Shantenu Jha

List of Publications by Year
in descending order

91 papers	1,687 citations	393982 19 h-index	414034 32 g-index
97 all docs	97 docs citations	97 times ranked	1921 citing authors

#	Article	IF	Citations
1	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	2.3	123
2	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
3	SAGA: A Simple API for Grid Applications. High-level application programming on the Grid. Computational Methods in Science and Technology, 2006, 12, 7-20.	0.3	77
4	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
5	Using clouds to provide grids with higher levels of abstraction and explicit support for usage modes. Concurrency Computation Practice and Experience, 2009, 21, 1087-1108.	1.4	55
6	A Tale of Two Data-Intensive Paradigms: Applications, Abstractions, and Architectures. , 2014, , .		54
7	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. Journal of Chemical Information and Modeling, 2022, 62, 116-128.	2.5	54
8	SAGA BigJob: An Extensible and Interoperable Pilot-Job Abstraction for Distributed Applications and Systems. , 2010, , .		46
9	A mechanism for S-adenosyl methionine assisted formation of a riboswitch conformation: a small molecule with a strong arm. Nucleic Acids Research, 2009, 37, 6528-6539.	6.5	44
10	DeepDriveMD: Deep-Learning Driven Adaptive Molecular Simulations for Protein Folding. , 2019, , .		42
11	Autonomic Management of Application Workflows on Hybrid Computing Infrastructure. Scientific Programming, 2011, 19, 75-89.	0.5	41
12	Exploring the Performance Fluctuations of HPC Workloads on Clouds. , 2010, , .		39
13	An Autonomic Approach to Integrated HPC Grid and Cloud Usage. , 2009, , .		36
14	A Comprehensive Perspective on Pilot-Job Systems. ACM Computing Surveys, 2019, 51, 1-32.	16.1	36
15	Determination of Free Energy Profiles for the Translocation of Polynucleotides through Î±-Hemolysin Nanopores using Non-Equilibrium Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 2135-2148.	2.3	33
16	SAGA: A standardized access layer to heterogeneous Distributed Computing Infrastructure. SoftwareX, 2015, 1-2, 3-8.	1.2	27
17	Harnessing the Power of Many: Extensible Toolkit for Scalable Ensemble Applications. , 2018, , .		26
18	Distributed Application Runtime Environment (DARE): A Standards-based Middleware Framework for Science-Gateways. Journal of Grid Computing, 2012, 10, 647-664.	2.5	25

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19	The Impact of a Ligand Binding on Strand Migration in the SAM-I Riboswitch. PLoS Computational Biology, 2013, 9, e1003069.	1.5	25
20	Adaptive ensemble simulations of biomolecules. Current Opinion in Structural Biology, 2018, 52, 87-94.	2.6	24
21	Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force. Journal of Computational Chemistry, 2014, 35, 692-702.	1.5	23
22	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	1.5	23
23	NEKTAR, SPICE and Vortonics: using federated grids for large scale scientific applications. Cluster Computing, 2007, 10, 351-364.	3.5	22
24	P∗: A model of pilot-abstractions. , 2012, , .		22
25	Efficient Runtime Environment for Coupled Multi-physics Simulations: Dynamic Resource Allocation and Load-Balancing. , 2010, , .		21
26	Understanding application-level interoperability: Scaling-out MapReduce over high-performance grids and clouds. Future Generation Computer Systems, 2011, 27, 590-599.	4.9	20
27	Ensemble Toolkit: Scalable and Flexible Execution of Ensembles of Tasks. , 2016, , .		20
28	CoCo-MD: A Simple and Effective Method for the Enhanced Sampling of Conformational Space. Journal of Chemical Theory and Computation, 2019, 15, 2587-2596.	2.3	20
29	A Systematic Framework for Data Management and Integration in a Continuous Pharmaceutical Manufacturing Processing Line. Processes, 2018, 6, 53.	1.3	19
30	Middleware Building Blocks for Workflow Systems. Computing in Science and Engineering, 2019, 21, 62-75.	1.2	19
31	Conformational Heterogeneity of the SAM-I Riboswitch Transcriptional ON State: A Chaperone-Like Role for S-Adenosyl Methionine. Journal of Molecular Biology, 2012, 418, 331-349.	2.0	18
32	Design and Performance Characterization of RADICAL-Pilot on Leadership-Class Platforms. IEEE Transactions on Parallel and Distributed Systems, 2022, 33, 818-829.	4.0	18
33	Force field validation for nucleic acid simulations: Comparing energies and dynamics of a DNA dodecamer. Journal of Computational Chemistry, 2005, 26, 1617-1627.	1.5	17
34	Rapid, Accurate, and Precise Calculation of Relative Binding Affinities for the SH2 Domain Using a Computational Grid. Journal of Chemical Theory and Computation, 2007, 3, 1193-1202.	2.3	16
35	Adaptive distributed replicaâ€"exchange simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 2595-2606.	1.6	15
36	Distributed computing practice for largeâ€scale science and engineering applications. Concurrency Computation Practice and Experience, 2013, 25, 1559-1585.	1.4	15

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37	ExTASY: Scalable and flexible coupling of MD simulations and advanced sampling techniques. , 2016, , .		15
38	Towards an Understanding of Facets and Exemplars of Big Data Applications. , 2014, , .		14
39	High-throughput binding affinity calculations at extreme scales. BMC Bioinformatics, 2018, 19, 482.	1.2	14
40	Extensible and Scalable Adaptive Sampling on Supercomputers. Journal of Chemical Theory and Computation, 2020, 16, 7915-7925.	2.3	14
41	Adaptive Ensemble Biomolecular Applications at Scale. SN Computer Science, 2020, 1, 1.	2.3	14
42	A Community Roadmap for Scientific Workflows Research and Development. , 2021, , .		14
43	Using Pilot Systems to Execute Many Task Workloads on Supercomputers. Lecture Notes in Computer Science, 2019, , 61-82.	1.0	13
44	Abstractions for Loosely-Coupled and Ensemble-Based Simulations on Azure. , 2010, , .		12
45	Scalable HPC & AI infrastructure for COVID-19 therapeutics. , 2021, , .		12
46	High-Throughput Computing on High-Performance Platforms: A Case Study. , 2017, , .		11
47	Pilot-Edge: Distributed Resource Management Along the Edge-to-Cloud Continuum. , 2021, , .		11
48	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	2.3	10
49	A parallel unidirectional coupled DEM-PBM model for the efficient simulation of computationally intensive particulate process systems. Computers and Chemical Engineering, 2018, 119, 128-142.	2.0	9
50	Supporting High-Performance and High-Throughput Computing for Experimental Science. Computing and Software for Big Science, 2019, 3, 1.	1.3	9
51	Exploring the RNA folding energy landscape using scalable distributed cyberinfrastructure. , 2010, , .		8
52	Energy landscape analysis for regulatory RNA finding using scalable distributed cyberinfrastructure. Concurrency Computation Practice and Experience, 2011, 23, 2292-2304.	1.4	8
53	Application skeletons: Construction and use in eScience. Future Generation Computer Systems, 2016, 59, 114-124.	4.9	8
54	Task-parallel Analysis of Molecular Dynamics Trajectories. , 2018, , .		8

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55	Characterizing the Performance of Executing Many-tasks on Summit. , 2019, , .		8
56	A Fresh Perspective on Developing and Executing DAG-Based Distributed Applications: A Case-Study of SAGA-Based Montage. , 2009, , .		7
57	Characterizing deep sequencing analytics using BFAST. , 2011, , .		7
58	Running many molecular dynamics simulations on many supercomputers. , 2012, , .		7
59	Pilot-Data: An abstraction for distributed data. Journal of Parallel and Distributed Computing, 2015, 79-80, 16-30.	2.7	7
60	Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations. , 2018, , .		7
61	Pilot-Streaming: A Stream Processing Framework for High-Performance Computing. , 2018, , .		7
62	Integrating Abstractions to Enhance the Execution of Distributed Applications. , 2016, , .		6
63	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations. , 2016, , .		6
64	Evaluating Distributed Execution of Workloads. , 2017, , .		6
65	Distributed Replica-Exchange Simulations on Production Environments Using SAGA and Migol. , 2008, , .		5
66	Developing eThread Pipeline Using SAGA-Pilot Abstraction for Large-Scale Structural Bioinformatics. BioMed Research International, 2014, 2014, 1-12.	0.9	5
67	Hacking at the Divide Between Polar Science and HPC: Using Hackathons as Training Tools. , 2017, , .		5
68	Synapse: Synthetic application profiler and emulator. Journal of Computational Science, 2018, 27, 329-344.	1.5	5
69	Learning Everywhere: A Taxonomy for the Integration of Machine Learning and Simulations. , 2019, , .		5
70	Understanding performance of distributed data-intensive applications. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 4089-4102.	1.6	4
71	A practical and comprehensive graduate course preparing students for research involving scientific computing. Procedia Computer Science, 2011, 4, 1927-1936.	1.2	4
72	Advancing nextâ€generation sequencing data analytics with scalable distributed infrastructure. Concurrency Computation Practice and Experience, 2014, 26, 894-906.	1.4	4

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73	Introducing distributed dynamic dataâ€intensive (D3) science: Understanding applications and infrastructure. Concurrency Computation Practice and Experience, 2017, 29, e4032.	1.4	4
74	Conceptualizing a Computing Platform for Science Beyond 2020: To Cloudify HPC, or HPCify Clouds?. , 2017, , .		4
75	Workflow Design Analysis for High Resolution Satellite Image Analysis. , 2019, , .		4
76	Coupling streaming AI and HPC ensembles to achieve 100â€"1000Ã— faster biomolecular simulations. , 2022, , .		4
77	Numerical methodologies for investigation of moderate-velocity flow using a hybrid computational fluid dynamics â€" molecular dynamics simulation approach. Journal of Mechanical Science and Technology, 2014, 28, 245-253.	0.7	3
78	A new hourly dataset for photovoltaic energy production for the continental USA. Data in Brief, 2022, 40, 107824.	0.5	3
79	An innovative application execution toolkit for multicluster grids. , 2009, , .		2
80	Synapse: Synthetic Application Profiler and Emulator. , 2016, , .		2
81	On the complexities of utilizing largeâ€scale lightpathâ€connected distributed cyberinfrastructure. Concurrency Computation Practice and Experience, 2017, 29, e3853.	1.4	2
82	Understanding ML Driven HPC: Applications and Infrastructure. , 2019, , .		2
83	Exploring Dynamic Enactment of Scientific Workflows Using Pilot-Abstractions. , 2013, , .		1
84	HPC enabled parallel, multi-scale & mechanistic model for high shear granulation using a coupled DEM-PBM framework. Computer Aided Chemical Engineering, 2018, 44, 1459-1464.	0.3	1
85	Parallel performance of molecular dynamics trajectory analysis. Concurrency Computation Practice and Experience, 2020, 32, e5789.	1.4	1
86	Comparing workflow application designs for high resolution satellite image analysis. Future Generation Computer Systems, 2021, 124, 315-329.	4.9	1
87	Application Skeleton: Generating Synthetic Applications for Infrastructure Research. Journal of Open Source Software, 2016, 1, 17.	2.0	1
88	A Scalable Pipeline for Transcriptome Profiling Tasks with On-Demand Computing Clouds. , 2016, , .		0
89	Methods and Experiences for Developing Abstractions for Data-intensive, Scientific Applications. , 2020, , .		0
90	Dynamic and Adaptive Monitoring and Analysis for Many-task Ensemble Computing. , 2021, , .		0

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91	ICEBERG: Imagery Cyber-infrastructure and Extensible Building blocks to Enhance Research in the Geosciences. (A Research Programmerâ€™s Perspective). , 2020, , .		0