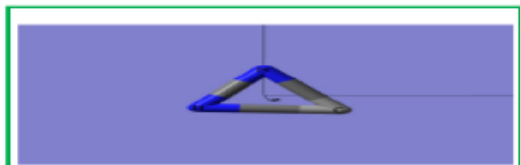
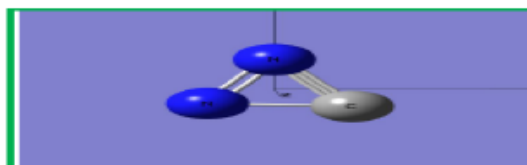




New Chemistry News



New News of Chem (NNC)



ChemNewsNew (CNN)

ExaScale (ES)

Computing, Memory Computers (CMC)

Extrapolating Single Organic Ion Solvation Thermochemistry from Simulated Water Nanodroplets	J. Phys. Chem. B, 2016, 120 (35), 9402–9409
Jonathan P. Coles, Céline Houriez, Michael Meot-Ner (Mautner), Michel Masella	
Placing Rigorous Bounds on Numerical Errors in Hartree–Fock Energy Computations	J. Chem. Theory Comput., 2011, 7 (6), 1631–1639
Pete P. Janes Alistair P. Rendell	
Scalability study of molecular dynamics simulation on Godson-T many-core architecture	J. Parallel Distributed Computing 73(11)(2013)1469-1482
Liu Peng Guangming Tan Rajiv K. Kalia Aiichiro Nakano Priya Vashishta Dongrui Fan Hao Zhang Fenglong Song	

Progress towards physics-based space weather forecasting with exascale computing	Advances in Engineering Software
Maria Elena Innocenti Alec Johnson Stefano Markidis Jorge Amaya Jan Deca Vyacheslav Olshevsky Giovanni Lapenta	
High-Order/Low-Order Methods for Ocean Modeling	Procedia Computer Science 51(2015)2086-2096
Christopher Newman Geoff Womeldorff Luis Chacón Dana A. Knoll	
Chapter 11 - Climate Analytics as a Service	Cloud Computing in Ocean Atmospheric Sciences, Academic Press, 2016(187-219)
J.L. Schnase	

Performance energy benchmarking of spectral solvers on hybrid multicore machines	Sustainable Computing: Informatics Systems 2016, 2210-5379
Tania Banerjee Jacob Rabb Sanjay Ranka	
Route to exascale: Novel mathematical methods, scalable algorithms Computational Science skills	J. Computational Science 14(2016)1-4
Vassil Alexandrov	
Balancing conflicting requirements for grid particle decomposition in continuum-Lagrangian solvers	Parallel Computing 52(2016)1-21
Hariswaran Sitaraman Ray Grout	
Unite conquer approach for high scale numerical computing	J. Computational Science 14(2014)5-14
Nahid Emad Serge Petiton	
Energy Study of Monte Carlo Quasi-Monte Carlo Algorithms for Solving Integral Equations	Procedia Computer Science 80(2016)1897-1905
Todor Gurov Aneta Karaivanova Vassil Alexandrov	
Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability	Computer Methods in Applied Mechanics Engineering 287(2015)262-289
Joseph E. Bishop John M. Emery Richard V. Field Christopher R. Weinberger David J. Littlewood	
7.05 - Numerical Methods for Mantle Convection	Treatise on Geophysics (Second Edition), Elsevier (2015) 197-222
S.J. Zhong D.A. Yuen L.N. Moresi M.G. Knepley	
Global communication schemes for the numerical solution of high-dimensional PDEs	Parallel Computing 52(2016)78-105
Philipp Hupp Mario Heene Riko Jacob Dirk Pflüger	
Energy-aware software: Challenges, opportunities strategies	J. Computational Science 4(6)(2013)444-449
Anne E. Trefethen Jeyarajan Thiyagalingam	
Facilitating analysis of Monte Carlo dense matrix inversion algorithm scaling behaviour through simulation	J. Computational Science 4(6)(2013)-473-479
Janko Straßburg Vassil N. Alexandrov	
FMM-based vortex method for simulation of isotropic turbulence on GPUs, compared with a spectral method	Computers & Fluids 80(2013)17-27
Rio Yokota L.A. Barba	
Developing a scalable hybrid MPI/OpenMP unstructured finite element model	Computers & Fluids 110(2015)227-234
Xiaohu Guo Michael Lange Gerard Gorman Lawrence Mitchell Michèle Weiland	

Multiscale high-order/low-order (HOLO) algorithms applications	J Computational Physics, 330, 1 February 2017,21-45
L. Chacón, G. Chen, D.A. Knoll, C. Newman, H. Park, W. Taitano, J.A. Willert, G. Womeldorff	
OpenSBLI: A framework for the automated derivation parallel execution of finite difference solvers on a range of computer architectures	J Computational Science, 18, 2017, 12-23
Christian T. Jacobs, Satya P. Jammy, Neil D. Sandham	

An efficient portable SIMD algorithm for charge/current deposition in Particle-In-Cell codes	Computer Physics Communications, 210, 2017, 145-154
H. Vincenti, M. Lobet, R. Lehe, R. Sasanka, J.-L. Vay	
On the energy footprint of I/O management in Exascale \{HPC\} systems	Future Generation Computer Systems 62(2016)17-28
Matthieu Dorier Orcun Yildiz Shadi Ibrahim Anne-Cécile Orgerie Gabriel Antoniu	
Education training for exascale	J. Computational Science 14(2016)69-73
Nia Alexandrov	
Research Trends in Big Data Analysis	Data Analysis in the Cloud, Computer Science Reviews Trends, Elsevier,(2016)123-138
Talia, Domenico Trunfio, Paolo Marozzo, Fabrizio	
Modeling Implementation of an Asynchronous Approach to Integrating \{HPC\} Big Data Analysis1	Procedia Computer Science 80(2016)52-62
Yuankun Fu Fengguang Song Luoding Zhu	
DOE Exascale Initiative	Briefing to the Secretary of Energy Advisory Board, September 13, 2013
Dimitri Kusnezov, Senior Advisor to the Secretary, US DOE Steve Binkley, Senior Advisor, Office of Science, US DOE Bill Harrod, Office of Science/ASCR Bob Meisner, Defense Programs/ASC	

Exascale Computing Systems, Methodologies, Applications	lums@indiana.edu
Andrew Lumsdaine	
ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems	DARPA IPTO September 28, 2008
Peter Kogge, Editor & Study Lead, Keren Bergman, Shekhar Borkar, Dan Campbell, William Carlson, William Dally, Monty Denneau, Paul Franzon, William Harrod, Kerry Hill, Jon Hiller, Sherman Karp, Stephen Keckler, Dean Klein, Robert Lucas, Mark Richards, Al Scarpelli, Steven Scott, Allan Snaveley, Thomas Sterling, R. Stanley Williams, Katherine Yelick	
Exascale Computing Technology Challenges	VECPAR 2010, LNCS 6449, pp. 1–25, 2011
John Shalf, Sudip Dosanjh, John Morrison	
The exascale draft plan has four high-level components	U S Dept of energy
The Opportunities, Challenges of Exascale Computing	U S Dept of energy,2010
Chapter 7 - Deep-Learning Numerical	High Performance Parallelism Pearls, Optimization (2015)129-142
Morgan Kaufmann	

Exascale design space exploration co-design	Future Generation Computer Systems 30(2014)46-58
S.S. Dosanjh R.F. Barrett D.W. Doerfler S.D. Hammond K.S. Hemmert M.A. Heroux P.T. Lin K.T. Pedretti A.F. Rodrigues T.G. Trucano J.P. Luitjens	
Scaling to a million cores beyond: Using light-weight simulation to understand the challenges ahead on the road to exascale	Future Generation Computer Systems 30(2014)9-65
Christian Engelmann	
Performance analysis of large scale parallel CFD computing based on Code_Saturne	Computer Physics Communications 184(2013)381-386
Zhi Shang	
Chapter Five - Optical Interconnects for Green Computers Data Centers	Advances in Computers 872(2012)125-201
Ali Hurson Atif Memon	
Trends in supercomputing: The European path to exascale	Computer Physics Communications 182(2011)2041-2046
N. Attig P. Gibbon Th. Lippert	

Parallel implementation of approximate atomistic models of the AMOEBA polarizable model	Chemical Physics Letters (2016)191-198
Omar Demerdash Teresa Head-Gordon	
Technological forecasting of supercomputer development: The March to Exascale computing	Omega 51(2015)128-135
Dong-Joon Lim Timothy R. Anderson Tom Shott	
Making the case for reforming the I/O software stack of extreme-scale systems	Advances in Engineering Software (2016) doi = http://dx.doi.org/10.1016/j.advengsoft.2016.07.003 ,
Florin Isaila Javier Garcia Jesus Carretero Rob Ross Dries Kimpe	
Manycore challenge in particle-in-cell simulation: How to exploit 1 TFlops peak performance for simulation codes with irregular computation	Computers & Electrical Engineering 46(2015)81-94
Hiroshi Nakashima	
Exaflop/s: The why the how	Comptes Rendus Mécanique 339(2-3)(2011)70-77
David E. Keyes	
An approach to exascale visualization: Interactive viewing of in-situ visualization	Computer Physics Communications 185(2014)79-85
Akira Kageyama Tomoki Yamada	
CAVE 3D: Software Extensions for Scientific Visualization of Large-scale Models	Procedia Computer Science 66(2015)679-688
Natalia Melnikova Stepan Orlov Nikolay Shabrov Vlad Kiev Aleksey Kuzin Michael Resch Uwe Woessner Martin Aumüller	

I have a DRIHM: A Case Study in Lifting Computational Science Services Up to the Scientific Mainstream	Procedia Computer Science 51(2015)2663-2667
Michael Schiffers Nils g.kmmtschen Felde Dieter Kranzlmüller	
The Route to Exascale: Novel Mathematical Methods, Scalable Algorithms Computational Science Skills	J. Computational Science 14(2016)85-89
Michael Schiffers Nils gentschen Felde Dieter Kranzlmüller	
An efficient portable $\{SIMD\}$ algorithm for charge/current deposition in Particle-In-Cell codes	Computer Physics Communications (2016) doi = http://dx.doi.org/10.1016/j.cpc.2016.08.023 ,
H. Vincenti M. Lobet R. Lehe R. Sasanka J.-L. Vay,	

Scalable Stochastic Hybrid Methods Algorithms for Extreme Scale Computing	Procedia Computer Science 29(2014)1888-1892
Vassil Alexandrov	
Computational homogenization at extreme scales	Extreme Mechanics Letters 6(2016)68-74
Matthew Mosby Karel Matouš	

A parameter-free dynamic alternative to hyper-viscosity for coupled transport equations: Application to the simulation of 3D squall lines using spectral elements	J. Computational Physics 283(2015)360-373
Simone Marras Francis X. Giraldo	
Chapter 1 - Energy-Aware High Performance Computing—A Survey	Green Sustainable Computing: Part II 88(2013)1-78
Michael Knobloch	
Monitoring Power Data: A first step towards a unified energy efficiency evaluation toolset for $\{HPC\}$ data centers	Environmental Modelling & Software 56(2014)13-26
Hayk Shoukourian Torsten Wilde Axel Auweter Arndt Bode	
Energy efficiency vs. performance of the numerical solution of PDEs: An application study on a low-power ARM-based cluster	J. Computational Physics 237(2013)132-150
Dominik Göddeke Dimitri Komatitsch Markus Geveler Dirk Ribbrock Nikola Rajovic Nikola Puzovic Alex Ramirez	



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