



SUMMERSOLSTICE 2014
International Conference On
Discrete Models Of Complex Systems

22-25 June 2014, Institute Jozef Stefan, Ljubljana, Slovenia

B O O K
O F
A B S T R A C T S

Edited by

Bosiljka Tadić & Milovan Šuvakov

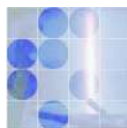
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Discrete Models of Complex Systems SUMMERSOLSTICE 2014

6th Edition



June 23—25, 2014, Institute Jožef Stefan, Ljubljana, Slovenia

BOOK OF ABSTRACTS

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CONTACT: Phone: +38614773767; FAX: +38614773724; E-mail: bosiljka.tadic@ijs.si

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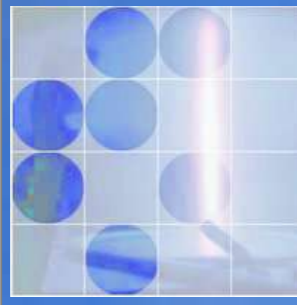
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6th Conference *Discrete Models of Complex Systems*

Program for Monday, 23rd June 2014

Monday 23. June 2014

Chair: Geoff Rodgers, Brunel University

TIME	Speaker	Title
09:00-09:30	Stefan Thurner Medical University Vienna	Entropies for Complex Systems
09:30-10:00	Milan Rajkovic Institute Vinca-Belgrade	Quantifying self-organization and complexity with a wavelet machine?
10:00-10:30	COFFEE BREAK	
10:30-11:00	Andrea Rapisarda University of Catania	Micro and Macro Benefits of Random Investments in Financial Markets
11:00-11:30	Jelena Grujic Imperial College London	Multi-strategy game as a complex system
11:30-12:00	Raul Rechtman UNAM Mexico	Topological bifurcations in a model of a society of reasonable contrarians
12:00-13:00	Lunch Break	

Monday 23. June 2014

Chair: Franco Bagnoli, University of Florence

TIME	Speaker	Title
13:00-13:30	Andrea Guazzini University of Florence	Sociophysics of Human Virtual Dynamics
13:30-14:00	Jiri Fiser Purkinje University	ETOS- domain specific language for discrete simulation
14:00-14:30	Anna Carbone Politecnico di Torino	Detrending Moving Average Algorithm: a Non-Random Walk through Complex Systems Science
14:30-15:00	Alexander Povolotsky BLTP, Dubna	Interacting particle systems: Integrability vs. universality
15:00-15:30	COFFEE BREAK	

Monday 23. June 2014

Chair: Matjaz Perc, University of Maribor

TIME	Speaker	Title
15:30-16:00	Alvaro Corral Barcelona University	Zipf's law and a scaling law, in texts and in music
16:00-16:30	Maria Letizia Bertotti Free University of Bozen	Correlation between economic inequality and mobility in kinetic models for social sciences
16:30-17:00	JiriSkvara J. E. Purkinje University	Stock Price Dynamics: Application of Simple Fluids Models and Percolation
17:00-17:30	Harbir Lamba George Mason University	Endogenous Dynamics in Financial and Economic Systems
17:00-19:00	Free time	

6th Conference *Discrete Models of Complex Systems*

Program for Tuesday, 24th June 2014

Tuesday 24. June 2014

Chair: Andrea Rapisarda, University of Catania

TIME	Speaker	Title
09:00-09:30	Matjaz Perc University of Maribor	Bargaining with discrete strategies
09:30-10:00	Marija Mitrovic Intitute of Physics Belgrade	Agent-Based Modeling and Social Structure in Bloggers' Dynamics
10:00-10:30	COFFEE BREAK	
10:30-11:00	Bruno Di Stefano Nuptek Systems, Toronto	Biomimicri As A Method For Developing Cognitive Agents
11:00-11:30	Anna T. Lawniczak University of Guelph	Model Of A Population Of Autonomous Simple Cognitive Agents And Their Performance In Various Environments
11:30-12:00	Rolf Hoffmann Tech. University Darmstadt	Ordering Colors into Strings by Agents
12:00-13:00	Lunch Break	

Tuesday 24. June 2014

Chair: Stefan Thurner, Medical University Vienna

TIME	Speaker	Title
13:00-14:00	Roderick Melnik WLU Waterloo, Canada	Interacting Scales and Coupled Phenomena in Nature and Models (<i>IJS Colloquium</i>)
14:00-14:30	Anton Grigoryev Saratov Technical University	DNA Sequencing by Discrete Dynamics DNA Elongation Monitoring
14:30-15:00	Luca Tubiana Jozef Stefan Institute	A simple one-dimensional model for composite polymer knots
15:00-15:30	COFFEE BREAK	

Tuesday 24. June 2014

Chair: Andrzej Krawiecki, Warsaw University Technol.

TIME	Speaker	Title
15:30-16:00	Jian Yuan, Tsinghua University Beijing	Understanding the Large Scale Urban Vehicular Mobility by Discrete Models
16:00-16:30	Pieter Van der Weeën Ghent University	Influence of the grid resolution on output accuracy and parameter sensitivity
16:30-17:00	Artem Badasyan University of Nova Gorica	Spin-based description of water in models of biological macromolecules
17:00-17:30	Natasa Adzic Jozef Stefan Institute	Field theoretic description of charge-regulation interaction
17:30-19:30	Short Excursion: <i>Ljubljana Castle, Guided tour</i>	
20:00-22:00	Conference Dinner	

6th Conference *Discrete Models of Complex Systems*

Program for Wednesday, 25th June 2014

Wednesday 25. June 2014

Chair: Rolf Hoffmann, Technical University Darmstadt

TIME	Speaker	Title
09:00-09:30	Jose F.F. Mendes University of Aveiro	Structural properties of complex networks
09:30-10:00	Geoff J. Rodgers Brunel University London	Network growth model with intrinsic vertex fitness
10:00-10:30	COFFEE BREAK	
10:30-11:00	Veronika Stoka Jozef Stefan Institute	A Structural and Functional Network as a Tool to Analyze Complex Biological Systems
11:00-11:30	Franco Bagnoli University of Florence	A self-organized method for risk perception in epidemic spreading on multiplex networks
11:30-12:00	Andrzej Krawiecki Warsaw Technology Univ	Dynamical Phase Transition in the Ising model on Scale-Free Networks
12:00-13:00	Lunch Break	

Wednesday 25. June 2014

Chair: Bosiljka Tadic, Jozef Stefan Institute

TIME	Speaker	Title
13:00-13:30	Joaquin Marro University of Granada	Non-equilibrium Phase Transitions in the Brain
13:30-14:00	Zeynep Kaya, Cognitive Neurosci. SISSA	Adding New Neurons on the Tail of a Binomial
14:00-14:30	Maximilian Sadilek Medical University of Vienna	From Wilson-Cowan to Kuramoto: Multiplex Formulation of Neural Activity
14:30-15:00	Zoran Levnajic University Novo Mesto	Reconstructing network structure from dynamical signals
15:00-15:30	COFFEE BREAK	

Wednesday 25. June 2014

Chair: Anna T. Lawniczak, University of Guelph

TIME	Speaker	Title
15:30-16:00	Benedikt Fuchs Medical University of Vienna	Behavioral and Network Origins of Wealth Inequality: Insights from a Virtual World
16:00-16:30	An Zeng University of Fribourg	Enhancing network functionalities by manipulating complex networks
16:30-17:00	Gamaliel Percino Medical University of Vienna	Complexity and the evolution of music-production networks
17:00-17:30	Bosiljka Tadic, Milovan Suvakov Jozef Stefan Institute	Triggering Mechanisms in Emotion Dynamics: From Brain Activity to Collective Social Behavior
17:30-17:40	Conference Closing	

Field theoretic description of charge-regulation interaction

Nataša Adžić¹, Rudolf Podgornik²

¹ Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana, Slovenia, natasa.adzic@ijs.si

² Department of Theoretical Physics, Jožef Stefan Institute, and Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia, rudolf.podgornik@fmf.uni-lj.si

In order to find the exact form of the electrostatic interaction between two proteins with dissociable charge groups in aqueous solution, we have studied a model system composed of two macroscopic surfaces with charge dissociation sites immersed in a counterion-only ionic solution [1]. We introduced a surface free energy corresponding to a simple model of charge regulation. Charge regulation is an old concept referring to the case, where the effective charge on a macroion, e.g. protein surface, responds to the local solution conditions, such as local pH, local electrostatic potential, salt concentration, dielectric constant variation and the presence of other charged groups. While in nanoscale interactions one often assumes constancy of surface macroion charge [2], in fact the charge state of the dissociable groups on the macroion surface always depends strongly on the acid-base equilibrium that defines the fraction of acidic (basic) groups that are dissociated and requires to be consistently included in any theoretical formulation. Due to it, we derived a theory, starting from the field-theoretic representation of the grand canonical partition function. It is evaluated within the mean field approximation giving the Poisson-Boltzmann theory with the Ninham-Parsegian boundary condition [3]. Gaussian fluctuations around the mean-field are then analyzed in the lowest order correction that we calculate *analytically* and *exactly*, using the path integral representation for the partition function of a harmonic oscillator with time-dependent frequency. Our general result gives attractive, long-ranged, fluctuation interaction which depends on the pH of the solution. The obtained attraction can overcome mean field repulsion when the surfaces reach their point of zero charge (PZC). Taking the proper limits, our result reduces to the zero-frequency van der Waals term, but also gives the correct Kirkwood-Shumaker result [4]-[5], which opens up the possibility to investigate the Kirkwood-Shumaker interaction in more general contexts where their original derivation fails.

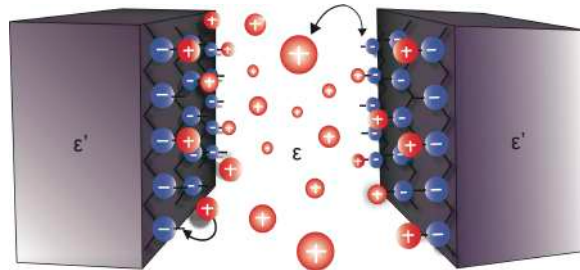


Figure 1: Graphical representation of the model: two charged planar surfaces with charge dissociation sites distributed uniformly along the surfaces and with counterions between the surfaces. The counterions originate from the charge dissociation of the dissociable groups (AC) through the reaction $AC \leftrightarrow A^- + C^+$.

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References

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- [2] A. Naji, M. Kanduč, J. Forsman, and R. Podgornik, J. Chem. Phys. **139** 150901 (2013).
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- [4] J. Kirkwood and J.B. Shumaker, Proc. Natl. Acad. Sci. USA **38** 855 (1952).
- [5] J. Kirkwood and J.B. Shumaker, Proc. Natl. Acad. Sci. USA **38** 863 (1952).