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	ANARI: A 3-D Rendering API Standard. Computing in Science and Engineering, 2022, 24, 7-18.	1.2	1
2	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
3	Analytic Rendering and Hardware-Accelerated Simulation for Scientific Applications. Computing in Science and Engineering, 2022, 24, 4-6.	1.2	0
4	Multiscale modeling and cinematic visualization of photosynthetic energy conversion processes from electronic to cell scales. Parallel Computing, 2021, 102, 102698.	1.3	10
5	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
6	Lessons Learned from Responsive Molecular Dynamics Studies of the COVID-19 Virus. , 2021, , .		2
7	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
8	Scalable Analysis of Authentic Viral Envelopes on FRONTERA. Computing in Science and Engineering, 2020, 22, 11-20.	1.2	10
9	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
10	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
11	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	9.0	149
12	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
13	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
14	GPU-accelerated molecular dynamics clustering analysis with OpenACC. , 2017, , 215-240.		2
15	Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. , 2016, 2016, 1048-1057.		22
16	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. Journal of Chemical Information and Modeling, 2016, 56, 1112-1116.	2.5	63
17	High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. , 2016, 2016, 1014-1023.		6
18	Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads. , 2016, 2016, 89-100.		23

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19	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
20	QwikMDâ€‰â€”â€‰Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	1.6	153
21	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37
22	Molecular dynamics-based refinement and validation for sub-5 Ã… cryo-electron microscopy maps. ELife, 2016, 5, .	2.8	136
23	Multilevel Summation Method for Electrostatic Force Evaluation. Biophysical Journal, 2015, 108, 183a.	0.2	1
24	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	2.3	46
25	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
26	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	1.5	42
27	Petascale Tcl with NAMD, VMD, and Swift/T. , 2014, , .		9
28	Stochastic Simulations of Cellular Processes: From Single Cells to Colonies. , 2014, , 277-293.		1
29	Stable Small Quantum Dots for Synaptic Receptor Tracking on Live Neurons. Angewandte Chemie - International Edition, 2014, 53, 12484-12488.	7.2	60
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	Methodologies for the analysis of instantaneous lipid diffusion in md simulations of large membrane systems. Faraday Discussions, 2014, 169, 455-475.	1.6	41
32	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
33	Lattice microbes: Highâ€performance stochastic simulation method for the reactionâ€diffusion master equation. Journal of Computational Chemistry, 2013, 34, 245-255.	1.5	112
34	GPU-accelerated molecular visualization on petascale supercomputing platforms. , 2013, , .		39
35	Early experiences scaling VMD molecular visualization and analysis jobs on blue waters. , 2013, , .		17
36	Fast Molecular Electrostatics Algorithms on GPUs. , 2011, , 43-58.		11

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37	GPU-Accelerated Computation and Interactive Display of Molecular Orbitals. , 2011, , 5-18.		15
38	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
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	An asymmetric distributed shared memory model for heterogeneous parallel systems. Computer Architecture News, 2010, 38, 347-358.	2.5	47
41	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	1.3	336
42	OpenCL: A Parallel Programming Standard for Heterogeneous Computing Systems. Computing in Science and Engineering, 2010, 12, 66-73.	1.2	959
43	Quantifying the impact of GPUs on performance and energy efficiency in HPC clusters. , 2010, , .		30
44	An asymmetric distributed shared memory model for heterogeneous parallel systems. , 2010, , .		110
45	Immersive Molecular Visualization and Interactive Modeling with Commodity Hardware. Lecture Notes in Computer Science, 2010, , 382-393.	1.0	30
46	Probing biomolecular machines with graphics processors. Communications of the ACM, 2009, 52, 34-41.	3.3	13
47	High performance computation and interactive display of molecular orbitals on GPUs and multi-core CPUs. , 2009, , .		41
48	Visualisation of cyclic and multi-branched molecules with VMD. Journal of Molecular Graphics and Modelling, 2009, 28, 131-139.	1.3	49
49	Multilevel summation of electrostatic potentials using graphics processing units. Parallel Computing, 2009, 35, 164-177.	1.3	118
50	GPU clusters for high-performance computing. , 2009, , .		141
51	Long time-scale simulations of in vivo diffusion using GPU hardware. , 2009, , .		29
52	Probing Biomolecular Machines with Graphics Processors. Queue, 2009, 7, 30-39.	0.8	6
53	GPU Computing. Proceedings of the IEEE, 2008, 96, 879-899.	16.4	1,266
54	Using VMD: An Introductory Tutorial. Current Protocols in Bioinformatics, 2008, 24, Unit 5.7.	25.8	116

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55	GPU acceleration of cutoff pair potentials for molecular modeling applications. , 2008, , .		74
56	Adapting a message-driven parallel application to GPU-accelerated clusters. , 2008, , .		84
57	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	1.5	619
58	A system for interactive molecular dynamics simulation. , 2001, , .		108