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List of Publications by Year
in descending order

163 papers	15,541 citations	19657 61 h-index	17592 121 g-index
163 all docs	163 docs citations	163 times ranked	8916 citing authors

#	Article	IF	Citations
1	A Mathematical Model for Universal Semantics. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2022, 44, 1124-1132.	13.9	0
2	The Barron Space and the Flow-Induced Function Spaces for Neural Network Models. Constructive Approximation, 2022, 55, 369-406.	3.0	26
3	Representation formulas and pointwise properties for Barron functions. Calculus of Variations and Partial Differential Equations, 2022, 61, 1.	1.7	5
4	Algorithms for solving high dimensional PDEs: from nonlinear Monte Carlo to machine learning. Nonlinearity, 2022, 35, 278-310.	1.4	37
5	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
6	Generalization error of GAN from the discriminatorâ€™s perspective. Research in Mathematical Sciences, 2022, 9, 1.	1.0	4
7	Deep potentials for materials science. Materials Futures, 2022, 1, 022601.	8.4	61
8	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
9	DeePKS: A Comprehensive Data-Driven Approach toward Chemically Accurate Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 170-181.	5.3	40
10	Coarse-grained spectral projection: A deep learning assisted approach to quantum unitary dynamics. Physical Review B, 2021, 103, .	3.2	3
11	Deep potential generation scheme and simulation protocol for the Li10GeP2S12-type superionic conductors. Journal of Chemical Physics, 2021, 154, 094703.	3.0	49
12	Phase Diagram of a Deep Potential Water Model. Physical Review Letters, 2021, 126, 236001.	7.8	140
13	Machine-learning-assisted modeling. Physics Today, 2021, 74, 36-41.	0.3	11
14	Kolmogorov width decay and poor approximators in machine learning: shallow neural networks, random feature models and neural tangent kernels. Research in Mathematical Sciences, 2021, 8, 1.	1.0	8
15	Multilevel Picard iterations for solving smooth semilinear parabolic heat equations. SN Partial Differential Equations and Applications, 2021, 2, 1.	0.6	14
16	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
17	Ground State Energy Functional with Hartreeâ€“Fock Efficiency and Chemical Accuracy. Journal of Physical Chemistry A, 2020, 124, 7155-7165.	2.5	42
18	Machine learning from a continuous viewpoint, I. Science China Mathematics, 2020, 63, 2233-2266.	1.7	24

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19	Machine-learning-based non-Newtonian fluid model with molecular fidelity. Physical Review E, 2020, 102, 043309.	2.1	15
20	A Priori Estimates of the Generalization Error for Autoencoders. , 2020, , .		0
21	A comparative analysis of optimization and generalization properties of two-layer neural network and random feature models under gradient descent dynamics. Science China Mathematics, 2020, 63, 1235-1258.	1.7	22
22	DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models. Computer Physics Communications, 2020, 253, 107206.	7.5	271
23	Modeling subgrid-scale forces by spatial artificial neural networks in large eddy simulation of turbulence. Physical Review Fluids, 2020, 5, .	2.5	68
24	Can Shallow Neural Networks Beat the Curse of Dimensionality? A Mean Field Training Perspective. IEEE Transactions on Artificial Intelligence, 2020, 1, 121-129.	4.7	19
25	Rademacher complexity and the generalization error of residual networks. Communications in Mathematical Sciences, 2020, 18, 1755-1774.	1.0	2
26	Solving many-electron SchrÃ¶dinger equation using deep neural networks. Journal of Computational Physics, 2019, 399, 108929.	3.8	108
27	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
28	Uniformly accurate machine learning-based hydrodynamic models for kinetic equations. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21983-21991.	7.1	51
29	Spatial feedbacks and the dynamics of savanna and forest. Theoretical Ecology, 2019, 12, 237-262.	1.0	20
30	On Multilevel Picard Numerical Approximations for High-Dimensional Nonlinear Parabolic Partial Differential Equations and High-Dimensional Nonlinear Backward Stochastic Differential Equations. Journal of Scientific Computing, 2019, 79, 1534-1571.	2.3	66
31	Machine Learning Approximation Algorithms for High-Dimensional Fully Nonlinear Partial Differential Equations and Second-order Backward Stochastic Differential Equations. Journal of Nonlinear Science, 2019, 29, 1563-1619.	2.1	160
32	Machine Learning Approximation Algorithms for High-Dimensional Fully Nonlinear Partial Differential Equations and Second-order Backward Stochastic Differential Equations. , 2019, 29, 1563.		1
33	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	2.4	299
34	Model Reduction with Memory and the Machine Learning of Dynamical Systems. Communications in Computational Physics, 2019, 25, .	1.7	39
35	<i>A priori</i> estimates of the population risk for two-layer neural networks. Communications in Mathematical Sciences, 2019, 17, 1407-1425.	1.0	40
36	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120, 143001.	7.8	1,006

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37	DeFine: deep convolutional neural networks accurately quantify intensities of transcription factor-DNA binding and facilitate evaluation of functional non-coding variants. Nucleic Acids Research, 2018, 46, e69-e69.	14.5	89
38	Reinforced dynamics for enhanced sampling in large atomic and molecular systems. Journal of Chemical Physics, 2018, 148, 124113.	3.0	48
39	DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. Computer Physics Communications, 2018, 228, 178-184.	7.5	727
40	Adaptive coupling of a deep neural network potential to a classical force field. Journal of Chemical Physics, 2018, 149, 154107.	3.0	11
41	Exponential convergence of the deep neural network approximation for analytic functions. Science China Mathematics, 2018, 61, 1733-1740.	1.7	41
42	Solving high-dimensional partial differential equations using deep learning. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8505-8510.	7.1	807
43	DeePCG: Constructing coarse-grained models via deep neural networks. Journal of Chemical Physics, 2018, 149, 034101.	3.0	141
44	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. Communications in Computational Physics, 2018, 23, .	1.7	164
45	Noisy Hegselmann-Krause Systems: Phase Transition and the 2R-Conjecture. Journal of Statistical Physics, 2017, 166, 1209-1225.	1.2	33
46	A Proposal on Machine Learning via Dynamical Systems. Communications in Mathematics and Statistics, 2017, 5, 1-11.	1.5	260
47	Deep Learning-Based Numerical Methods for High-Dimensional Parabolic Partial Differential Equations and Backward Stochastic Differential Equations. Communications in Mathematics and Statistics, 2017, 5, 349-380.	1.5	402
48	Renormalized powers of Ornsteinâ€“Uhlenbeck processes and well-posedness of stochastic Ginzburgâ€“Landau equations. Nonlinear Analysis: Theory, Methods & Applications, 2016, 142, 152-193.	1.1	11
49	A thermodynamic study of the two-dimensional pressure-driven channel flow. Discrete and Continuous Dynamical Systems, 2016, 36, 4349-4366.	0.9	0
50	Study of the instability of the Poiseuille flow using a thermodynamic formalism. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 9518-9523.	7.1	11
51	On the distinguished limits of the Navier slip model of the moving contact line problem. Journal of Fluid Mechanics, 2015, 772, 107-126.	3.4	19
52	The Free Action of Nonequilibrium Dynamics. Journal of Statistical Physics, 2015, 161, 300-325.	1.2	1
53	Sampling saddle points on a free energy surface. Journal of Chemical Physics, 2014, 140, 164109.	3.0	18
54	Microscopic mechanisms of equilibrium melting of a solid. Science, 2014, 346, 729-732.	12.6	111

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55	Mathematical theory of solids: From quantum mechanics to continuum models. Discrete and Continuous Dynamical Systems, 2014, 34, 5085-5097.	0.9	0
56	Exact Renormalization Group Analysis of Turbulent Transport by the Shear Flow. Journal of Statistical Physics, 2013, 153, 553-571.	1.2	1
57	Asymptotic analysis of quantum dynamics in crystals: the Bloch-Wigner transform, Bloch dynamics and Berry phase. Acta Mathematicae Applicatae Sinica, 2013, 29, 465-476.	0.7	7
58	Efficient iterative method for solving the Diracâ€“Kohnâ€“Sham density functional theory. Journal of Computational Physics, 2013, 245, 205-217.	3.8	6
59	Optimization-Based String Method for Finding Minimum Energy Path. Communications in Computational Physics, 2013, 14, 265-275.	1.7	18
60	The heterogeneous multiscale method. Acta Numerica, 2012, 21, 1-87.	10.7	334
61	Atomistic simulations of rare events using gentlest ascent dynamics. Journal of Chemical Physics, 2012, 136, 124104.	3.0	31
62	Subcritical bifurcation in spatially extended systems. Nonlinearity, 2012, 25, 761-779.	1.4	8
63	Stability and the continuum limit of the spin-polarized Thomas-Fermi-Dirac-von WeizsÃcker model. Journal of Mathematical Physics, 2012, 53, .	1.1	2
64	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
65	Optimized local basis set for Kohnâ€“Sham density functional theory. Journal of Computational Physics, 2012, 231, 4515-4529.	3.8	9
66	Contact line dynamics on heterogeneous surfaces. Physics of Fluids, 2011, 23, .	4.0	33
67	Effective Maxwell equations from time-dependent density functional theory. Acta Mathematica Sinica, English Series, 2011, 27, 339-368.	0.6	6
68	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
69	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
70	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
71	A numerical method for the study of nucleation of ordered phases. Journal of Computational Physics, 2010, 229, 1797-1809.	3.8	26
72	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

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73	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
74	Nucleation of Ordered Phases in Block Copolymers. Physical Review Letters, 2010, 104, 148301.	7.8	106
75	Continuum models for the contact line problem. Physics of Fluids, 2010, 22, .	4.0	87
76	Transition-Path Theory and Path-Finding Algorithms for the Study of Rare Events. Annual Review of Physical Chemistry, 2010, 61, 391-420.	10.8	481
77	Study of noise-induced transitions in the Lorenz system using the minimum action method. Communications in Mathematical Sciences, 2010, 8, 341-355.	1.0	29
78	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
79	Density-gradient-corrected embedded atom method. Physical Review B, 2009, 79, .	3.2	9
80	Probabilistic framework for network partition. Physical Review E, 2009, 80, 026106.	2.1	25
81	A general strategy for designing seamless multiscale methods. Journal of Computational Physics, 2009, 228, 5437-5453.	3.8	80
82	Pole-Based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics Series B, 2009, 30, 729-742.	0.4	46
83	On the Crystallization of 2D Hexagonal Lattices. Communications in Mathematical Physics, 2009, 286, 1099-1140.	2.2	57
84	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
85	The Andersen thermostat in molecular dynamics. Communications on Pure and Applied Mathematics, 2008, 61, 96-136.	3.1	29
86	Adaptive minimum action method for the study of rare events. Journal of Chemical Physics, 2008, 128, 104111.	3.0	84
87	Optimal partition and effective dynamics of complex networks. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7907-7912.	7.1	91
88	Breakdown of homogenization for the random Hamilton-Jacobi equations. Communications in Mathematical Sciences, 2008, 6, 189-197.	1.0	3
89	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
90	Noise can play an organizing role for the recurrent dynamics in excitable media. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 702-707.	7.1	33

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91	Simplified and improved string method for computing the minimum energy paths in barrier-crossing events. Journal of Chemical Physics, 2007, 126, 164103.	3.0	516
92	Numerical study of metastability due to tunneling: The quantum string method. Physica A: Statistical Mechanics and Its Applications, 2007, 379, 491-502.	2.6	13
93	The local microscale problem in the multiscale modeling of strongly heterogeneous media: Effects of boundary conditions and cell size. Journal of Computational Physics, 2007, 222, 556-572.	3.8	82
94	A discontinuous Galerkin implementation of a domain decomposition method for kinetic-hydrodynamic coupling multiscale problems in gas dynamics and device simulations. Journal of Computational Physics, 2007, 225, 1314-1330.	3.8	14
95	Boundary conditions for the moving contact line problem. Physics of Fluids, 2007, 19, 022101.	4.0	186
96	Cauchyâ€“Born Rule and the Stability of Crystalline Solids: Static Problems. Archive for Rational Mechanics and Analysis, 2007, 183, 241-297.	2.4	163
97	The Elastic Continuum Limit of the Tight Binding Model*. Chinese Annals of Mathematics Series B, 2007, 28, 665-676.	0.4	7
98	Nested stochastic simulation algorithms for chemical kinetic systems with multiple time scales. Journal of Computational Physics, 2007, 221, 158-180.	3.8	101
99	Seamless multiscale modeling via dynamics on fiber bundles. Communications in Mathematical Sciences, 2007, 5, 649-663.	1.0	12
100	The continuum limit and QM-continuum approximation of quantum mechanical models of solids. Communications in Mathematical Sciences, 2007, 5, 679-696.	1.0	2
101	A sub-linear scaling algorithm for computing the electronic structure of materials. Communications in Mathematical Sciences, 2007, 5, 999-1026.	1.0	17
102	Towards a Theory of Transition Paths. Journal of Statistical Physics, 2006, 123, 503-523.	1.2	375
103	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
104	Modified models of polymer phase separation. Physical Review E, 2006, 73, 061801.	2.1	36
105	Uniform accuracy of the quasicontinuum method. Physical Review B, 2006, 74, .	3.2	86
106	Analysis of the Local Quasicontinuum Method. Series in Contemporary Applied Mathematics, 2006, , 18-32.	0.8	12
107	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
108	Heterogeneous multiscale method for the modeling of complex fluids and micro-fluidics. Journal of Computational Physics, 2005, 204, 1-26.	3.8	157

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109	Numerical methods for multiscale transport equations and application to two-phase porous media flow. Journal of Computational Physics, 2005, 210, 656-675.	3.8	20
110	Self-induced stochastic resonance in excitable systems. Physica D: Nonlinear Phenomena, 2005, 210, 227-240.	2.8	90
111	Transition pathways in complex systems: Reaction coordinates, isocommittor surfaces, and transition tubes. Chemical Physics Letters, 2005, 413, 242-247.	2.6	187
112	The Heterogeneous Multiscale Method Based on the Discontinuous Galerkin Method for Hyperbolic and Parabolic Problems. Multiscale Modeling and Simulation, 2005, 3, 871-894.	1.6	24
113	Lattice Boltzmann Methods for Multiscale Fluid Problems. , 2005, , 2475-2486.		2
114	Transition pathways in complex systems: Application of the finite-temperature string method to the alanine dipeptide. Journal of Chemical Physics, 2005, 123, 134109.	3.0	168
115	Finite Temperature String Method for the Study of Rare Eventsâ€. Journal of Physical Chemistry B, 2005, 109, 6688-6693.	2.6	397
116	Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates. Journal of Chemical Physics, 2005, 123, 194107.	3.0	135
117	Multiscale simulations in simple metals:â€ƒA density-functional-based methodology. Physical Review B, 2005, 71, .	3.2	103
118	Multiscale Modeling Of Crystalline Solids. , 2005, , 1491-1506.		5
119	Lattice Boltzmann Methods for Multiscale Fluid Problems. , 2005, , 2475-2486.		0
120	Analysis of the heterogeneous multiscale method for elliptic homogenization problems. Journal of the American Mathematical Society, 2004, 18, 121-156.	3.9	196
121	Well-Posedness for the Dumbbell Model of Polymeric Fluids. Communications in Mathematical Physics, 2004, 248, 409-427.	2.2	81
122	Minimum action method for the study of rare events. Communications on Pure and Applied Mathematics, 2004, 57, 637-656.	3.1	185
123	Heterogenous multiscale method for locally self-similar problems. Communications in Mathematical Sciences, 2004, 2, 137-144.	1.0	5
124	Analysis of the heterogeneous multiscale method for gas dynamics. Methods and Applications of Analysis, 2004, 11, 557-572.	0.5	10
125	Coupling kinetic Monte-Carlo and continuum models with application to epitaxial growth. Journal of Computational Physics, 2003, 189, 197-211.	3.8	59
126	Finite difference heterogeneous multi-scale method for homogenization problems. Journal of Computational Physics, 2003, 191, 18-39.	3.8	98

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127	A note on generalized flows. Physica D: Nonlinear Phenomena, 2003, 183, 159-174.	2.8	12
128	Heterogeneous multiscale method: A general methodology for multiscale modeling. Physical Review B, 2003, 67, .	3.2	182
129	Improved gauss-seidel projection method for micromagnetics simulations. IEEE Transactions on Magnetics, 2003, 39, 1766-1770.	2.1	21
130	Energy landscape and thermally activated switching of submicron-sized ferromagnetic elements. Journal of Applied Physics, 2003, 93, 2275-2282.	2.5	83
131	The Heterognous Multiscale Methods. Communications in Mathematical Sciences, 2003, 1, 87-132.	1.0	826
132	Gauge Method for Viscous Incompressible Flows. Communications in Mathematical Sciences, 2003, 1, 317-332.	1.0	90
133	Analysis of the heterogeneous multiscale method for ordinary differential equations. Communications in Mathematical Sciences, 2003, 1, 423-436.	1.0	74
134	Theory of phase separation kinetics in polymerâ€“liquid crystal systems. Journal of Chemical Physics, 2002, 116, 4723-4734.	3.0	15
135	String method for the study of rare events. Physical Review B, 2002, 66, .	3.2	843
136	Nonlinear evolution equation for the stress-driven morphological instability. Journal of Applied Physics, 2002, 91, 9414-9422.	2.5	45
137	Brownian motors in the photoalignment of liquid crystals. Applied Physics A: Materials Science and Processing, 2002, 75, 293-300.	2.3	40
138	A Dynamic Atomisticâ€“Continuum Method for the Simulation of Crystalline Materials. Journal of Computational Physics, 2002, 182, 234-261.	3.8	102
139	Convergence of a Stochastic Method for the Modeling of Polymeric Fluids. Acta Mathematicae Applicatae Sinica, 2002, 18, 529-536.	0.7	12
140	Gibbsian Dynamics and Invariant Measures for Stochastic Dissipative PDEs. Journal of Statistical Physics, 2002, 108, 1125-1156.	1.2	21
141	Effective dynamics for ferromagnetic thin films. Journal of Applied Physics, 2001, 90, 370-374.	2.5	37
142	Matching Conditions in Atomistic-Continuum Modeling of Materials. Physical Review Letters, 2001, 87, 135501.	7.8	125
143	Gibbsian Dynamics and ErgodicityÂ¶for the Stochastically Forced Navierâ€“Stokes Equation. Communications in Mathematical Physics, 2001, 224, 83-106.	2.2	174
144	A Gaussâ€“Seidel Projection Method for Micromagnetics Simulations. Journal of Computational Physics, 2001, 171, 357-372.	3.8	131

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145	Ergodicity for the Navier-Stokes equation with degenerate random forcing: Finite-dimensional approximation. Communications on Pure and Applied Mathematics, 2001, 54, 1386-1402.	3.1	85
146	A continuum model for the growth of epitaxial films. Journal of Crystal Growth, 2001, 222, 414-425.	1.5	13
147	Continuum Theory of Epitaxial Crystal Growth. I. Journal of Statistical Physics, 2001, 104, 221-253.	1.2	29
148	Generalized flows, intrinsic stochasticity, and turbulent transport. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 8200-8205.	7.1	62
149	Invariant Measures for Burgers Equation with Stochastic Forcing. Annals of Mathematics, 2000, 151, 877.	4.2	236
150	Another note on forced burgers turbulence. Physics of Fluids, 2000, 12, 149-154.	4.0	12
151	Kinetic model for a step edge in epitaxial growth. Physical Review E, 1999, 59, 6879-6887.	2.1	69
152	Asymptotic Theory for the Probability Density Functions in Burgers Turbulence. Physical Review Letters, 1999, 83, 2572-2575.	7.8	61
153	On the statistical solution of the Riemann equation and its implications for Burgers turbulence. Physics of Fluids, 1999, 11, 2149-2153.	4.0	8
154	Domain size in the presence of random fields. Physical Review E, 1998, 57, 135-137.	2.1	4
155	Probability Distribution Functions for the Random Forced Burgers Equation. Physical Review Letters, 1997, 78, 1904-1907.	7.8	120
156	Thermodynamically driven incompressible fluid mixtures. Journal of Chemical Physics, 1997, 107, 10177-10184.	3.0	33
157	Finite Difference Schemes for Incompressible Flows in the Velocityâ€“Impulse Density Formulation. Journal of Computational Physics, 1997, 130, 67-76.	3.8	32
158	Finite Difference Methods for 3D Viscous Incompressible Flows in the Vorticityâ€“Vector Potential Formulation on Nonstaggered Grids. Journal of Computational Physics, 1997, 138, 57-82.	3.8	40
159	Vorticity Boundary Condition and Related Issues for Finite Difference Schemes. Journal of Computational Physics, 1996, 124, 368-382.	3.8	170
160	Essentially Compact Schemes for Unsteady Viscous Incompressible Flows. Journal of Computational Physics, 1996, 126, 122-138.	3.8	113
161	Dynamics of vortex liquids in Ginzburg-Landau theories with applications to superconductivity. Physical Review B, 1994, 50, 1126-1135.	3.2	53
162	Correctors for the homogenization of conservation laws with oscillatory forcing terms. Asymptotic Analysis, 1992, 5, 311-316.	0.5	15

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163	Probabilistic framework for network partition. , 0, .		1