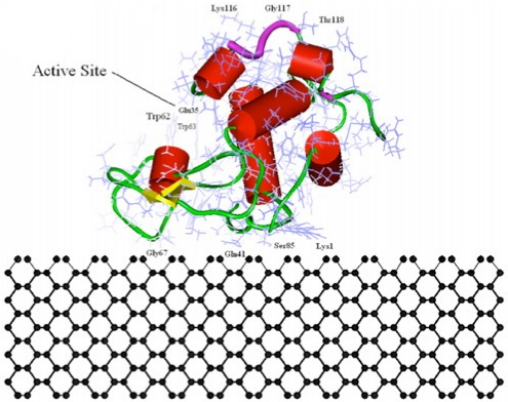
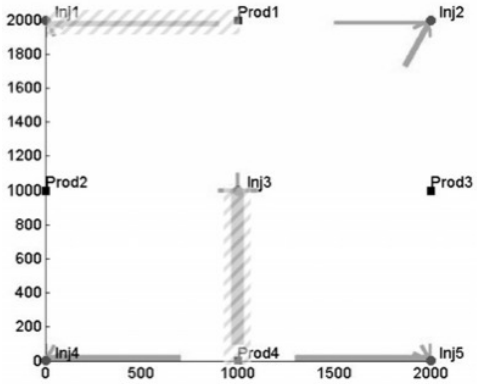
Final-Project Publications (1)

Computer Physics Communications 180 (2009) 669–674

A hybrid multi-loop genetic-algorithm/simplex/spatial-grid method for locating the optimum orientation of an adsorbed protein on a solid surface

Tao Wei [a], Shengjing Mu [b], Aiichiro Nakano [c], Katherine Shing [a,*]



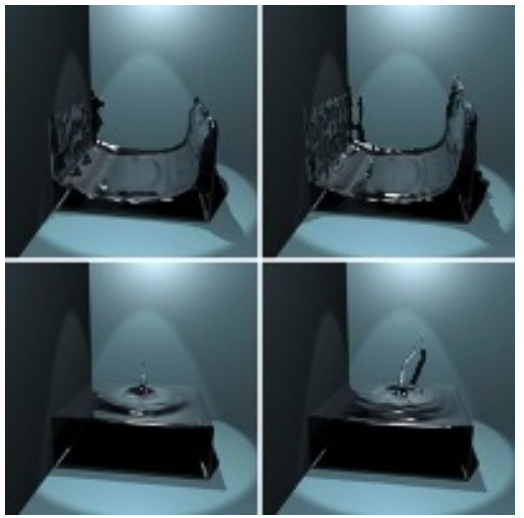


Hyokyeong Lee, Ke-Thia Yao, Aiichiro Nakano: **Dynamic Structure Learning of Factor Graphs and Parameter Estimation of a Constrained Nonlinear Predictive Model for Oilfield Optimization.** IC-AI 2010: 633-639

Hybrid Lattice-Boltzmann/Level-set Method for Liquid Simulation and Visualization

International Journal of Computational Science

Youngmin Kwak[1]*, C.-C. Jay Kuo[1], Aiichiro Nakano[2]



Final-Project Publications (2)

APPLIED PHYSICS LETTERS **100**, 163108 (2012)

Critical dimensions of highly lattice mismatched semiconductor nanowires grown in strain-releasing configurations

Suzana Sburlan,[1] P. Daniel Dapkus,[1,2] and Aiichiro Nakano[2,3]

JOURNAL OF APPLIED PHYSICS **111**, 054907 (2012)

Effect of substrate strain on critical dimensions of highly lattice mismatched defect-free nanorods

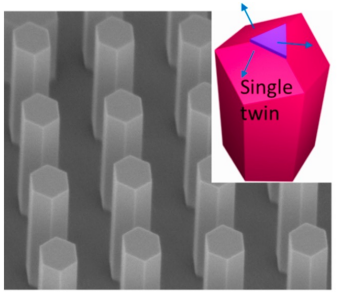
Suzana Sburlan,[1,a)] Aiichiro Nakano,[2,3] and P. Daniel Dapkus[1,3]

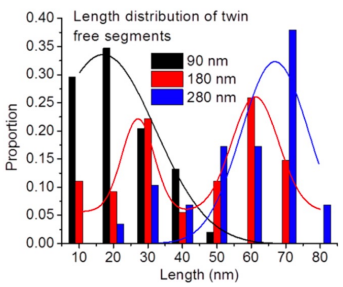
ACSNANO www.acsnano.org

ARTICLE

Facile Five-Step Heteroepitaxial Growth of GaAs Nanowires on Silicon Substrates and the Twin Formation Mechanism

Maoqing Yao,[†,∥] Chunyang Sheng,[‡,∥] Mingyuan Ge,[§] Chun-Yung Chi,[†,∥] Sen Cong,[†,∥] Aiichiro Nakano,[‡,∥] P. Daniel Dapkus,[*,†,∥] and Chongwu Zhou[*,†,∥]

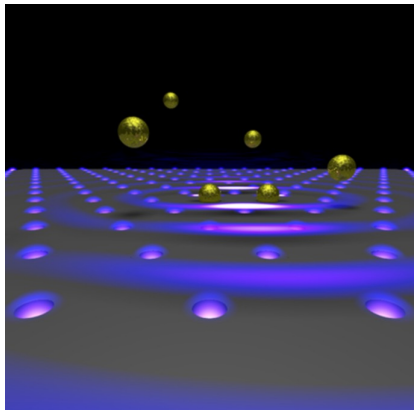




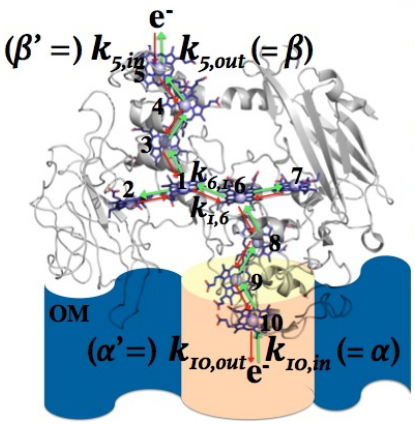
NANO LETTERS Letter pubs.acs.org/NanoLett

Optical Epitaxial Growth of Gold Nanoparticle Arrays

Ningfeng Huang,[†] Luis Javier Martínez,[†] Eric Jaquay,[†] Aiichiro Nakano,[‡] and Michelle L. Povinelli[*,†]



Final-Project Publications (3)



Kinetic Monte Carlo Simulations and Molecular Conductance Measurements of the Bacterial Decaheme Cytochrome MtrF

Hye Suk Byun[1], Sahand Pirbadian[1], Prof. Aiichiro Nakano[1,2], Dr. Liang Shi[3] and Prof. Mohamed Y. El-Naggar[1,*]

Article first published online: 5 SEP 2014

DOI: 10.1002/celc.201402211

Issue

ChemElectroChem

Special Issue: Biofuel Cells

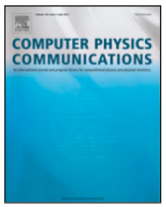
Volume 1, Issue 11, pages 1932–1939, November 11, 2014

Computer Physics Communications 219 (2017) 246–254

Contents lists available at ScienceDirect

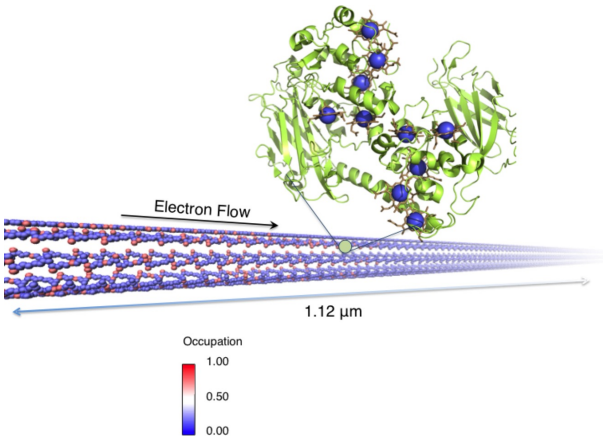
Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc



A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics

Hye Suk Byun [a], Mohamed Y. El-Naggar [a,b,c], Rajiv K. Kalia [a,d,e,f], Aiichiro Nakano [a,b,d,e,f,*], Priya Vashishta [a,d,e,f]

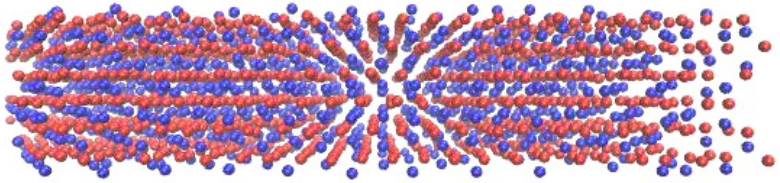


Final-Project Publications (4)

Directional Melting of Alumina via Polarized Microwave Heating

Yuan Hu,[1] Aiichiro Nakano,[2] and Joseph Wang[1]

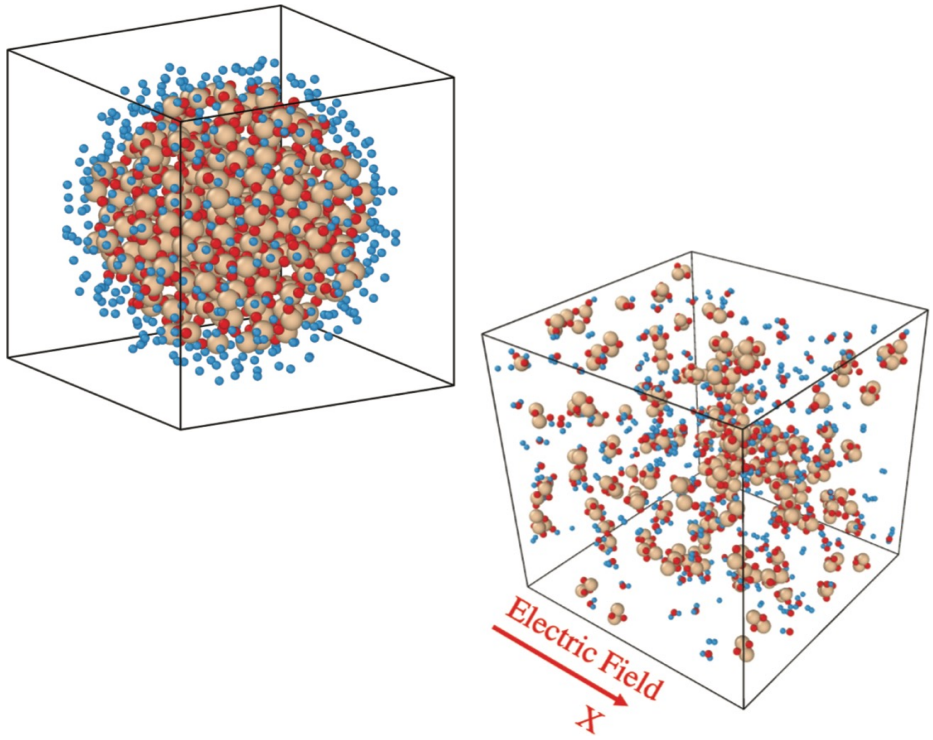
Appl. Phys. Lett. **110,** 044102 (2017)



Geophysical Research Letters **48**, e2020GL091681 (2021)

Molecular Dynamics Simulations of Dielectric Breakdown of Lunar Regolith: Implications for Water Ice Formation on Lunar Surface

Ziyu Huang[1], Ken-ichi Nomura[2], Aiichiro Nakano[3], and Joseph Wang[1]



Final-Project Publications (5)

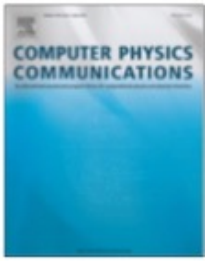
Submitted to *Computer Physics Communications*

Computer Physics Communications 207 (2016) 186–192

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

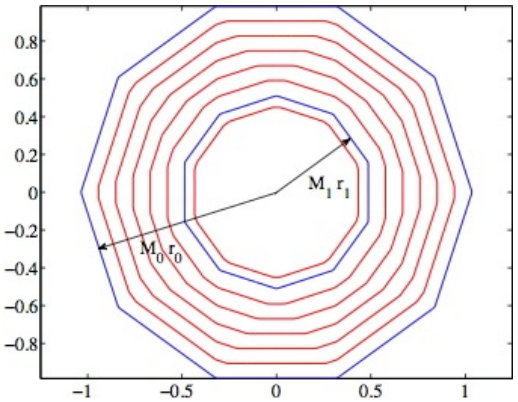


Parallel implementation of geometrical shock dynamics for two dimensional converging shock waves

Shi Qiu, Kuang Liu, Veronica Eliasson *

Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089-1191, USA

Team project is encouraged



More Class Projects (1)

Computer Physics Communications 239 (2019) 265–271

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

PAR^2: Parallel Random Walk Particle Tracking Method for solute transport in porous media☆

Calogero B. Rizzo [a,*], Aiichiro Nakano [b], Felipe P.J. de Barros [a]

Computer Physics Communications 244 (2019) 324–328

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

WaterAlignment: Identification of displaced water molecules in molecular docking using Jonker and Volgenant shortest path augmentation for linear assignment☆

Dab Brill [c,e,*], Jason B. Giles [e], Ian S. Haworth [e], Aiichiro Nakano [a,b,c,d,f]

Computational Materials Science 173 (2020) 109429

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Boltzmann machine modeling of layered MoS_2 synthesis on a quantum annealer

Jeremy Liu [a,b], Ankith Mohan [a], Rajiv K. Kalia [c], Aiichiro Nakano [c], Ken-ichi Nomura [c,*], Priya Vashishta [c], Ke-Thia Yao [a]

Buildings **9**, 44 (2019)

Article

Adaptive Kinetic Architecture and Collective Behavior: A Dynamic Analysis for Emergency Evacuation

Angella Johnson [1,*], Size Zheng [2], Aiichiro Nakano [3], Goetz Schierle [1] and Joon-Ho Choi [1]

Computer Physics Communications 247 (2020) 106873

sDMD: An open source program for discontinuous molecular dynamics simulation of protein folding and aggregation☆

Size Zheng [a,*], Leili Javidpour [b], Muhammad Sahimi [c], Katherine S. Shing [c], Aiichiro Nakano [c]

Quantum Science & Technology **6**, 014007 (2021)

Domain-specific compilers for dynamic simulations of quantum materials on quantum computers

Lindsay Bassman[5,1], Sahil Gulania[2], Connor Powers[1], Rongpeng Li[3], Thomas Linker[1], Kuang Liu[1], T K Satish Kumar[4], Rajiv K Kalia[1], Aiichiro Nakano[1] and Priya Vashishta[1]

Phys. Chem. Chem. Phys. **24**, 10378 (2022)

Probing the presence and absence of metal-fullerene electron transfer reactions in helium nanodroplets by deflection measurements†

John W. Niman, [a] Benjamin S. Kamerin, [a] Thomas H. Villers,[a] Thomas M. Linker,[b] Aiichiro Nakano[b] and Vitaly V. Kresin *[a]

More Class Projects (2)

Article https://doi.org/10.1038/s41467-024-47685-8

Scalable computation of anisotropic vibrations for large macromolecular assemblies

Jordy Homing Lam [1,2,3], Aiichiro Nakano [1,4,5] & Vsevolod Katritch [1,2,3,6]

Nature Communications | (2024)15:3479

https://github.com/jhmlam/Inching

PHYSICAL REVIEW B **110**, 075116 (2024)

Dynamics of symmetry-protected topological matter on a quantum computer

Miguel Mercado [1,*] Kyle Chen,[2] Parth Hemant Darekar [3,4] Aiichiro Nakano [5] Rosa Di Felice [1,6] and Stephan Haas [1]

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING COMPUTATIONAL CHEMISTRY | September 11, 2024

pubs.acs.org/jcim Article

Exploring the Global Reaction Coordinate for Retinal Photoisomerization: A Graph Theory-Based Machine Learning Approach

Goran Giudetti,[⊥] Madhubani Mukherjee,[⊥] Samprita Nandi, Sraddha Agrawal, Oleg V. Prezhdo, and Aiichiro Nakano*

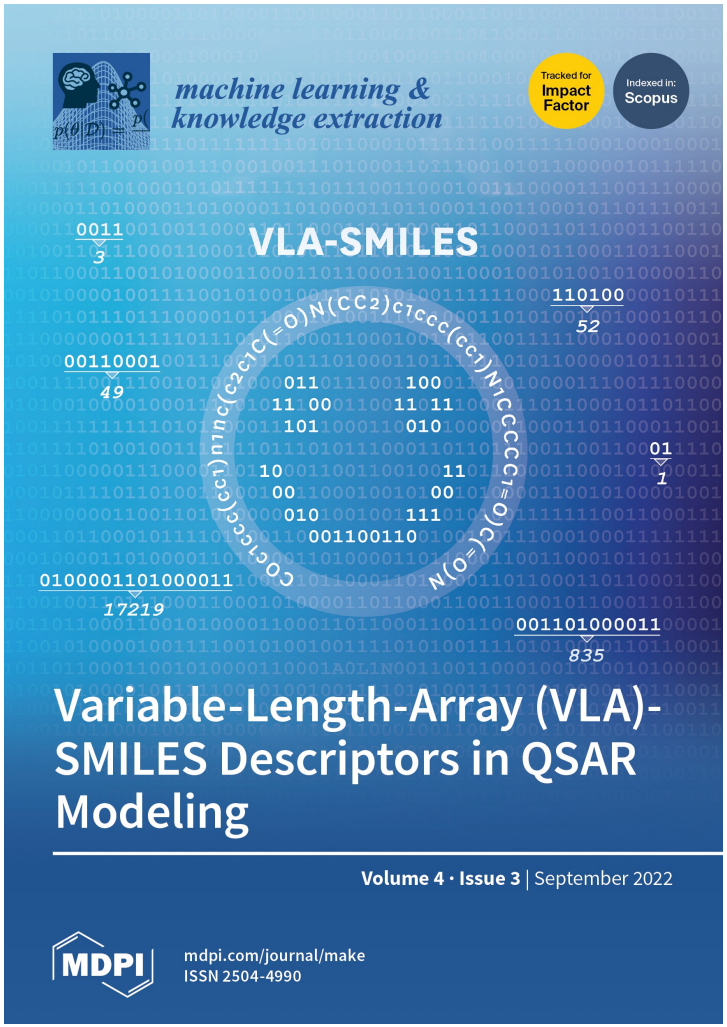
Cite This: https://doi.org/10.1021/acs.jcim.4c00325 Read Online

Journal Cover

Dielectric polymer property prediction using recurrent neural networks with optimizations

Antonina L. Nazarova, L. Yang, K. Liu, A. Mishra, R. K. Kalia, K. Nomura, A. Nakano, P. Vashishta, and P. Rajak

Journal of Chemical Information and Modeling **61**, 2175 ('21)



VLA-SMILES: Variable-Length-Array SMILES Descriptors in Neural Network-Based QSAR Modeling

Antonina L. Nazarova [1,*,†] and Aiichiro Nakano [2,*]

Journal of Machine Learning and Knowledge Extraction **4**, 715 (2022)

Not Quite from This Class

nature computational science

Article

https://doi.org/10.1038/s43588-022-00370-6

Fast multi-source nanophotonic simulations using augmented partial factorization

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Check for updates

Ho-Chun Lin, Zeyu Wang & Chia Wei Hsu

Numerical solutions of Maxwell's equations are indispensable for nanophotonics and electromagnetics but are constrained when it comes to large systems, especially multi-channel ones such as disordered media, aperiodic metasurfaces and densely packed photonic circuits where the many inputs require many large-scale simulations. Conventionally, before extracting the quantities of interest, Maxwell's equations are first solved on every element of a discretization basis set that contains much more information than is typically needed. Furthermore, such simulations are often performed one input at a time, which can be slow and repetitive. Here we propose to bypass the full-basis solutions and directly compute the quantities of interest while also eliminating the repetition over inputs. We do so by augmenting the Maxwell operator with all the input source profiles and all the output projection profiles, followed by a single partial factorization that yields the entire generalized scattering matrix via the Schur complement, with no approximation beyond discretization. This method applies to any linear partial differential equation. Benchmarks show that this approach is 1,000–30,000,000 times faster than existing methods for two-dimensional systems with about 10,000,000 variables. As examples, we demonstrate simulations of entangled photon backscattering from disorder and high-numerical-aperture metalenses that are thousands of wavelengths wide.

Parallelized in CSCI 653