

24th IUPAP Conference on Computational Physics

(IUPAP-CCP 2012)

Journal of Physics: Conference Series Volume 454

**Kobe, Japan
14-18 October 2012**

**ISBN: 978-1-62993-092-3
ISSN: 1742-6588**

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© by the Institute of Physics
All rights reserved.

Printed by Curran Associates, Inc. (2013)

For permission requests, please contact the Institute of Physics
at the address below.

Institute of Physics
Dirac House, Temple Back
Bristol BS1 6BE UK

Phone: 44 1 17 929 7481
Fax: 44 1 17 920 0979

techtracking@iop.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

FINITE-DIFFERENCE, FINITE-VOLUME, FINITE-ELEMENT METHODS

012001 Numerical Simulations of Dynamics and Emission from Relativistic Astrophysical Jets	1
<i>P Mimica, M A Aloy, J M Rueda-Becerril, S Tabik, C Aloy</i>	
012002 BSSN Equations in Spherical Coordinates Without Regularization: Spherically Symmetric Spacetimes	11
<i>P J Montero, I Cordero-Carrión</i>	
012003 Symmetry-preserving Momentum Remap for ALE Hydrodynamics	21
<i>J Velechovský, M Kucharík, R Liska, M Shashkov</i>	
012004 Fluid-orbit Coupling Calculation for Flight Analysis of Impulsively Driven Laser Vehicle	31
<i>M Takahashi, N Ohnishi</i>	
012005 Global Vlasov Simulation on Magnetospheres of Astronomical Objects	38
<i>T Umeda, Y Ito, K Fukazawa</i>	
012006 Modelling Migration in Multilayer Systems by a Finite Difference Method: the Spherical Symmetry Case	46
<i>C I Hojbota, V Tosa, P V Mercea</i>	
012007 Kinetic Energy Spectrum of Low-reynolds-number Turbulence with Polymer Additives	51
<i>T Watanabe, T Gotoh</i>	
012008 Radiation Hydrodynamics Simulation of High-Z Doped ICF Targets	59
<i>T Shioto, N Ohnishi, A Sunahara, S Fujioka</i>	
012009 Fluid Simulation of Plume Head-on Collision Dynamics During Pulsed Laser Ablation	65
<i>R Fujii, K Doi, Y Yokoyama, H Fukuoka, A Sugimura, N Tominaga, H Susa, I Umezu</i>	
012010 Finite Difference Simulations of Seismic Wave Propagation for Understanding Earthquake Physics and Predicting Ground Motions: Advances and Challenges	73
<i>H Aochi, T Ulrich, A Ducellier, F Dupros, D Michea</i>	
012011 Finite Difference Time Domain Method for Calculating the Band Structure of a 2D Photonic Crystal and Simulating the Lensing Effect	82
<i>S R Dastjerdi, M Ghanaatshoar</i>	

PARTICLE METHODS

012012 Resolving the Outer Density Profile of Dark Matter Halo in Andromeda Galaxy	86
<i>T Kirihara, Y Miki, M Mori</i>	
012013 Hunting a Wandering Black Hole in M31 Halo Using GPU Cluster	92
<i>Y Miki, M Mori, T Kawaguchi</i>	
012014 Studying the Core-cusp Problem in Cold Dark Matter Halos Using N-body Simulations on GPU Clusters	100
<i>G Ogiya, M Mori, Y Miki, T Boku, N Nakasato</i>	
012015 Exploiting Parallelism in Many-core Architectures: Lattice Boltzmann Models As a Test Case	110
<i>F Mantovani, M Pivanti, S F Schifano, R Tripiccion</i>	
012016 Plasma Particle-in-cell Simulations with QED Reactions for Pair Production Experiments Using a High-Z Solid Target	121
<i>T Moritaka, L Baiotti, A Lin, L Weiwu, Y Sakawa, Y Kuramitsu, T Morita, H Takabe</i>	
012017 Electron Behavior in Ion Beam Neutralization in Electric Propulsion: Full Particle-in-cell Simulation	133
<i>H Usui, A Hashimoto, Y Miyake</i>	

MOLECULAR DYNAMICS

012018 High Performance Computing for Drug Development on K Computer	141
<i>H Fujitani, K Shinoda, T Yamashita, T Kodama</i>	
012019 Development of a First-principles Code Based on the Screened KKR Method for Large Super-cells	147
<i>S Doi, M Ogura, H Akai</i>	

012020 Optimization of the Jastrow Factor in the Correlated Wave Function of Electrons Using the First-principles Transcorrelated Method for Solid-state Calculations	157
<i>M Ochi, S Tsuneyuki</i>	
012021 First-principles Band Structure and FLEX Approach to the Pressure Effect on T_c of the Cuprate Superconductors	166
<i>H Sakakibara, K Suzuki, H Usui, K Kuroki, R Arita, D J Scalapino, H Aoki</i>	
012022 Ab Initio Study of Dissociation Reaction of Ethylene Molecules on Ni Cluster.....	174
<i>K Shimamura, T Oguri, Y Shibuta, S Ohmura, F Shimojo, S Yamaguchi</i>	
012023 Variational Path Integral Molecular Dynamics Study of a Water Molecule	181
<i>S Miura</i>	
012024 Shape Transition of Micelles in Amphiphilic Solution: A Molecular Dynamics Study.....	187
<i>S Fujiwara, M Hashimoto, T Itoh, H Nakamura, Y Tamura</i>	
012025 A Graph Theoretical Approach to Fluctuating Networks in Glass-forming Liquids: A Molecular Dynamics Study with Applications of the Pebble Game Algorithm.....	191
<i>Y Takéuchi</i>	
012026 Order Parameter by Instantaneous Normal Mode Analysis for Melting Behaviour of Cluster $Ag_{17}Cu_2$.....	197
<i>P-H Tang, T-M Wu, S K Lai</i>	
012027 Molecular Dynamics with Atomic Transitions and Nuclear Reactions.....	204
<i>R More, F Wang</i>	
012028 Evaluations of the Conformational Search Accuracy of CAMDAS Using Experimental Three-dimensional Structures of Protein-ligand Complexes.....	219
<i>A Oda, N Yamaotsu, S Hirono, Y Takano, S Fukuyoshi, R Nakagaki, O Takahashi</i>	
012029 Photoexcited Electron and Hole Dynamics in Semiconductor Quantum Dots: Phonon-induced Relaxation, Multiple Exciton Generation and Recombination	229
<i>K Hyeon-Deuk</i>	
012030 An Efficient Computational Method for the Implementation of a Semi-classical Instanton Approach Using Discretized Path Integrals	232
<i>T Kawatsu, S Miura</i>	

MONTE CARLO METHODS

012031 Sampling from a Polytope and Hard-disk Monte Carlo.....	239
<i>S C Kapfer, W Krauth</i>	
012032 Fourier Monte Carlo Simulation of Crystalline Membranes in the Flat Phase.....	251
<i>A Tröster</i>	
012033 Validity of the Rayleigh Hypothesis for Two-dimensional Randomly Rough Metal Surfaces	268
<i>T Nordam, P A Letnes, I Simonsen</i>	
012034 Multicanonical Simulation of Coupled Folding and Binding of Intrinsically Disordered Protein Using an Ising-like Protein Model.....	278
<i>K Matsushita, M Kikuchi</i>	
012035 Stochastic and Fractal Properties of Silicon and Porous Silicon Rough Surfaces.....	285
<i>S Hosseinabadi, M Rajabi</i>	
012036 Monte Carlo Simulation of InAs HEMTs Considering Strain and Quantum Confinement Effects	292
<i>A Endoh, I Watanabe, A Kasamatsu, T Mimura</i>	
012037 Conformational Analysis Investigation Into the Influence of Nano-porosity of Ultra-permeable Ultra-selective Polyimides on Its Diffusivity As Potential Membranes for Use in the "Green" Separation of Natural Gases	300
<i>T M Madkour</i>	
012038 GPGPU Simulations of 2D Lattice Neutral Models in Ecology.....	312
<i>T Oura, K Tokita</i>	
012039 Multicanonical Simulation of the Domb-joyce Model and the Go Model: New Enumeration Methods for Self-avoiding Walks	319
<i>N C Shirai, M Kikuchi</i>	
012040 Empirical Study of the GARCH Model with Rational Errors	329
<i>T T Chen, T Takaishi</i>	
012041 Analysis of Spin Financial Market by GARCH Model.....	339
<i>T Takaishi</i>	

QUANTUM MONTE CARLO METHODS

012042 Lattice Computations for High Energy and Nuclear Physics	349
<i>K Jansen</i>	
012043 a First Look at Quasi-monte Carlo for Lattice Field Theory Problems	368
<i>K Jansen, H Leovey, A Nube, A Griewank, M Mueller-Preussker</i>	
012044 Simulation of Lattice QCD with Domain-wall Fermions	380
<i>T-W Chiu</i>	
012045 Quantum Monte Carlo Study of the Half-filled Hubbard Model on the Honeycomb Lattice	393
<i>Y Otsuka, S Yunoki, S Sorella</i>	
012046 Improved Multi-variable Variational Monte Carlo Method Examined by High-precision Calculations of One-dimensional Hubbard Model	399
<i>R Kaneko, S Morita, M Imada</i>	
012047 Variational Monte Carlo Study for the Insulating Mechanism of Sr₂IrO₄: from the Viewpoint of Energy Gain	408
<i>H Watanabe, T Shirakawa, S Yunoki</i>	
012048 Fermion-induced Decoherence of Bosons in Optical Lattices	414
<i>A Masaki, H Mori</i>	
012049 a Study of Parallelizing O(N) Green-function-based Monte Carlo Method for Many Fermions Coupled with Classical Degrees of Freedom	418
<i>S Zhang, S Yamagia, S Yunoki</i>	
012050 Cluster Structure in Monte Carlo Shell Model	433
<i>T Yoshida, N Shimizu, T Abe, T Otsuka</i>	
012051 Computational Particle Physics for Event Generators and Data Analysis	437
<i>D Perret-Gallix</i>	

DENSITY FUNCTIONAL THEORY

012052 Time Evolution of Heisenberg Operators of Nuclei and Electrons of QED System Based on Field Theory	457
<i>M Senami, T Miyazato, S Takada, Y Ikeda, A Tachibana</i>	
012053 Coupled Perturbed Hartree-fock Method for Non-hermitian Hamiltonians	464
<i>Y Ikeda, M Senami, A Tachibana</i>	
012054 Simulation of Heavy Ion Collision Using a Time-dependent Density Functional Theory Including Nuclear Superfluidity	473
<i>S Ebata</i>	
012055 How to Determine Boundaries for QM/MM Calculations: a Guideline Based on Linear Response Function for Glutathione	477
<i>S Yamanaka, K Ueda, K Nakata, M Okumura, K Yamaguchi, H Nakamura</i>	
012056 Checking the Validity of the Correlated Thomas-fermi Functional in the Pair Density Functional Theory	483
<i>K Higuchi, M Higuchi</i>	
012057 Structural Relaxation and Binding Energy Calculations of FK506 Binding Protein Complexes Using the Large-scale DFT Code CONQUEST	490
<i>T Otsuka, N Okimoto, M Taiji, D R Bowler, T Miyazaki</i>	
012058 Quantum Chemical Study of Conformational Preferences of Intermediates and Transition States in the Alkaline Hydrolysis of Dimethyl Phosphate	495
<i>Y Takano, M Kita, H Nakamura</i>	
012059 Effect of Atomic Adsorption of Catalytic Metals on Mechanical Properties of Graphene	504
<i>R Iwata, M Aoki</i>	
012060 Ab-initio Calculations of the Photoelastic Constants of the Cubic Sic Polytype	511
<i>P Djemia, K Bouamama</i>	
012061 Hybrid Functional Study on Diffusion of Silicate Cathode Material Li₂NiSiO₄	519
<i>K M Bui, V A Dinh, T Ohno</i>	
012062 Density Functional Study for Optical Properties of Blue Silicate Phosphor: BaCa₂MgSi₂O₈	525
<i>M Ishida, Y Imanari, T Isobe, S Kuze, T Ezuhara, T Umeda, K Ohno, S Miyazaki</i>	

DENSITY MATRIX RENORMALIZATION GROUP (INCLUDING DIRECT MATRIX DIAGONALIZATION, MATRIX PRODUCT STATES, PEPS, MERA)

012063 No Core CI Calculations for Light Nuclei with Chiral 2- and 3-body Forces	534
<i>P Maris, H M Aktulga, S Binder, A Calci, Ü V Catalyürek, J Langhammer, E Ng, E Saule, R Roth, J P Vary, C Yang</i>	
012064 A Multiprecision C++ Library for Matrix-product-state Simulation of Quantum Computing: Evaluation of Numerical Errors	549
<i>A Saitoh</i>	
012065 Computational Issues of Configuration Interaction Frameworks Describing Open Quantum Systems	559
<i>N Michel</i>	
012066 Recent Development of Monte Carlo Shell Model and Its Application to No-core Calculations	569
<i>T Abe, P Maris, T Otsuka, N Shimizu, Y Tsunoda, Y Utsuno, J P Vary, T Yoshida</i>	
012067 Superfluidity of One-dimensional Trapped Fermionic Optical Lattices with Spatially Alternating Interactions	582
<i>A Yamamoto, S Yunoki</i>	
012068 Theoretical Studies of a Three-band Hubbard Model with a Strong Spin-orbit Coupling for 5d Transition Metal Oxide Sr₂IrO₄	587
<i>T Shirakawa, H Watanabe, S Yunoki</i>	
012069 Correlated Theory of Linear Optical Absorption of Octacene and Nonacene	595
<i>H Chakraborty, A Shukla</i>	

BIO-COMPUTING

012070 Percolation Phenomena in Disordered Topological Networks	603
<i>V Rodriguez, Y Diau, J Arsuaga</i>	
012071 Thermodynamics and Structural Properties of a Confined HP Protein Determined by Wang-landau Simulation	616
<i>B Pattanasiri, Y W Li, D P Landau, T Wüst, W Triampo</i>	

CLIMATE AND DISASTER PREVENTION

012072 Challenge Toward the Prediction of Typhoon Behaviour and Down Pour	625
<i>K Takahashi, R Onishi, Y Baba, S Kida, K Matsuda, K Goto, H Fuchigami</i>	
012073 Super High-resolution Mesoscale Weather Prediction	635
<i>K Saito, T Tsuyuki, H Seko, F Kimura, T Tokioka, T Kuroda, L Duc, K Ito, T Oizumi, G Chen, J Ito</i>	

EDUCATION IN COMPUTATIONAL PHYSICS

012074 Probing the Extensive Nature of Entropy	641
<i>T Salagaram, N Chetty</i>	
012075 the Challenges of Developing Computational Physics: The Case of South Africa	649
<i>T Salagaram, N Chetty</i>	

VISUALIZATION

012076 3d Visualization of Atomistic Simulations on Every Desktop	658
<i>D Peled, A Silverman, J Adler</i>	
012077 Applications and a Three-dimensional Desktop Environment for an Immersive Virtual Reality System	663
<i>A Kageyama, Y Masada</i>	
012078 Irreversible Data Compression Concepts with Polynomial Fitting in Time-order of Particle Trajectory for Visualization of Huge Particle System	673
<i>H Ohtani, K Hagita, A M Ito, T Kato, T Saitoh, T Takeda</i>	

OTHER METHODS AND TOPICS

012079 Photoinduced Spin-order Destructions in One-dimensional Extended Hubbard Model	684
<i>H Lu, S Sota, H Matsueda, J Bonca, T Tohyama</i>	
012080 A Fitting Formula for Radiative Cooling Based on Non-local Thermodynamic Equilibrium Population from Weakly-ionized Air Plasma	691
<i>Y Ogino, A Nagano, T Ishihara, N Ohnishi</i>	
012081 Acceleration of Feynman Loop Integrals in High-energy Physics on Many Core GPUs	701
<i>F Yuasa, T Ishikawa, N Hamaguchi, T Koike, N Nakasato</i>	
012082 Multi-threaded Adaptive Extrapolation Procedure for Feynman Loop Integrals in the Physical Region	708
<i>E De Doncker, F Yuasa, R Assaf</i>	
012083 Exact Partition Functions of a Polymer on a Square Lattice Up to Chain Length 38	718
<i>J H Lee, S-Y Kim, J Lee</i>	
012084 Double-layer Evolutionary Algorithm for Distributed Optimization of Particle Detection on the Grid	725
<i>A Padée, K Kurek, K Zaremba</i>	
012085 A Numerical Calculation Method for Frequency-shift of a Plasma Wave Using Wave Digital Filters	737
<i>T Utsunomiya, M Shimokawabe</i>	
012086 Wavelet Transform and Huffman Coding Based Electrocardiogram Compression Algorithm: Application to Telecardiology	747
<i>S A Chouakri, O Djaafri, A Taleb-Ahmed</i>	
Author Index	