal, 2011, 6, 11527.	0.3	15
164	Frozen Gaussian approximation for high frequency wave propagation. Communications in Mathematical Sciences, 2011, 9, 663-683.	1.0	33
165	Electronic structure of smoothly deformed crystals: Cauchyâ€born rule for the nonlinear tightâ€binding model. Communications on Pure and Applied Mathematics, 2010, 63, 1432-1468.	3.1	20
166	Localized bases of eigensubspaces and operator compression. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1273-1278.	7.1	52
167	Linear-scaling subspace-iteration algorithm with optimally localized nonorthogonal wave functions for Kohn-Sham density functional theory. Physical Review B, 2009, 79, .	3.2	32
168	Multipole representation of the Fermi operator with application to the electronic structure analysis of metallic systems. Physical Review B, 2009, 79, .	3.2	23
169	Pole-Based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics Series B, 2009, 30, 729-742.	0.4	46
170	Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems. Communications in Mathematical Sciences, 2009, 7, 755-777.	1.0	59
171	The Elastic Continuum Limit of the Tight Binding Model*. Chinese Annals of Mathematics Series B, 2007, 28, 665-676.	0.4	7
172	Seamless multiscale modeling via dynamics on fiber bundles. Communications in Mathematical Sciences, 2007, 5, 649-663.	1.0	12
173	The continuum limit and QM-continuum approximation of quantum mechanical models of solids. Communications in Mathematical Sciences, 2007, 5, 679-696.	1.0	2
174	A sub-linear scaling algorithm for computing the electronic structure of materials. Communications in Mathematical Sciences, 2007, 5, 999-1026.	1.0	17
175	Uniform accuracy of the quasicontinuum method. Physical Review B, 2006, 74, .	3.2	86
176	Tensorization of the strong data processing inequality for quantum chi-square divergences. Quantum - the Open Journal for Quantum Science, 0, 3, 199.	0.0	1