Hasan Metin Aktulga

List of Publications by Citations

40 papers	2,465 citations	14 h-index	45 g-index
45 ext. papers	3,786 ext. citations	3.4 avg, IF	4.95 L-index

#	Paper	IF	Citations
40	The ReaxFF reactive force-field: development, applications and future directions. *Npj Computational Materials*, **2016**, 2,	10.9	858
39	Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques. *Parallel Computing*, **2012**, 38, 245-259	1	508
38	A reactive molecular dynamics simulation of the silica-water interface. *Journal of Chemical Physics*, **2010**, 132, 174704	3.9	359
37	LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, **2021**, 271, 108171	4.2	315
36	Improving the scalability of a symmetric iterative eigensolver for multi-core platforms. *Concurrency Computation Practice and Experience*, **2014**, 26, 2631-2651	1.4	46
35	Reactive Molecular Dynamics: Numerical Methods and Algorithmic Techniques. *SIAM Journal of Scientific Computing*, **2012**, 34, C1-C23	2.6	45
34	Efficient global optimization of reactive force-field parameters. *Journal of Computational Chemistry* , **2015**, 36, 1550-61	3.5	37
33	Optimizing Sparse Matrix-Multiple Vectors Multiplication for Nuclear Configuration Interaction Calculations **2014**,		36
32	PuReMD-GPU: A reactive molecular dynamics simulation package for GPUs. *Journal of Computational Physics*, **2014**, 272, 343-359	4.1	35
31	Accelerating nuclear configuration interaction calculations through a preconditioned block iterative eigensolver. *Computer Physics Communications*, **2018**, 222, 1-13	4.2	22
30	Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method. *Parallel Computing*, **2014**, 40, 195-212	1	19
29	Topology-Aware Mappings for Large-Scale Eigenvalue Problems. *Lecture Notes in Computer Science*, **2012**, 830-842	0.9	19
28	Large-scale ab initio configuration interaction calculations for light nuclei. *Journal of Physics: Conference Series*, **2012**, 403, 012019	0.3	17
27	Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 3237-3251	6.4	17
26	Optimizing the performance of reactive molecular dynamics simulations for many-core architectures. *International Journal of High Performance Computing Applications*, **2019**, 33, 304-321	1.8	14
25	. *IEEE Transactions on Parallel and Distributed Systems*, **2017**, 28, 202-214	3.7	11
24	Exploring the future of out-of-core computing with compute-local non-volatile memory **2013**,		11

23	An Out-of-Core Dataflow Middleware to Reduce the Cost of Large Scale Iterative Solvers **2012**,		9
22	No Core CI calculations for light nuclei with chiral 2- and 3-body forces. *Journal of Physics: Conference Series*, **2013**, 454, 012063	0.3	9
21	Identifying statistical dependence in genomic sequences via mutual information estimates. *Eurasip Journal on Bioinformatics and Systems Biology*, **2007**, 14741		9
20	A High Performance Block Eigensolver for Nuclear Configuration Interaction Calculations. *IEEE Transactions on Parallel and Distributed Systems*, **2017**, 28, 1550-1563	3.7	8
19	. *IEEE Transactions on Antennas and Propagation*, **2019**, 67, 1094-1107	4.9	8
18	Fast Solvers for Charge Distribution Models on Shared Memory Platforms. *SIAM Journal of Scientific Computing*, **2020**, 42, C1-C22	2.6	6
17	An Out-of-Core Eigensolver on SSD-equipped Clusters **2012**,		6
16	Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. *Journal of Chemical Physics*, **2020**, 153, 084107	3.9	5
15	ReaxFF/AMBER-A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7645-7654	6.4	5
14	Toward scalable many-body calculations for nuclear open quantum systems using the Gamow Shell Model. *Computer Physics Communications*, **2020**, 247, 106978	4.2	5
13	Large-scale parallel null space calculation for nuclear configuration interaction **2011**,		4
12	Scalable nuclear density functional theory with Sky3D. *Computer Physics Communications*, **2018**, 223, 34-44	4.2	4
11	Towards Fast Scalable Solvers for Charge Equilibration in Molecular Dynamics Applications **2016**,		3
10	Performance optimization of reactive molecular dynamics simulations with dynamic charge distribution models on distributed memory platforms **2019**,		3
9	Evaluation of Directive-Based GPU Programming Models on a Block Eigensolver with Consideration of Large Sparse Matrices. *Lecture Notes in Computer Science*, **2020**, 66-88	0.9	2
8	Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. *Journal of Chemical Theory and Computation*, **2021**, 17, 3955-3966	6.4	2
7	Fast and scalable evaluation of pairwise potentials. *Computer Physics Communications*, **2020**, 255, 107248	4.2	1
6	Performance analysis of distributed symmetric sparse matrix vector multiplication algorithm for multi-core architectures. *Concurrency Computation Practice and Experience*, **2015**, 27, 5019-5036	1.4	1

5	On Reducing I/O Overheads in Large-Scale Invariant Subspace Projections. *Lecture Notes in Computer Science*, **2012**, 305-314	0.9	1
4	An Out-of-Core Task-based Middleware for Data-Intensive Scientific Computing **2015**, 647-667		1
3	Parallel Non-Uniform MLFMA for Multiscale Electromagnetic Simulation **2018**,		1
2	Water in an External Electric Field: Comparing Charge Distribution Methods Using ReaxFF Simulations.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1
1	High Performance Evaluation of Helmholtz Potentials using the Multi-Level Fast Multipole Algorithm. *IEEE Transactions on Parallel and Distributed Systems*, **2022**, 1-1	3.7	