CCP2021

XXXII IUPAP Conference on Computational Physics

2-5 August 2021, ~~Coventry, England~~ online

Preface

CCP2021 is the 32nd conference in a series of meetings on computational physics that have been held annually and under the auspices of the International Union for Pure and Applied Physics (IUPAP) for more than 20 years now. The conference has a tradition of following a triannual cycle between the European, American and Asian/Pacific (plus maybe more frequently in the future also: African) regions, according to which it should have been held in Coventry in 2020. While preparations were well advanced, the meeting was called off in April 2020 due to the restrictions relating to the coronavirus pandemic. We were quite confident back then that the meeting could be held face-to-face in 2021, but the virus proved to be more persistent than we had envisaged, such that CCP2021 will be held entirely online. While we are rather disappointed that we cannot welcome you to Coventry in person, we are also excited about the new opportunities afforded by the online format: it is more inclusive, more ecological, more diverse, and more family friendly than any CCP conference before! At the same time, thanks to the many and varied contributions, we are glad to be able to present an excellent representation of where computational physics stands in the summer of 2021.

We are grateful for the kind sponsorship of a number of prestigious academic bodies, and leading publishing and software houses (listed on page 12). We thank you for participating and we warmly welcome you (virtually) to the ancient city of Coventry.

Coventry/Chemnitz, July 2021

Damien Foster
Nikolaos G. Fytas
Charo del Genio
Ran Holtzman
Susanne Horn
Abhishek Kumar
Alban Potherat
Martin Weigel (chair)
Taras Yavors'kii

Previous CCP conferences

2019 Hong Kong (CN)

2018 Davies (US)

2017 Paris (FR)

2016 Pretoria (ZA)

2015 Guhawati (IN)

2014 Boston (US)

2013 Moscow (RU)

2012 Kobe (JP)

2011 Gatlinburg (US)

2010 Trondheim (NO)

2009 Kaohsiung (TW)

2008 Ouro Preto (BR)

2007 Brussels (BE)

2006 Gyeongju (KR)

2005 Los Angeles (US)

2004 Genova (IT)

2003 Beijing (CN)

2002 Dan Diego (US)

2001 Aachen (DE)

2000 Brisbane (AU)

1999 Atlanta (US)

1998 Grenada (ES)

1997 Santa Cruz (US)

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14:45 – 15:00	**Masayuki Takahashi**	Coupling Simulation on Two-dimensional Axisymmetric Beaming Propulsion System
15:00 – 15:15	**Tomo-Hiko Watanabe**	Kinetic simulation of multi-scale turbulence interactions and diffusion in magnetized plasma

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 2

Parallel Session: Materials and non-science 1

13:45 – 14:15	**Boris Kozinsky (invited)**	Towards ex-machina computations of transport and transformations in complex materials
14:15 – 14:30	**Nobuhiko Akino**	Optical Properties of OLED Materials by TDDFT
14:30 – 14:45	**James Boust**	*Ab initio* theory of $Nd_2Fe_{14}B$-based hard magnetic materials
14:45 – 15:00	**Hyeon-Deuk Kim**	Anomalous Properties of Condensed Hydrogen Systems under Extreme Thermodynamic Conditions Revealed by the Non-Empirical Ab Initio Molecular Dynamic Simulation Method
15:00 – 15:15	**Martin Matas**	Role of the M choice in Hf(M)SiBCN (M = Y, Ho, Ta, Mo) thin films: DFT, ab-initio molecular dynamics and experiment

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 1

Parallel Session: Statistical physics and complex systems 1

(Chairs: Wolfhard Janke, Yuko Okamoto)

13:45 – 14:00	**Lev Shchur**	Acceptance rate is a thermodynamic function in local Monte Carlo algorithms
14:00 – 14:15	**Nir Schreiber**	Changeover phenomenon in randomly colored Potts models
14:15 – 14:30	**Tasrief Surungan**	Phase diagram of the polyhedral spin models on square lattice with diluted bonds
14:30 – 14:45	**Thomas Prellberg**	Entropy of Dense Trails on the Square Lattice

Vu Sinh	Deep attention model for extracting material structure-property relationships
Lilih SIti Solihat	Theoretical Study of Dynamics and Infra-Red Spectra of Myosins
Mario Spera	A new high-performance N-body code to study merging compact-object binaries
Miles Stoudenmire	Simulating Near-Term Quantum Computers with Approximate Tensor Network Algorithms
Tasrief Surungan	Phase diagram of the polyhedral spin models on square lattice with diluted bonds
Hidemaro Suwa	Geometric allocation approach to accelerating directed worm algorithm
Soichiro Suzuki	Plasma Propagation via Radiation Transfer in Millimeter-wave Discharge under Subcritical Condition
Daisuke Suzuki	Thermodynamic folding transition of a small protein molecule
Yusuke Suzumura	Molecular-Dynamics Simulation of Liquid Sulfur by Artificial Neural Network Potentials
Masayuki Takahashi	Coupling Simulation on Two-dimensional Axisymmetric Beaming Propulsion System
Jun Takahashi	Multicriticality of the deconfined quantum critical point
Mykhailo Tatochenko	Confinement effects on packings of disco-rectangles in slit pores
Dave Thirumalai	Sub-diffusive glassy dynamics to super-diffusion in an evolving cell colony
Synge Todo	Novel approaches for tensor renormalization group method - ATRG and BTRG

SP1.2 – Changeover phenomenon in randomly colored Potts models

Nir Schreiber, Reuven Cohen , Gideon Amir, Simi Haber
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A hybrid Potts model where a random concentration p of the spins assume q_0 colors (Potts states) and a random concentration $1-p$ of the spins assume $q > q_0$ colors is introduced. It is known that when the system is homogeneous, with an integer spin number q_0 or q, it undergoes a second or a first order transition, respectively. It is argued that there is a concentration p^* such that the transition nature of the model is changed at p^*. This idea is demonstrated analytically and by simulations for two different types of interaction: the usual square lattice nearest neighboring and the mean field all-to-all interaction. Exact expressions for the second order critical line in concentration-temperature parameter space of the mean field model together with some other related critical properties, are derived.

[1] N. Schreiber, R. Cohen, G. Amir and S. Haber, arXiv:2105.05442 (2021).
[2] N. Schreiber, R. Cohen, S. Haber, G. Amir and B. Barzel, Phys. Rev. E 100 (2019) 52119.

SP1.3 – Phase diagram of the polyhedral spin models on square lattice with diluted bonds

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The study of phase transition is an important subject in condensed matter physics as some materials are more versatile when they are at certain phase. The low temperature ferromagnetic phase of magnetic material is a firm example of these. Passing by the Curie temperature, the paramagnetic phase of magnetic materials will change to a ferromagnetic phase. There are three main variables controlling a magnetic phase transition, namely the symmetry of spins, coupling interaction and the lattice structure. It is known that the discreteness can create low temper-

ature magnetic order, exemplified by the existence of a true- long range order for the 2D 6-state clock model at lower temperature [1, 2] In this talk we present our study of the ferromagnetic polyhedral spins model on square lattice with bond dilution. Polyhedral spins are the discrete counterpart of the continuous Heisenberg spin model. Two polyhedral spin models, i.e., the icosahedoron and dodecahedron model are discussed. As previously reported, the non-diluted (pure) ferromagnetic case of these models exhibits finite temperature phase transition [3]. We use Monte Carlo simulation with a newly introduced algorithm, two-size PCC algorithm [4]; and probe whether the existing phase transitions are significantly affected by the bond dilution. We simulate the models with various bond concentrations and calculate their corresponding critical temperatures. The phase diagram of the models are presented as a plot of the obtained critical temperatures with respect to their corresponding bond concentrations.

[1] T. Surungan and Y. Okabe, Phys. Rev. B 71, 188428 (2005).
[2] T. Surungan et al., J. Phys. A: Math. Theor. 52, 275002 (2019).
[3] T. Surungan and Y. Okabe, arXiv.org, cond-mat:1709.03720.
[4] T. Surungan and Y. Okabe, J. Phys. A: Math. Theor. 53, 505002 (2020).

SP1.4 – Entropy of Dense Trails on the Square Lattice

Lucas Rodrigues[1], Jurgen Stilck[1], Thomas Prellberg[2]

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We estimate the entropy of self-avoiding trails on the square lattice in the dense limit, where a single trail passes through all edges of the lattice, as a function of the density of crossings.

For this, the largest eigenvalues of transfer matrices of size up to 6.547×10^8 was obtained, utilising 76GB memory.