John E Stone

List of Publications by Year in descending order

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58 papers	7,370 citations	236612 25 h-index	315357 38 g-index
64 all docs	64 docs citations	64 times ranked	8064 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
2	GPU Computing. Proceedings of the IEEE, 2008, 96, 879-899.	16.4	1,266
3	OpenCL: A Parallel Programming Standard for Heterogeneous Computing Systems. Computing in Science and Engineering, 2010, 12, 66-73.	1.2	959
4	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	1.5	619
5	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	1.3	336
6	Fast analysis of molecular dynamics trajectories with graphics processing unitsâ€”Radial distribution function histogramming. Journal of Computational Physics, 2011, 230, 3556-3569.	1.9	200
7	QwikMDâ€‰â€”â€‰Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	1.6	153
8	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	9.0	149
9	GPU clusters for high-performance computing. , 2009, , .		141
10	Molecular dynamics-based refinement and validation for sub-5 Ã… cryo-electron microscopy maps. ELife, 2016, 5, .	2.8	136
11	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
12	Multilevel summation of electrostatic potentials using graphics processing units. Parallel Computing, 2009, 35, 164-177.	1.3	118
13	Using VMD: An Introductory Tutorial. Current Protocols in Bioinformatics, 2008, 24, Unit 5.7.	25.8	116
14	Lattice microbes: Highâ€performance stochastic simulation method for the reactionâ€diffusion master equation. Journal of Computational Chemistry, 2013, 34, 245-255.	1.5	112
15	An asymmetric distributed shared memory model for heterogeneous parallel systems. , 2010, , .		110
16	A system for interactive molecular dynamics simulation. , 2001, , .		108
17	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	2.4	91
18	Adapting a message-driven parallel application to GPU-accelerated clusters. , 2008, , .		84

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19	GPU acceleration of cutoff pair potentials for molecular modeling applications. , 2008, , .		74
20	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. Journal of Chemical Information and Modeling, 2016, 56, 1112-1116.	2.5	63
21	Stable Small Quantum Dots for Synaptic Receptor Tracking on Live Neurons. Angewandte Chemie - International Edition, 2014, 53, 12484-12488.	7.2	60
22	Visualisation of cyclic and multi-branched molecules with VMD. Journal of Molecular Graphics and Modelling, 2009, 28, 131-139.	1.3	49
23	An asymmetric distributed shared memory model for heterogeneous parallel systems. Computer Architecture News, 2010, 38, 347-358.	2.5	47
24	Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations. Parallel Computing, 2014, 40, 86-99.	1.3	46
25	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	2.3	46
26	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	1.5	42
27	High performance computation and interactive display of molecular orbitals on GPUs and multi-core CPUs. , 2009, , .		41
28	Methodologies for the analysis of instantaneous lipid diffusion in md simulations of large membrane systems. Faraday Discussions, 2014, 169, 455-475.	1.6	41
29	GPU-accelerated molecular visualization on petascale supercomputing platforms. , 2013, , .		39
30	GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. Faraday Discussions, 2014, 169, 265-283.	1.6	37
31	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37
32	Quantifying the impact of GPUs on performance and energy efficiency in HPC clusters. , 2010, , .		30
33	Immersive Molecular Visualization and Interactive Modeling with Commodity Hardware. Lecture Notes in Computer Science, 2010, , 382-393.	1.0	30
34	Long time-scale simulations of in vivo diffusion using GPU hardware. , 2009, , .		29
35	Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads. , 2016, 2016, 89-100.		23
36	Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software to GPU-Accelerated OpenPOWER Platforms. Lecture Notes in Computer Science, 2016, 9945, 188-206.	1.0	23

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37	Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. , 2016, 2016, 1048-1057.		22
38	Early experiences scaling VMD molecular visualization and analysis jobs on blue waters. , 2013, , .		17
39	Immersive Out-of-Core Visualization of Large-Size and Long-Timescale Molecular Dynamics Trajectories. Lecture Notes in Computer Science, 2011, , 1-12.	1.0	16
40	GPU-Accelerated Computation and Interactive Display of Molecular Orbitals. , 2011, , 5-18.		15
41	Challenges of Integrating Stochastic Dynamics and Cryo-Electron Tomograms in Whole-Cell Simulations. Journal of Physical Chemistry B, 2017, 121, 3871-3881.	1.2	14
42	Probing biomolecular machines with graphics processors. Communications of the ACM, 2009, 52, 34-41.	3.3	13
43	Fast Molecular Electrostatics Algorithms on GPUs. , 2011, , 43-58.		11
44	Scalable Analysis of Authentic Viral Envelopes on FRONTERA. Computing in Science and Engineering, 2020, 22, 11-20.	1.2	10
45	Multiscale modeling and cinematic visualization of photosynthetic energy conversion processes from electronic to cell scales. Parallel Computing, 2021, 102, 102698.	1.3	10
46	py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. Journal of Chemical Theory and Computation, 2022, 18, 4983-4994.	2.3	10
47	Petascale Tcl with NAMD, VMD, and Swift/T. , 2014, , .		9
48	High-Performance Analysis of Biomolecular Containers to Measure Small-Molecule Transport, Transbilayer Lipid Diffusion, and Protein Cavities. Journal of Chemical Information and Modeling, 2019, 59, 4328-4338.	2.5	9
49	Best Practices in Running Collaborative GPU Hackathons: Advancing Scientific Applications with a Sustained Impact. Computing in Science and Engineering, 2018, 20, 95-106.	1.2	8
50	Probing Biomolecular Machines with Graphics Processors. Queue, 2009, 7, 30-39.	0.8	6
51	Runtime and Architecture Support for Efficient Data Exchange in Multi-Accelerator Applications. IEEE Transactions on Parallel and Distributed Systems, 2015, 26, 1405-1418.	4.0	6
52	High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. , 2016, 2016, 1014-1023.		6
53	GPU-accelerated molecular dynamics clustering analysis with OpenACC. , 2017, , 215-240.		2
54	Lessons Learned from Responsive Molecular Dynamics Studies of the COVID-19 Virus. , 2021, , .		2

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55	Stochastic Simulations of Cellular Processes: From Single Cells to Colonies. , 2014, , 277-293.		1
56	Multilevel Summation Method for Electrostatic Force Evaluation. Biophysical Journal, 2015, 108, 183a.	0.2	1
57	ANARI: A 3-D Rendering API Standard. Computing in Science and Engineering, 2022, 24, 7-18.	1.2	1
58	Analytic Rendering and Hardware-Accelerated Simulation for Scientific Applications. Computing in Science and Engineering, 2022, 24, 4-6.	1.2	0