List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	A multiphysics and multiscale software environment for modeling astrophysical systems. New Astronomy, 2009, 14, 369-378.	1.8	146
2	Chemically Specific Multiscale Modeling of Clay–Polymer Nanocomposites Reveals Intercalation Dynamics, Tactoid Selfâ€Assembly and Emergent Materials Properties. Advanced Materials, 2015, 27, 966-984.	21.0	98
3	Computer simulations reveal complex distribution of haemodynamic forces in a mouse retina model of angiogenesis. Journal of the Royal Society Interface, 2014, 11, 20140543.	3.4	87
4	THE COSMOGRID SIMULATION: STATISTICAL PROPERTIES OF SMALL DARK MATTER HALOS. Astrophysical Journal, 2013, 767, 146.	4.5	76
5	Distributed multiscale computing with MUSCLE 2, the Multiscale Coupling Library and Environment. Journal of Computational Science, 2014, 5, 719-731.	2.9	57
6	Survey of Multiscale and Multiphysics Applications and Communities. Computing in Science and Engineering, 2014, 16, 34-43.	1.2	56
7	A generalized simulation development approach for predicting refugee destinations. Scientific Reports, 2017, 7, 13377.	3.3	55
8	Multiscale computing in the exascale era. Journal of Computational Science, 2017, 22, 15-25.	2.9	54
9	Choice of boundary condition for lattice-Boltzmann simulation of moderate-Reynolds-number flow in complex domains. Physical Review E, 2014, 89, 023303.	2.1	48
10	Ten Simple Rules for Effective Computational Research. PLoS Computational Biology, 2014, 10, e1003506.	3.2	47
11	Analysing and modelling the performance of the HemeLB lattice-Boltzmann simulation environment. Journal of Computational Science, 2013, 4, 412-422.	2.9	46
12	Ten Simple Rules for a Successful Cross-Disciplinary Collaboration. PLoS Computational Biology, 2015, 11, e1004214.	3.2	46
13	Mechanism of Exfoliation and Prediction of Materials Properties of Clay–Polymer Nanocomposites from Multiscale Modeling. Nano Letters, 2015, 15, 8108-8113.	9.1	45
14	The impact of uncertainty on predictions of the CovidSim epidemiological code. Nature Computational Science, 2021, 1, 128-135.	8.0	45
15	Impact of blood rheology on wall shear stress in a model of the middle cerebral artery. Interface Focus, 2013, 3, 20120094.	3.0	41
16	Flexible composition and execution of high performance, high fidelity multiscale biomedical simulations. Interface Focus, 2013, 3, 20120087.	3.0	35
17	FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures. Computer Physics Communications, 2016, 207, 375-385.	7.5	32
18	Performance of distributed multiscale simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130407.	3.4	31

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19	Mastering the scales: a survey on the benefits of multiscale computing software. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180147.	3.4	30
20	FACS: A geospatial agent-based simulator for analysing COVID-19 spread and public health measures on local regions. Journal of Simulation, 2022, 16, 355-373.	1.5	30
21	Simulating Refugee Movements: Where would You Go?. Procedia Computer Science, 2016, 80, 2251-2255.	2.0	26
22	Science hackathons for developing interdisciplinary research and collaborations. ELife, 2015, 4, e09944.	6.0	23
23	Validation of Patient-Specific Cerebral Blood Flow Simulation Using Transcranial Doppler Measurements. Frontiers in Physiology, 2018, 9, 721.	2.8	22
24	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21
25	Patterns for High Performance Multiscale Computing. Future Generation Computer Systems, 2019, 91, 335-346.	7.5	20
26	Multiscale Computing with the Multiscale Modeling Library and Runtime Environment. Procedia Computer Science, 2013, 18, 1097-1105.	2.0	18
27	Simulating the Universe on an Intercontinental Grid. Computer, 2010, 43, 63-70.	1.1	16
28	Community effort endorsing multiscale modelling, multiscale data science and multiscale computing for systems medicine. Briefings in Bioinformatics, 2019, 20, 1057-1062.	6.5	15
29	VECMAtk: a scalable verification, validation and uncertainty quantification toolkit for scientific simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200221.	3.4	15
30	An automated multiscale ensemble simulation approach for vascular blood flow. Journal of Computational Science, 2015, 9, 150-155.	2.9	14
31	Introducing VECMAtk - Verification, Validation and Uncertainty Quantification for Multiscale and HPC Simulations. Lecture Notes in Computer Science, 2019, , 479-492.	1.3	14
32	How Policy Decisions Affect Refugee Journeys in South Sudan: A Study Using Automated Ensemble Simulations. Jasss, 2020, 23, .	1.8	14
33	A lightweight communication library for distributed computing. Computational Science & Discovery, 2010, 3, 015002.	1.5	11
34	A Serious Video Game To Support Decision Making On Refugee Aid Deployment Policy. Procedia Computer Science, 2017, 108, 205-214.	2.0	11
35	A parallel gravitational N-body kernel. New Astronomy, 2008, 13, 285-295.	1.8	10
36	High-performance gravitational N -body simulations on a planet-wide-distributed supercomputer. Computational Science & Discovery, 2011, 4, 015001.	1.5	9

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37	Distributed Infrastructure for Multiscale Computing. , 2012, , .		9
38	Towards an automated framework for agent-based simulation of refugee movements. , 2017, , .		9
39	Reliability and reproducibility in computational science: implementing validation, verification and uncertainty quantification <i>in silico</i> . Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200409.	3.4	9
40	Running Parallel Applications with Topology-Aware Grid Middleware. , 2009, , .		8
41	Support for Multiscale Simulations with Molecular Dynamics. Procedia Computer Science, 2013, 18, 1116-1125.	2.0	7
42	Multiscale Modelling and Simulation Workshop:12 Years of Inspiration. Procedia Computer Science, 2015, 51, 1082-1087.	2.0	7
43	Sensitivity-driven simulation development: a case study in forced migration. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200077.	3.4	7
44	Distributed Multiscale Simulations of Clay-Polymer Nanocomposites. Materials Research Society Symposia Proceedings, 2012, 1470, 6.	0.1	6
45	A Multiphysics and Multiscale Software Environment for Modeling Astrophysical Systems. Lecture Notes in Computer Science, 2008, , 207-216.	1.3	6
46	Taxonomy of Multiscale Computing Communities. , 2011, , .		5
47	Anatomy and Physiology of Multiscale Modeling and Simulation in Systems Medicine. Methods in Molecular Biology, 2016, 1386, 375-404.	0.9	5
48	On the Origin of Grid Species: The Living Application. Lecture Notes in Computer Science, 2009, , 205-212.	1.3	5
49	Distributed N-body simulation on the grid using dedicated hardware. New Astronomy, 2008, 13, 348-358.	1.8	4
50	A route pruning algorithm for an automated geographic location graph construction. Scientific Reports, 2021, 11, 11547.	3.3	4
51	Tutorial applications for Verification, Validation and Uncertainty Quantification using VECMA toolkit. Journal of Computational Science, 2021, 53, 101402.	2.9	4
52	Computational Engineering on the Grid: Crafting a Distributed Virtual Reactor. , 2006, , .		3
53	The Living Application: a Self-Organizing System for Complex Grid Tasks. International Journal of High Performance Computing Applications, 2010, 24, 185-193.	3.7	3
54	Building Global Research Capacity in Public Health: The Case of a Science Gateway for Physical Activity Lifelong Modelling and Simulation. , 2019, , .		3

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55	Weighted Decomposition in High-Performance Lattice-Boltzmann Simulations: Are Some Lattice Sites More Equal than Others?. Lecture Notes in Computer Science, 2015, , 28-38.	1.3	3
56	Modelling Distributed Multiscale Simulation Performance: An Application to Nanocomposites. , 2011, , .		2
57	From Thread to Transcontinental Computer: Disturbing Lessons in Distributed Supercomputing. , 2015, , .		2
58	Development of a Multiscale Simulation Approach for Forced Migration. Lecture Notes in Computer Science, 2018, , 869-875.	1.3	2
59	Towards Modelling the Effect of Evolving Violence on Forced Migration. , 2019, , .		2
60	Hybrid Simulation Development $\hat{a} \in $ Is It Just Analytics?. , 2019, , .		2
61	Simulating N-Body Systems on the Grid Using Dedicated Hardware. Lecture Notes in Computer Science, 2008, , 86-95.	1.3	2
62	Developing an infrastructure to support multiscale modelling and simulation. , 2011, , .		1
63	Multiscale Modelling and Simulation, 13th International Workshop. Procedia Computer Science, 2016, 80, 1242-1243.	2.0	1
64	Uncertainty quantification of dynamic earthquake rupture simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200076.	3.4	1
65	Experience with the International Testbed in the CrossGrid Project. Lecture Notes in Computer Science, 2005, , 98-110.	1.3	1
66	STAMINA: Bioinformatics Platform for Monitoring and Mitigating Pandemic Outbreaks. Technologies, 2022, 10, 63.	5.1	1
67	On-Line Application Performance Monitoring of Blood Flow Simulation in Computational Grid Architectures. , 0, , .		0
68	A platform independent communication library for distributed computing. Procedia Computer Science, 2010, 1, 2699-2706.	2.0	0
69	Towards a computational system to support clinical treatment decisions for diagnosed cerebral aneurysms. , 2014, , .		0
70	Multiscale Modelling and Simulation, 14th International Workshop. Procedia Computer Science, 2017, 108, 1811-1812.	2.0	0
71	Impact of immigrants on a multi-agent economical system. PLoS ONE, 2018, 13, e0197509.	2.5	0

P-Flee: An Efficient Parallel Algorithm for Simulating Human Migration., 2021,,.

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73	Towards Accurate Simulation of Global Challenges on Data Centers Infrastructures via Coupling of Models and Data Sources. Lecture Notes in Computer Science, 2020, , 410-424.	1.3	0