List of Publications by Year in descending order

29 papers	19,018 citations	535685 17 h-index	843174 20 g-index
30 all docs	30 docs citations	30 times ranked	26153 citing authors

#	Article	IF	Citations
1	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
2	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
3	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
4	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	9.0	149
5	What You Should Know About NAMD and Charm++ But Were Hoping to Ignore. , 2018, , .		0
6	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
7	NAMD: Scalable Molecular Dynamics Based on the Charm++ Parallel Runtime System. , 2017, , 119-144.		4
8	Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads. , 2016, 2016, 89-100.		23
9	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
10	QwikMDâ€‰â€”â€‰Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.	1.6	153
11	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37
12	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	2.3	46
13	Petascale Tcl with NAMD, VMD, and Swift/T. , 2014, , .		9
14	Mapping to Irregular Torus Topologies and Other Techniques for Petascale Biomolecular Simulation. , 2014, 2014, 81-91.		24
15	Multiple-Replica Strategies for Free-Energy Calculations in NAMD: Multiple-Walker Adaptive Biasing Force and Walker Selection Rules. Journal of Chemical Theory and Computation, 2014, 10, 5276-5285.	2.3	66
16	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	3.0	115
17	Optimizing fine-grained communication in a biomolecular simulation application on Cray XK6. , 2012, , .		7
18	GPU/CPU Algorithm for Generalized Born/Solvent-Accessible Surface Area Implicit Solvent Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2521-2530.	2.3	49

#	Article	IF	Citations
19	Parallel Generalized Born Implicit Solvent Calculations with NAMD. Journal of Chemical Theory and Computation, 2011, 7, 3635-3642.	2.3	137
20	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	2.1	233
21	Enabling and scaling biomolecular simulations of 100 million atoms on petascale machines with a multicore-optimized message-driven runtime. , 2011, , .		26
22	Quantifying the impact of GPUs on performance and energy efficiency in HPC clusters. , 2010, , .		30
23	Probing biomolecular machines with graphics processors. Communications of the ACM, 2009, 52, 34-41.	3.3	13
24	Probing Biomolecular Machines with Graphics Processors. Queue, 2009, 7, 30-39.	0.8	6
25	Adapting a message-driven parallel application to GPU-accelerated clusters. , 2008, , .		84
26	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	1.5	619
27	Correcting mesh-based force calculations to conserve both energy and momentum in molecular dynamics simulations. Journal of Computational Physics, 2007, 225, 1-5.	1.9	26
28	Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 2005, 26, 1781-1802.	1.5	15,208
29	Avoiding Algorithmic Obfuscation in a Message-Driven Parallel MD Code. Lecture Notes in Computational Science and Engineering, 1999, , 472-482.	0.1	5