David Bernholdt

List of Publications by Year in descending order

26 papers	1,968 citations	759233 12 h-index	713466 21 g-index
35 all docs	35 docs citations	35 times ranked	2244 citing authors

#	Article	IF	Citations
1	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
2	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
3	Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. Chemical Physics Letters, 1996, 250, 477-484.	2.6	214
4	A Component Architecture for High-Performance Scientific Computing. International Journal of High Performance Computing Applications, 2006, 20, 163-202.	3.7	154
5	Automatic code generation for many-body electronic structure methods: the tensor contraction engineâ€¡â€¡. Molecular Physics, 2006, 104, 211-228.	1.7	104
6	Parallel computational chemistry made easier: The development of NWChem. International Journal of Quantum Chemistry, 1995, 56, 475-483.	2.0	69
7	A survey of MPI usage in the US exascale computing project. Concurrency Computation Practice and Experience, 2020, 32, e4851.	2.2	49
8	Continuum-scale modeling of helium bubble bursting under plasma-exposed tungsten surfaces. Nuclear Fusion, 2018, 58, 126034.	3.5	38
9	Space-time trade-off optimization for a class of electronic structure calculations. , 2002, , .		37
10	Performance Optimization of Tensor Contraction Expressions for Many-Body Methods in Quantum Chemistry. Journal of Physical Chemistry A, 2009, 113, 12715-12723.	2.5	24
11	The Design and Implementation of the SWIM Integrated Plasma Simulator. , 2010, , .		24
12	Benchmarks and Tests of a Multidimensional Cluster Dynamics Model of Helium Implantation in Tungsten. Fusion Science and Technology, 2017, 71, 84-92.	1.1	20
13	Data redistribution and remote method invocation for coupled components. Journal of Parallel and Distributed Computing, 2006, 66, 931-946.	4.1	15
14	Analysis of OpenMP 4.5 Offloading in Implementations: Correctness and Overhead. Parallel Computing, 2019, 89, 102546.	2.1	15
15	Strategies for Fault Tolerance in Multicomponent Applications. Procedia Computer Science, 2011, 4, 2287-2296.	2.0	10
16	A framework for characterizing overlap of communication and computation in parallel applications. Cluster Computing, 2008, 11, 75-90.	5.0	9
17	Many-task applications in the Integrated Plasma Simulator. , 2010, , .		6
18	Realization of User Level Fault Tolerant Policy Management through a Holistic Approach for Fault Correlation. , 2011, , .		6

#	Article	IF	Citations
19	Data Grid discovery and Semantic Web technologies for the earth sciences. International Journal on Digital Libraries, 2005, 5, 72-83.	1.5	5
20	Parameter Sweep and Optimization of Loosely Coupled Simulations Using the DAKOTA Toolkit. , 2012, , .		5
21	Integrated model predictions on the impact of substrate damage on gas dynamics during ITER burning-plasma operations. Nuclear Fusion, 2021, 61, 116051.	3.5	5
22	Teaching Software Sustainability for High Performance Computing at ATPESC. , 2020, , .		3
23	Application health monitoring for extremeâ€scale resiliency using cooperative fault management. Concurrency Computation Practice and Experience, 2020, 32, e5449.	2.2	2
24	Research initiatives for plug-and-play scientific computing. Journal of Physics: Conference Series, 2007, 78, 012046.	0.4	0
25	Programmer-Guided Reliability for Extreme-Scale Applications. , 2015, , .		0
26	Programmer-guided reliability for extreme-scale applications. International Journal of High Performance Computing Applications, 2018, 32, 598-612.	3.7	0