

# **25th IUPAP Conference on Computational Physics**

**(CCP 2013)**

**Journal of Physics: Conference Series Volume 510**

**Moscow, Russia  
20 – 24 August 2013**

**ISBN: 978-1-63439-290-7  
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. (2014)

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](mailto: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](mailto:curran@proceedings.com)  
Web: [www.proceedings.com](http://www.proceedings.com)

# TABLE OF CONTENTS

## HIGH ENERGY PHYSICS

<b>SEARCH FOR THE HIGGS BOSON: A STATISTICAL ADVENTURE OF EXCLUSION AND DISCOVERY</b> .....	1
<i>D Horváth</i>	

## SOFT CONDENSED MATTER / NANOSCIENCE

<b>SIMULATIONS OF INTERFACIAL PHENOMENA IN SOFT CONDENSED MATTER AND NANOSCIENCE</b> .....	15
<i>K Binder</i>	

## EDUCATION IN COMPUTATIONAL PHYSICS

<b>HOW DO I SIMULATE PROBLEM X?</b> .....	30
<i>J Adler, Y Artzi, L Ben Bashat, T Y Izraeli, M Kreif, I Lavi, A Leibenzon, A Levi, I Schlesinger, E Toledano, U Peretz, Y Weisler, A Yagil</i>	

## IT AND HPC FOR PHYSICS AND EDUCATION

<b>EXPERIMENTAL RESEARCH CONTROL SOFTWARE SYSTEM</b> .....	36
<i>I A Cohn, A G Kovalenko, A N Vystavkin</i>	
<b>AUTOMATED CODE GENERATION FOR LATTICE QUANTUM CHROMODYNAMICS AND BEYOND</b> .....	40
<i>D Barthou, O Brand-Foissac, O Pène, G Grosdidier, R Dolbeau, C Eisenbeis, M Kruse, K Petrov, C Tadonki</i>	
<b>MULTI-AGENT TASKS SCHEDULING SYSTEM IN SOFTWARE DEFINED NETWORKS</b> .....	50
<i>P O Skobelev, O N Granichin, D S Budaev, V B Laryukhin, I V Mayorov</i>	
<b>AUTOMATIC POST PROCESSING ALGORITHM FOR PASSIVE SEISMIC MONITORING DATA</b> .....	61
<i>K Nepeina</i>	

## BIOLOGICAL PHYSICS / MONTE CARLO METHODS

<b>FOURIER MONTE CARLO SIMULATION OF HEXATIC MEMBRANES</b> .....	70
<i>A Tröster</i>	

## DIFFERENTIAL EQUATIONS AND CHAOS

<b>SYNC OR ANTI-SYNC – DYNAMICAL PATTERN SELECTION IN COUPLED SELF-SUSTAINED OSCILLATOR SYSTEMS</b> .....	78
<i>L Davidova, S Újvári, Z Nédá</i>	

## SOLID STATE PHYSICS / MATERIAL SCIENCE

<b>RADIATION DAMAGE THIN COATING OF SILICON CARBIDE</b> .....	86
<i>A Bondareva, G Zmievskaya, T Levchenko</i>	

## **ASTROPHYSICS AND COSMOLOGY**

<b>NUMERICAL CODE FOR MULTI-COMPONENT GALAXIES: FROM N-BODY TO CHEMISTRY AND MAGNETIC FIELDS</b> .....	96
<i>S A Khoperskov, E O Vasiliev, A V Khoperskov, V N Lubimov</i>	

## **MONTE CARLO METHODS**

<b>A NEW PARADIGM FOR PETASCALE MONTE CARLO SIMULATION: REPLICAS EXCHANGE WANG-LANDAU SAMPLING</b> .....	109
<i>Y W Li, T Vogel, T Wüst, D P Landau</i>	
<b>DYNAMIC CONNECTIVITY ALGORITHMS FOR MONTE CARLO SIMULATIONS OF THE RANDOM-CLUSTER MODEL</b> .....	120
<i>E M Elçi, M Weigel</i>	
<b>NON-EQUILIBRIUM CRITICAL DYNAMICS OF PURE AND DILUTED 2D XY-MODEL</b> .....	130
<i>P V Prudnikov, I S Popov</i>	
<b>AGEING PROPERTIES OF THREE-DIMENSIONAL PURE AND SITE-DILUTED ISING FERROMAGNETS</b> .....	139
<i>V V Prudnikov, P V Prudnikov, E A Pospelov</i>	
<b>MELTING SCENARIO OF THE TWO-DIMENSIONAL CORE-SOFTENED SYSTEM: FIRST-ORDER OR CONTINUOUS TRANSITION?</b> .....	149
<i>D E Dudalov, Y D Fomin, E N Tsiok, V N Ryzhov</i>	
<b>APPLICATION OF THE PARALLEL MULTICANONICAL METHOD TO LATTICE GAS CONDENSATION</b> .....	158
<i>J Zierenberg, M Wiedenmann, W Janke</i>	
<b>NON-EQUILIBRIUM CRITICAL BEHAVIOUR OF ULTRATHIN MAGNETIC AND METAMAGNETIC ISING FILMS</b> .....	166
<i>S P V Prudnikov, A S Elin, M A Medvedeva</i>	
<b>MONTE CARLO RENORMALIZATION GROUP OF DILUTE 3D ISING DYNAMICS</b> .....	173
<i>V V Prudnikov, A N Vakilov, S A Zolotarev</i>	
<b>AGEING AND NON-EQUILIBRIUM CRITICAL PHENOMENA IN MONTE CARLO SIMULATIONS</b> .....	180
<i>V V Prudnikov, P V Prudnikov</i>	
<b>IMITATION MONTE CARLO METHODS FOR PROBLEMS OF THE BOLTZMANN EQUATION WITH SMALL KNUDSEN NUMBERS, PARALLELIZING ALGORITHMS WITH SPLITTING</b> .....	194
<i>A I Khisamutdinov, N N Velker</i>	
<b>BOND ORIENTATION PROPERTIES IN LIPID MOLECULES OF MEMBRANES: MOLECULAR DYNAMICS SIMULATIONS</b> .....	203
<i>A L Rabinovich, A P Lyubartsev</i>	
<b>INTRAMOLECULAR STRUCTURES IN A SINGLE COPOLYMER CHAIN CONSISTING OF FLEXIBLE AND SEMIFLEXIBLE BLOCKS: MONTE CARLO SIMULATION OF A LATTICE MODEL</b> .....	213
<i>J A Martemyanova, V A Ivanov, W Paul</i>	
<b>MONTE CARLO SIMULATION OF CRITICAL PROPERTIES OF ULTRATHIN ANISOTROPIC HEISENBERG FILMS</b> .....	221
<i>M A Medvedeva, P V Prudnikov</i>	
<b>THE FLUCTUATION-DISSIPATION THEOREM OF COLLOIDAL PARTICLE'S ENERGY ON 2D PERIODIC SUBSTRATES: A MONTE CARLO STUDY OF THERMAL NOISE-LIKE FLUCTUATION AND DIFFUSION LIKE BROWNIAN MOTION</b> .....	229
<i>A Najafi</i>	
<b>FRUSTRATIONS AND PHASE TRANSITIONS IN THE ISING MODEL ON SQUARE LATTICE</b> .....	239
<i>A K Murtazaev, M K Ramazanov, F A Kassar-Ogly</i>	

## **DENSITY FUNCTIONAL THEORY**

<b>OPTICAL SPECTRUM ANALYSIS OF REAL-TIME TDDFT USING THE MAXIMUM ENTROPY METHOD</b> .....	248
<i>M Toogoshi, M Kato, S S Kano, Y Zempo</i>	

<b>PRESSURE-INDUCED SEMIMETALLIC BEHAVIOR OF CALCIUM FROM AB INITIO CALCULATIONS</b> .....	256
<i>M V Magnitskaya, N L Matsko, V S Baturin, Y A Uspenskii</i>	
<b>TRULY SELF-CONSISTENT SOLUTION OF KOHN-SHAM EQUATIONS FOR EXTENDED SYSTEMS WITH INHOMOGENEOUS ELECTRON GAS</b> .....	263
<i>A Ya Shul'Man, D V Posvyanskii</i>	
<b>EFFECT OF NITROGEN IMPURITY ON THE STRUCTURAL, MECHANICAL AND PHONON PROPERTIES OF DIAMOND FROM FIRST-PRINCIPLE STUDY</b> .....	274
<i>T A Ivanova, B N Mavrin</i>	

## QUANTUM PHYSICS AND LOW TEMPERATURE PHYSICS

<b>CRYSTAL EQUIVALENT TEMPERATURE MODEL IN PROCESS OF NONLINEAR CONVERSION OF LASER RADIATION</b> .....	283
<i>O A Ryabushkin, D V Myasnikov, A I Baranov</i>	
<b>STRUCTURAL AND ELECTRONIC PROPERTIES OF SMALL SILICON CLUSTERS</b> .....	291
<i>V S Baturin, S V Lepeshkin, M V Magnitskaya, N L Matsko, Yu A Uspenskii</i>	
<b>CONCEPT OF EQUIVALENT TEMPERATURE OF THE NONLINEAR-OPTICAL CRYSTAL INTERACTING WITH NONUNIFORM LASER RADIATION</b> .....	300
<i>O A Ryabushkin, D V Myasnikov, A V Konyashkin, I S Ulyanov</i>	
<b>DYNAMICS OF TWO-DIMENSIONAL ELECTRON GAS IN NON-UNIFORM MAGNETIC FIELD</b> .....	311
<i>O G Balev, I A Larkin</i>	
<b>FLUCTUATION-DISSIPATION THEOREM IN ISOLATED QUANTUM SYSTEMS OUT OF EQUILIBRIUM</b> .....	319
<i>E Khatami, G Pupillo, M Srednicki, M Rigol</i>	
<b>NOVEL METHOD FOR IDENTIFICATION OF INTRINSIC VIBRATION MODES IN PIEZOELECTRIC CRYSTALS</b> .....	325
<i>O A Ryabushkin, D V Myasnikov, A V Konyashkin</i>	
<b>SMOOTHED PARTICLE METHOD FOR REAL-SPACE ELECTRONIC STRUCTURE CALCULATIONS</b> .....	334
<i>S Sugimoto, Y Zempo</i>	

## MOLECULAR DYNAMICS

<b>ABOUT THE ENERGY LEVELS OF GAAS</b> .....	341
<i>K Iskakova, R Akhmaltdinov, A Amanova</i>	
<b>AB INITIO MOLECULAR-DYNAMICS STUDY OF DISSOCIATION MECHANISM OF HIGHLY CHARGED MOLECULES</b> .....	351
<i>S Ohmura, K Nagaya, F Shimojo, M Yao</i>	
<b>VALIDITY OF MOLECULAR DYNAMICS FOR THE SIMULATION OF SOFT MATTER</b> .....	359
<i>S Kim</i>	

## PLASMA PHYSICS

<b>ULTRAFAST LASERS AND SOLIDS IN HIGHLY EXCITED STATES: RESULTS OF HYDRODYNAMICS AND MOLECULAR DYNAMICS SIMULATIONS</b> .....	364
<i>N A Inogamov, V V Zhakhovsky, V A Khokhlov, S I Ashitkov, Y N Emirov, K V Khichshenko, A Y Faenov, T A Pikuz, M Ishino, M Kando, N Hasegawa, M Nishikino, P S Komarov, B J Demaske, M B Agranat, S I Anisimov, T Kawachi, I I Oleynik</i>	
<b>IMPLEMENTATION OF THE KINETIC PLASMA CODE WITH LOCALLY RECURSIVE NON-LOCALLY ASYNCHRONOUS ALGORITHMS</b> .....	379
<i>A Y Perepelkina, V D Levchenko, I A Goryachev</i>	
<b>MODEL KINETIC DESCRIPTION FOR MANY-COMPONENT PLASMA</b> .....	390
<i>V V Belyi</i>	
<b>DEVELOPMENTS OF LARGE EDDY SIMULATION FOR COMPRESSIBLE SPACE PLASMA TURBULENCE</b> .....	400
<i>A A Chernyshov, K V Karelsky, A S Petrosyan</i>	
<b>EXPLORING PHASE SPACE TURBULENCE IN MAGNETIC FUSION PLASMAS</b> .....	411
<i>T-H Watanabe, Y Idomura, S Maeyama, M Nakata, H Sugama, M Nunami, A Ishizawa</i>	

<b>NONLINEAR OSCILLATIONS IN THE KNUDSEN PLASMA DIODES</b> .....	422
<i>A Y Ender, V I Kuznetsov</i>	

## **HYDRODYNAMICS**

<b>MMALE NUMERICAL SIMULATION FOR MULTI-MATERIAL LARGE DEFORMATION FLUID FLOWS</b> .....	434
<i>Q Zeng</i>	
<b>NONLINEAR GENERATION OF SURFACE WAVES AGAINST THE WIND IN A LIMITED FETCH GROWTH MODEL</b> .....	442
<i>A Pushkarev</i>	
<b>OPTIMIZATION OF SOLVER FOR GAS FLOW MODELING</b> .....	452
<i>D Savichkin, O Dodulad, Y Kloss</i>	
<b>FREAK WAVES AT THE SURFACE OF DEEP WATER</b> .....	461
<i>A I Dyachenko, D I Kachulin, V E Zakharov</i>	
<b>Author Index</b>	