

# Summer Solstice 2018

# Conference on Discrete Models of Complex Systems

Book of abstracts

Gdańsk, June 25-27, 2018

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# Main informations

# Commitees

### **Conference Chairs**

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# Sponsors



**Invited Speakers** 

#### Andreas Deutsch

# Biological lattice-gas cellular automaton models for the analysis of collective behaviour in interacting cell populations

Andreas Deutsch, Centre for Information Services and High Performance Computing, TU Dresden

As a cellular automaton, a BIO-LGCA is defined on a regular lattice, where the nodes of the lattice take a certain number of discrete states. As a lattice-gas, the state space of a BIO-LGCA is related to the lattice geometry. Each node can be occupied by "biological agents", e.g. biological cells, characterized by their velocities which are restricted to the unit vectors connecting a node to its nearest neighbors. Agents move along the links and interact on the nodes of the lattice. This interaction can change the number of agents at individual nodes (birth/death processes) and may depend on the states in neighboring nodes which allows to model collective effects. Meanwhile, the BIO-LGCA has been established as discrete lattice- and agent-based model which permits multi-scale analysis and efficient large-simulations.

Ref.: Deutsch, A., Dormann, S.: Cellular automaton modeling of biological pattern formation: characterization, applications, and analysis. Birkhauser, Boston, 2018

#### Nazim Fatès

# How difficult is it to self-diagnose? On synchronisation phenomena in various cellular automata

Nazim Fatès, INRIA Nancy-Grand-Est/LORIA

Reflexivity is a fundamental property of complex systems. This word is in itself an enigma: if we consider an artificial system built by an engineer, it is a huge task to imagine how such a system may have an "image" of itself. If we think about biological organisms, which are usually described as an assembly of cells, it is still a mystery to know how these "systems" can self-diagnose and self-repair. Our purpose is to examine these questions in the context of cellular automata. We will describe mathematical models that allow a group of cells which are all identical to perform various tasks in a decentralised way. We examine phase synchronisation (blinking at the same pace), topology diagnosis (detecting the introduction of defects) and self-correction of k-colourings (stable states where two adjacents cells have different colours). We underline the limits of the classical deterministic solutions and show how randomness is often an elegant solution to deal with the difficulties.

#### Pietro Lio'

### Data integration: exploring the link between complex networks and neural networks

Pietro Lio', University of Cambridge

We are immersed in a Big Data ocean that contains many different data streams: molecular, images, clinical, social, behavioral, biometric, environmental, etc. Therefore data integration is nowadays one of the most important scientific and technological challenges. I will highlight similarities and differences among four useful methodologies in data integration. The first type of analysis we propose is a multilayer network approach. Another methodology is deep learning neural networks (supervise and unsupervised). The third approach is matrix factorisation and finally network regression. In particular I will show how cooupling between multilayer networks and deep learning could lead to cross modal and attention Networks. I will end with practical issues related to implementation and coding.

#### Andrea Rapisarda

#### If you are so smart why you are not so successful?

Andrea Rapisarda, INFN and University of Catania, Italy

The largely dominant meritocratic paradigm of highly competitive Western cultures is rooted on the belief that success is due mainly, if not exclusively, to personal qualities such as talent, intelligence, skills, efforts or risk taking. Sometimes, we are willing to admit that a certain degree of luck could also play a role in achieving significant material success. But, as a matter of fact, it is rather common to underestimate the importance of external forces in individual successful stories. It is very well known that intelligence or talent exhibit a Gaussian distribution among the population, whereas the distribution of wealth - considered a proxy of success follows typically a power law (Pareto law). Such a discrepancy between a Normal distribution of inputs, with a typical scale, and the scale invariant distribution of outputs, suggests that some hidden ingredient is at work behind the scenes. In this paper, with the help of a very simple agent-based model, we suggest that such an ingredient is just randomness. In particular, we show that, if it is true that some degree of talent is necessary to be successful in life, almost never the most talented people reach the highest peaks of success, being overtaken by mediocre but sensibly luckier individuals. As to our knowledge, this counterintuitive result although implicitly suggested between the lines in a vast literature is quantified here for the first time. It sheds new light on the effectiveness of assessing merit on the basis of the reached level of success and underlines the risks of distributing excessive honors or resources to people who, at the end of the day, could have been simply luckier than others. With the help of this model, several policy hypotheses are also addressed and compared to show the most efficient strategies for public funding of research in order to improve meritocracy, diversity and innovation.

# M. Ángeles Serrano

# Multiscale unfolding of complex networks by geometric renormalization

#### M. Ángeles Serrano, ICREA - Universitat de Barcelona

Complex networks display a hidden metric structure, which determines the likelihood and intensity of interactions. This quality has been exploited to map real networks, producing geometric representations that can be used as a guide for their efficient navigation and that shed light on pivotal forces –like preferentiality, localization, and hierarchization– that rule their structure and evolution. Now, the powerful methods that unveil network geometry enable to disentangle the multiple scales coexisting in real networks, strongly intertwined due to the small world property. We have defined a geometric renormalization group for complex networks embedded in an underlying space that allows for a rigorous investigation of networks as viewed at different length scales. We find that real scale-free networks show geometric scaling under this renormalization group transformation. This feature enables us to unfold them in a self-similar multilayer shell which reveals the coexisting scales and their interplay. The multiscale unfolding brings about immediate practical applications. Among many possibilities, it yields a natural way of building high-fidelity smaller-scale replicas of large real networks, and sustains the design of a new multiscale navigation protocol in hyperbolic space which boosts the success of single-layer versions.

# Program

# Sunday, June 24, 2018

Get Together Party (18:00-22:00) Faculty of Social Science



# Monday, June 25, 2018

Morning Session I: Theory of discrete systems (9:00-11:00)

# Biological lattice-gas cellular automaton models for the analysis of collective behaviour in interacting cell populations

Andreas Deutsch, Centre for Information Services and High Performance Computing, TU Dresden

As a cellular automaton, a BIO-LGCA is defined on a regular lattice, where the nodes of the lattice take a certain number of discrete states. As a lattice-gas, the state space of a BIO-LGCA is related to the lattice geometry. Each node can be occupied by "biological agents", e.g. biological cells, characterized by their velocities which are restricted to the unit vectors connecting a node to its nearest neighbors. Agents move along the links and interact on the nodes of the lattice. This interaction can change the number of agents at individual nodes (birth/death processes) and may depend on the states in neighboring nodes which allows to model collective effects. Meanwhile, the BIO-LGCA has been established as discrete lattice- and agent-based model which permits multi-scale analysis and efficient large-simulations.

Ref.: Deutsch, A., Dormann, S.: Cellular automaton modeling of biological pattern formation: characterization, applications, and analysis. Birkhauser, Boston, 2018

### Boundary control of Cellular Automata

Franco Bagnoli, University of Florence, Italy

We address the problem of regional controllability of cellular automata via boundary actions, i.e., we investigate the characteristics of a cellular automaton so that it can be controlled inside a given region only acting on the value of sites at its boundaries. We shall examine the conditions for deterministic and probabilistic cellulare automata, for what concerns the possibility of driving a systems towards a configuration (reachability problem) and inducing it in following a given trajectory (drivability problem).

#### Explorations of ternary cellular automata

Henryk Fukś, Brock University

While binary nearest-neighbour cellar automata (CA) have been studied in detail and from many different angles, the same cannot be said about ternary (three-state) CA rules. We will present some results of the explorations of the vast space of ternary rules, paying special attention to selected classes of rules, such as those which exhibit conservations laws as well as rules which are "reducible" to binary rules. The underlying question will be as follows: are there any ternary rules which could be useful in "complexity engineering", for example, to construct solutions of problems similar to the density classification problem?

# Morning Session II: Theory of discrete systems (11:30-13:30)

# How difficult is it to self-diagnose? On synchronisation phenomena in various cellular automata

Nazim Fatès, INRIA Nancy-Grand-Est/LORIA

Reflexivity is a fundamental property of complex systems. This word is in itself an enigma: if we consider an artificial system built by an engineer, it is a huge task to imagine how such a system may have an "image" of itself. If we think about biological organisms, which are usually described as an assembly of cells, it is still a mystery to know how these "systems" can self-diagnose and self-repair. Our purpose is to examine these questions in the context of cellular automata. We will describe mathematical models that allow a group of cells which are all identical to perform various tasks in a decentralised way. We examine phase synchronisation (blinking at the same pace), topology diagnosis (detecting the introduction of defects) and self-correction of k-colourings (stable states where two adjacents cells have different colours). We underline the limits of the classical deterministic solutions and show how randomness is often an elegant solution to deal with the difficulties.

## Cellular automaton models for analyzing the collective migration of heterogeneous cell populations

Anja Voss-Böhme, Hochschule für Technik und Wirtschaft Dresden, University of Applied Sciences, Friedrich-List-Platz 1, 01069 Dresden, Germany

Cell migration and cell proliferation are fundamental processes of tissue dynamics. They essentially determine the spatio-temporal density patterns which are observed in populations of interacting cells but often depend themselves on the cell density profile as well as the composition of the extracellular matrix in the local neighborhood of the cells. Probabilistic cellular automata and their extensions provide a model framework which allows to numerically and analytically study the tissue dynamics which results from the feedback between scales. Considering specifically heterogeneous cell populations where cell plasticity plays a major role, it is shown that cell-based cellular automaton modeling allows to estimate the contribution of heterogeneity on the dissemination and growth the whole cell population at the tissue scale.

References:

K. Talkenberger, E. Ada Cavalcanti-Adamda, A. Voss-Böhme, A. Deutsch. Amoeboidmesenchymal migration plasticity promotes invasion only in complex heterogeneous microenvironments. Scientific Reports 7: Article number: 9237 (2017) doi:10.1038/s41598-017-09300-3

D. Reher, B. Klink, A. Deutsch, A. Voss-Böhme. Cell adhesion heterogeneity reinforces tumour cell dissemination: novel insights from a mathematical model. Biology Direct 12:18 (2017) doi: 10.1186/s13062-017-0188-z

K. Böttger, H. Hatzikirou, A. Voss-Böhme, E. Ada Cavalcanti-Adam, M. A. Herrero, A. Deutsch. An Emerging Allee effect is critical for tumor initiation and persistance. PLOS Computational Biology 11(9):E1004366 (2015) doi:10.1371/journal.pcbi.1004366

#### Forming domino patterns by uniform cellular automata

Rolf Hoffmann, TU Darmstadt Germany

Forming Domino Patterns by Uniform Cellular Automata Rolf Hoffmann, TU Darmstadt

Here a domino is considered as a pair of black cells, surrounded by white cells. The task is to form a maximum number of dominoes (horizontal or vertically oriented) in a square field of cells. This task can by solved by cellular automata agents [1] which are moving around and acting according to an embedded finite state machine that was evolved by genetic algorithm. Applications are for example: finding a filter for domino particles with high throughput, or packing a maximum number of domino packets in a container.

Now it is the question how this task can be solved without intelligent agents, just with an uniform cellular automata rule. In a methodical way, the aimed global pattern is scanned for valid local neighborhood patterns, so-called templates. Then the rule is designed in a probabilistic way that the new cell state converges to the templates and through them to the aimed global pattern. Starting from any random initial configuration, the effectiveness and efficiency of the designed rules are studied through simulations using synchronous and asynchronous updating schemes. The used method is also illustrated by the simpler task to form a checkerboard pattern [2,3].

 Hoffmann R., Désérable D. (2017) Generating Maximal Domino Patterns by Cellular Automata Agents. In: Malyshkin V. (eds) Parallel Computing Technologies 2017. LNCS 10421, pp 18-31

[2] Fatès N., Marcovici I., Taati S. (2016) Two-Dimensional Traffic Rules and the Density Classification Problem. In: Cook M., Neary T. (eds) Cellular Automata and Discrete Complex Systems. AUTOMATA 2016. LNCS, vol 9664. pp 135-148

[3] Hoffmann R. (2018) Checkerboard Pattern Formed by Cellular Automata Agents. In: Adamatzky A. (eds) Shortest Path Solvers. From Software to Wetware. Emergence, Complexity and Computation, vol 32. pp 239-264

# Afternoon Session I: Theory of discrete systems (15:00-17:00)

# Pulsing dynamics in randomly wired complex cellular automata

Andrew Wuensche, Discrete Dynamics Lab, www.ddlab.org

A novel and remarkable phenomenon, sustained rhythmic oscillations, pulsing dynamics, directly emerge when the local connection scheme is randomised in 3-value complex cellular automata — those characterised by emergent gliders. With random wiring, time-plots of pulsing measures for each complex rule maintain a particular frequency-amplitude-waveform, and scatter plots of entropy/density and the density return-map show unique signatures, which have the characteristics of chaotic strange attractors.

In this talk I will describe and demonstrate the pulsing phenomena and measures in the context of samples of 3-value k-totalistic rules on a 2D hexagonal lattice, present case studies showing a diversity of pulsing rhythms, the emergence of spiral density waves as random wiring is locally confined, discuss possible mechanisms, and insights into bio-oscillations in nature.

References: http://arxiv.org/abs/1806.06416

# Solving the relaxed density classification problem by means of two-dimensional affine continuous cellular automata.

Marcin Dembowski, University of Gdańsk

We consider particular two-dimensional cellular automata (CAs) for solving the density classification problem (DCP) in some generalized sense. It is said that a d-dimensional binary CA solves the DCP if it evolves to the homogeneous state (all 0s or all 1s) that corresponds to the majority state of the initial configuration. The first formulation of the DCP concerns one-dimensional binary CAs. It was proved for any dimension that there exists no d-dimensional binary CA that solves the DCP. The proof follows from the fact that one of the necessary conditions for a binary CA to classify density for all initial configurations (of any size) is that it must be density-conserving, conflicting the goal of the DCP.

To overcome this hurdle, researchers have modified the original DCP by allowing two CAs instead of a single, adding memory, using non-deterministic CAs or by defining a different output specification. In our previous work we considered Continuous CAs (CCAs), i.e. CAs with real-valued states, which are also known as coupled-map lattices and look for an infallible classifier for one dimension. We focused on one of the simplest families of CCAs, so-called Affine CCAs (ACCAs), in which the local rule is affine in each variable and the values are in the range [0,1]. In this family there is no rule that solves the classical DCP, but by a slight relaxation of the output specification, we found an entire family of density-

conserving ACCAs solving this relaxed DCP. Our simulations showed that for such ACCAs with a range one neighbourhood the best performing ACCA, acts as the traffic rule that is mixed with the identity rule.

Now we consider two-dimensional ACCAs, which implies a very high computational complexity. We examine which two-dimensional density-conserving ACCAs are performing the best. The answer to this question is interesting because in two dimensions there is no rule that solves the spacing problem like the traffic rule does for one dimension.

## On the reversibility problem of finite hexagonal cellular automata over Z3

Adam Dzedzej, Institute of Mathematics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk, 80-308 Gdańsk, Poland

Barbara Wolnik, Institute of Mathematics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk, 80-308 Gdańsk, Poland

Antoni Augustynowicz, Institute of Mathematics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk, 80-308 Gdańsk, Poland

Maciej Dziemiańczuk, Institute of Informatics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk

Jan M. Baetens, *KERMIT*, Department of Data Analysis and Mathematical Modelling, Ghent University Bernard De Baets, *KERMIT*, Department of Data Analysis and Mathematical Modelling, Ghent University

Reversible cellular automata (CAs) are of particular interest in CA applications since they can be used to simulate, for instance, gas or fluid dynamics. Unfortunately, determining whether a CA is reversible is an intricate task, especially in two or more dimensions. Moreover, in general, reversibility is not decidable [1]. However, in the case of CAs with the state set Z3 on two-dimensional hexagonal grids (HCAs), the problem of reversibility has been regarded as completely resolved. For null boundary conditions Siap et al. [2] claimed to have classified the HCAs and sizes of grids on which they are reversible. It appears that the results presented in [2] are not valid. The problem of reversibility of HCAs with periodic boundary conditions was studied in [3]. Nevertheless, the tools introduced there do not allow to decide whether a given HCA is reversible or not. Additionally, they apply to a restricted list of HCAs by imposing conditions on local rule coefficients.

We give counterexamples to theorems stated in [2] and present a correct and extended classification of HCAs over Z3 with periodic boundary conditions.

References:

[1] Kari, J.: Reversibility of 2D cellular automata is undecidable. Physica D: Nonlinear Phenomena 45(1), 379-385 (1990)

[2] Siap, I., Akin, H., Uguz, S.: Structure and reversibility of 2D hexagonal cellular automata. Computers and Mathematics with Applications 62(11), 4161-4169 (2011)

[3] Uguz, S., Siap, I., Akin, H.: 2-dimensional reversible hexagonal cellular automata with periodic boundary. Acta Physica Polonica A 123(2), 480-483 (2013)

# Statistical modeling of genotype-phenotype relationship through gene family analysis

Krzysztof Bartoszek, Department of Computer and Information Science, Linköping University, Sweden

Pietro Lio', Computer Laboratory, University of Cambridge, UK

Quantitative genetics aims to understand the genetic bases of traits (phenotype) coded by many genes, or complex traits. This kind of trait includes most traits of interest in medical science (e.g. complex diseases), animal and plant breeding (e.g. growth, productivity) and evolutionary biology (e.g. life-history traits). Gene families have extraordinary importance in elucidating genome architecture and dynamics: they combine the study of traits at pathway level with the evolutionary mutational divergence and selection trajectories. We propose an Ornstein-Uhlenbeck model to study genotype-phenotype mapping and the relations of genes within large families of duplicated genes scattered in the human genomes. This model is also suitable to investigate patterns of speciation. We discuss our model in the context of the infinitesimal model (Fisher 1918), the recent omnigene model and we describe a tutorial of a related software.

References

R. A. Fisher. The correlation between relatives on the supposition of Mendelian inheritance. Proc. Roy. Soc. Edinburgh 52 (1918), 399-433.

## Poster Session (17:30-19:00)

## A study of cellular automata in reservoir computing on real-valued datasets

Levi Fussell, University of Edinburgh

Reservoir computing (RC) is a computational paradigm in which a dynamical system is used to drive computation. In this work we explore how cellular automata (CA), which have been shown to exhibit edge of chaos behavior and manifest complex patterns and dynamics, can be utilised as the reservoir in an reservoir computer. To the best of our knowledge, previous research has studied only one or two-dimensional binary cellular automata reservoirs, evaluated on binary data. Our work explores real-valued, high-dimensional CA rules trained on a variety of complex time series data sets: Mackey-Glass, NARMA, and the SILSO monthly sunspots dataset. For each model we use one or two-dimensional lattices and a more general N-dimensional lattice. These results are then compared to an echo state network (ESN) baseline. We show it can be difficult to achieve comparable performance to an ESN and provide insight into how CA should be designed for reservoir computing.

# Predicting language diversity with the agent-based model on complex network

Tomasz Gubiec, University of Warsaw

Evolution and propagation of the world's languages is a complex phenomenon, driven, to a large extent, by social interactions. Multilingual society can be seen as a system of interacting agents, where the interaction leads to a modification of the language spoken by the individuals. Here we address the issue of the language diversity in societies of different sizes, and we show that local interactions are crucial to capturing characteristics of the empirical data. We propose a model [1] that cancels the contradiction between previous models and the Solomon Islands case. Our results demonstrate the importance of the topology of the network, and the rewiring mechanism in the process of language change.

[1] T. Raducha, T. Gubiec, Accepted to PlosOne (arXiv:1704.0835) (2018)

#### Line graphs for fractals

Malgorzata Krawczyk, AGH University of Science and Technology, Poland

Fractals are very interesting and ubiquitous objects. One of methods which allow for a fractal construction is the Lindenmayer system [1]. For each analysed graph we construct its line graph [2]. Nodes in a line graph constructed for a given graph replace its edges, and two nodes in a new graph are connected if they have a common node in the original graph. The question we ask is if the obtained line graphs show fractal properties. In this case we should be able to find the Lindenmayer system which allows for the line graph construction.

In our earlier paper [3] some symmetric fractals were analysed in terms of the number of classes of nodes. Now, the method is applied for graphs and their line graphs constructed on fractals to compare their symmetry.

We have shown that line graphs constructed on fractal graphs demonstrate fractal properties. We found the related Lindenmayer systems and calculated the fractal dimension for a set of line graphs, which for all analysed examples is equal to the fractal dimension of original graphs. As the structure of cyclic and linear graphs and their line graphs is very similar, the related number of classes is also the same. This is no more true for higher order fractals. Also in this case pattern of a change of the number of classes with the graph size is not trivial. For the fractals analysed in this paper the number of classes is much lower than the number of nodes; this means that the ratio of the reduction of the system size when described by classes is high. This is due to the high symmetry of the considered examples.

This work was (partially) supported by the AGH UST statutory tasks No. 11.11.220.01/2 within subsidy of the Ministry of Science and Higher Education

1. Prusinkiewicz, P. and Lindenmayer, A., The Algorithmic Beauty of Plants, Springer-Verlag 1990

2. Diestel, R., Graph Theory, Springer-Verlag New York 1997, 2000

3. Krawczyk M.J., IJMPC 26 (2015) 1550025

## Spatial evolution of Hindmarsh–Rose neural network with time delays

Michał Łepek, Warsaw University of Technology

Spatial relations between neurons in the network with time delays play a crucial role in determining dynamics of the system. During the development of the nervous system different types of neurons group together to enable specific functions of the network. Right spatial distances, thus right time delays between cells are crucial for an appropriate functioning of the system. To model the process of neural migration we proposed simple but effective model of network spatial evolution based on Hindmarsh–Rose neurons and Metropolis–Hastings Monte Carlo algorithm. Under the specific assumptions and using appropriate parameters of the neural evolution the network can converge to the desirable state giving the opportunity of achieving large variety of spectra. We show that there is a specific range of network size in space which allows it to generate assumed output. A network or generally speaking a system with time delays (corresponding to the arrangement in the physical space) of specific output properties has a specific spatial dimension that allows it to function properly.

#### Cartesian genetic programming with memory

Maciej J. Mrowinski, Faculty of Physics, Warsaw University of Technology

Cartesian Genetic Programming (CGP) is an evolutionary programming algorithm whose purpose is to evolve computer programs using concepts inspired by natural selection. It's range of applications is wide and includes problems like optimisation or image processing. Programs in CGP are encoded as graphs. The structure of an encoded CGP program is very similar to a multilayer perceptron network with different activation functions assigned to nodes and with equal weights of all connections. A CGP program is evolved using the so called 4+1 algorithm, which tries to maximise a user-provided fitness function by creating, via mutation, new generations of programs.

Recurrent Cartesian Genetic Programming (RCGP) is a variant of CGP which allows cycles in the graphs representing programs, which implicitly introduces memory into CGP. The addition of memory broadens the range of applications of CGP and makes it a more viable tool for problems like time series forecasting. In our work, we propose a modification of CGP which results in an explicit inclusion of memory. We achieve this by directly including a shift register in each node of the CGP graph and constantly providing these registers with values processed by nodes. Thanks to this approach (which we call SRMCGP – Shift Register Memory CGP), users gain fine-grained control over the memory in the program, which is not possible in RCGP, and avoid forward, recurrent connections. In order to study the memory capabilities of RCGP and SRMCGP, we performed numerical simulations of programs whose purpose was to memorise and repeat the input signal after a given number of time steps. Our results suggest that SRMCGP is much more efficient than RCGP usable solutions/programs can be acquired faster through SRMCGP. Additionally, SRMCGP results in a smaller number of active nodes which makes SRMCGP programs less costly (it terms of computation time) to decode. SRMCGP is also more likely to actually create usable solutions/programs.

# Modeling atrial fibrillation formation by multilayer cellular automata

Krzysztof Pastuszak, Gdańsk University of Technology Danuta Makowiec, University of Gdańsk

Atrial fibrillation is one of the most common sustained abnormal heart rhytm (1). Continuous models have been shown to reproduce the macroscopic behaviour (2), however they fail to capture the microscopic effects of fibrosis (2). Discrete, cellular automata based models have been successfully used to reproduce the phenomena of spiral waves formation in atrial fibrillation (3),(4),(5),(6).

In the following a multilayer cellular automata model, inspired by (5), is presented. Fibrosis is simulated by the introduction of collagen fibers, and by regulation of a number of lateral crossconnections. Effects on spiral waves formation and wave propagation speed are examined. Single and multilayer models are compared.

The results were obtained by performing numerical simulations. Bibliography:

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# Healthcare system network model for simulations of interhospital multidrug-resistant pathogen spread

Konrad Sakowski, Institute of High Pressure Physics, PAS Monika Piotrowska, Institute of Applied Mathematics and Mechanics, University of Warsaw

Widespread use of medicines and antibiotics in modern treatment leads to development of resistance of pathogens to some drugs due to natural selection. Such effect is particularly noticeable in the hospital environment. Spread of the multidrug-resistant Enterobacteriaceae (MDR-E) became an important problem for European healthcare systems. The standard approach to this problem is to focus on preventing of transmission of MDR-E locally, on the single facility level. However, there is growing evidence that the inter-hospital patient transfers may be the an important factor contributing to the MDR-E spread within healthcare systems. In this study, we present a network model of patient traffic in healthcare systems, which can be a basis of systematic study of transmission dynamics of MDR-E and the effectiveness of infection control strategies to prevent their spread through these systems. This model takes into account direct transfers between healthcare facilities as well as indirect transfers, where the patients stay at home for some time between discharge and readmission. To model the pathogen spread within single facilities, we use standard SIS differential model. We show results of simulations preformed with the proposed model and we show what is the impact of various model parameters on the MDR-E transmission dynamics. An important problem in this study is how to build a network corresponding to a realistic healthcare system having access only to limited (privacy reasons) patient hospitalization records. We would like to present the problems and limitations of recovering of patient transfer network from such records. Examples of derived networks will be presented and discussed.

Acknowledgements:

This work was supported by grant no. 2016/22/Z/ST1/00690 of National Science Centre, Poland within the transnational research programme JPI-EC-AMR (Joint Programming Initiative on Antimicrobial Resistance).

# Analyzing the impact of cell turnover on the plasticity of tissue polarity patterns by cellular automaton modeling: The dynamically diluted alignment model

Anja Voss-Böhme, Hochschule für Technik und Wirtschaft Dresden, University of Applied Sciences, Friedrich-List-Platz 1, 01069 Dresden, Germany

Authors: Karl B. Hoffmann, Anja Voss-Böhme, Jochen C. Rink and Lutz Brusch Abstract: Understanding the polarisation of cells and tissues is key for decoding the principles of tissue morphogenesis during biological development and regeneration. We argue that a deeper understanding of biological polarity pattern formation can be gained from the consideration of pattern reorganisation in response to an opposing instructive cue. Considering experimentally inducible body axis inversions in planarian flatworms, we define a dynamically diluted alignment model linking three processes: entrainment of cell polarity by a global signal, local cell-cell coupling aligning polarity among neighbours, and cell turnover replacing polarised cells by initially unpolarised cells. The model is related to an 8-Potts model with annealed site-dilution but explicitly describes the dynamics on the cellular scale. Numerical and theoretical model analysis shows that a persistent global orienting signal determines the final mean polarity orientation at the tissue scale. Neighbour coupling retards polarity pattern reorganisation whereas cell turnover accelerates it. These results can be subsumed in linear dependency relation between the time of polarity reorganisation and some e?ective neighbour coupling strength which integrates both effects. Our results allow to determine neighbour coupling strengths from experimental observations.

Reference: K. Hoffmann, A. Voss-Böhme, J. C. Rink, L. Brusch. (2017) A Dynamically Diluted Alignment Model Reveals the Impact of Cell Turnover on the Plasticity of Tissue Polarity Patterns. Journal of the Royal Society Interface, 14 20170466 (2017)

## Does data preprocessing affect the analysis of couplings in the cardiovascular system?

Dorota Wejer, University of Gdańsk

Shannon entropy (ShE) is a recognized tool for studying the organization of time series. Transfer entropy (TE) allows the assessment of dependencies between coupled systems. It occurs that both entropies reveal a strong dependence on the preprocessing method used for the signal.

We considered two types of symbolization. The first type refers to the variability of the signal. The second type exposes the trends of dynamics. Both symbolizations were applied to basic physiological signals: the rhythm of heart rate (RR) and systolic blood pressure (SBP) in order to assess the organization of the cardiovascular system. The signals were registered in healthy people during the tilt test (HUT) - a medical procedure often used to evoked autonomic reflexes - here baroreflex, provoked by the sudden change of a body position. Systematic studies were supported by simulations with shuffled data to distinguish the real features of signals from random fluctuations. The obtained results were also confronted with the physiological facts of the cardiovascular response to the HUT test.

We have found that ShE obtained for signals with the preprocessing method based on variability is indistinguishable from ShE obtained from randomly shuffled signals. But when symbolization with coding dynamical trends was used then the expected distinction between real signals (lower entropy) and randomly shuffled signals (higher entropy) ocurrs.

Also, the high percentage of zero values obtained for TE seems to be the effect of preprocessing. TE = 0 means that studied signals are not coupled (rather rare event) or couplings do not achieve statistical significance. Nevertheless, we found the time periods in the HUT recordings with statistically significant invluence of the heart rhythm on the vascular system (so-called, feed-forward bareflex arm), and the effects of the vascular system on the cardiac system (so-called, feed-back baroreflex arm).

In summary, any inference based on entropy measures must always be supported by the rules used in the preprocessing of data.

# Tuesday, June 26, 2018

# Morning Session I: Networks (9:00-11:00)

# Multiscale unfolding of complex networks by geometric renormalization

M. Ángeles Serrano, ICREA - Universitat de Barcelona

Complex networks display a hidden metric structure, which determines the likelihood and intensity of interactions. This quality has been exploited to map real networks, producing geometric representations that can be used as a guide for their efficient navigation and that shed light on pivotal forces –like preferentiality, localization, and hierarchization– that rule their structure and evolution. Now, the powerful methods that unveil network geometry enable to disentangle the multiple scales coexisting in real networks, strongly intertwined due to the small world property. We have defined a geometric renormalization group for complex networks embedded in an underlying space that allows for a rigorous investigation of networks as viewed at different length scales. We find that real scale-free networks show geometric scaling under this renormalization group transformation. This feature enables us to unfold them in a self-similar multilayer shell which reveals the coexisting scales and their interplay. The multiscale unfolding brings about immediate practical applications. Among many possibilities, it yields a natural way of building high-fidelity smaller-scale replicas of large real networks, and sustains the design of a new multiscale navigation protocol in hyperbolic space which boosts the success of single-layer versions.

# Geometrical self-assembly of networks with large simplicial complexes

#### Bosiljka Tadic, Jozef Stefan Institute

Structured networks representing a variety of complex systems, from functional materials [1] and brain activity patterns [2] to online social graphs [3], exhibit a hidden structure that can be attributed to the occurrence of significant simplicial complexes and the emergent hyperbolicity [4]. Q-analysis based on the algebraic topology of graphs can decipher this complex architecture by identifying elementary simplexes beyond nodes and links (triangles, tetrahedrons, and higher order cliques), and revealing the ways that they combine into

a particular mesoscopic complex. To understand how such hidden geometries of networks can emerge, we have recently devised a model of geometrical self-assembly of pre-formatted groups of nodes, which are described by simplexes of different sizes [5]. In the model, the geometric compatibility of the attaching simplex with the suitable binding site on the growing network plays a decisive role in addition to the chemical affinity of the system towards adding a number of new nodes. In this lecture, we will describe the model's rules and parameters; then we will demonstrate how different structures are generated by varying the related parameters (see online demo: http://suki.ipb.ac.rs/ggraph/) and distinguish them by determining the appropriate algebraic-topology measures.

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#### Finding the optimal nets for self-folding Kirigami

Jose Fernando Mendes, University of Aveiro

Three-dimensional shells can be synthesized from the spontaneous self-folding of twodimensional templates of interconnected panels, called nets. The yield is maximized following sequentially two design rules: (i) maximum number of vertices with a single-edge cut and (ii) minimum radius of gyration of the net. Previous methods to identify the optimal net are based on random search and thus limited to very simple shell structures and not guaranteeing a unique solution. Here, we show that the optimal net can be found using a deterministic algorithm. We map the connectivity of the shell into a shell graph, where the nodes and links of the graph represent the vertices and edges of the shell, respectively. Applying the design rule (i) corresponds then to finding the set of maximum leaf spanning trees of the shell graph, to which (ii) can be applied straightforwardly. This method allows not only to designing the self-assembly of much larger shell structures but also to apply additional design rules, as a complete catalog of the maximum leaf spanning trees is obtained.

# Morning Session II: Applications of discrete models (11:30-13:30)

#### If you are so smart why you are not so successful?

Andrea Rapisarda, INFN and University of Catania, Italy

The largely dominant meritocratic paradigm of highly competitive Western cultures is rooted on the belief that success is due mainly, if not exclusively, to personal qualities such as talent, intelligence, skills, efforts or risk taking. Sometimes, we are willing to admit that a certain degree of luck could also play a role in achieving significant material success. But, as a matter of fact, it is rather common to underestimate the importance of external forces in individual successful stories. It is very well known that intelligence or talent exhibit a Gaussian distribution among the population, whereas the distribution of wealth - considered a proxy of success follows typically a power law (Pareto law). Such a discrepancy between a Normal distribution of inputs, with a typical scale, and the scale invariant distribution of outputs, suggests that some hidden ingredient is at work behind the scenes. In this paper, with the help of a very simple agent-based model, we suggest that such an ingredient is just randomness. In particular, we show that, if it is true that some degree of talent is necessary to be successful in life, almost never the most talented people reach the highest peaks of success, being overtaken by mediocre but sensibly luckier individuals. As to our knowledge, this counterintuitive result although implicitly suggested between the lines in a vast literature is quantified here for the first time. It sheds new light on the effectiveness of assessing merit on the basis of the reached level of success and underlines the risks of distributing excessive honors or resources to people who, at the end of the day, could have been simply luckier than others. With the help of this model, several policy hypotheses are also addressed and compared to show the most efficient strategies for public funding of research in order to improve meritocracy, diversity and innovation.

## The coevolving voter model with spin-dependent rewiring probability – mean field approach

Krzysztof Kułakowski, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology

Recent generalization of the coevolving voter model [1] for the case of spin-dependent node degree is further generalized here, including spin-dependent probability of rewiring. Mean field results [2] indicate that either the system splits into two separate networks with different spins, or one of spin orientation goes extinct. In both cases, the density of active links is equal to zero. The results are discussed in terms of homophily in social contacts.

[1] J. Toruniewska, K. Kułakowski, K. Suchecki and J. Hołyst, Phys. Rev. E 96 (2017) 042306

[2] K. Kułakowski, M. Stojkow, D. Żuchowska-Skiba and P. Gawroński, submitted (arXiv: 1804.06650)

# Can banks default overnight? Modelling endogenous contagion on the O/N interbank market

Tomasz Gubiec, University of Warsaw

We propose [1] a new model of the liquidity-driven banking system focusing on overnight interbank loans. This significant branch of the interbank market is commonly neglected in the banking system modeling and systemic risk analysis. We construct a model where banks are allowed to use both the interbank and the securities markets to manage their liquidity demand and supply as driven by prudential requirements in a volatile environment. The network of interbank loans is dynamic and simulated every day. We show how the intrasystem cash fluctuations alone, without any external shocks, may lead to systemic defaults, and what may be a symptom of the self-organized criticality of the system. We also analyze the impact of different prudential regulations and market conditions on the interbank market resilience. We confirm that the central bank's asset purchase programmes, limiting the declines in government bond prices, can successfully stabilize banks' liquidity demands. The model can be used to analyze the interbank market impact of macroprudential tools.

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# Afternoon Session I: Applications of discrete models (15:00-17:00)

## Social clusters: role of memory and opinion alignment

Bartłomiej Dybiec, Institute of Physics, Jagiellonian University

Individuals building social systems are characterized by complex states, and interactions among individuals can align their opinions. The Axelrod model describes how local interactions can result in emergence of cultural domains. We discuss two variants of the Axelrod model where local consensus is reached either by listening and accepting one of neighbors' opinion or two agents discuss their opinion and achieve an agreement with mixed opinions. It is shown that the local agreement rule affects the character of the transition between the single culture and the multiculture regimes.

In the accepting model, during each interaction the receiver accepts the whole providers opinion while in the discussing model the opinions are aligned in the democratic way: on average, each interacting agents accepts half of traits of its interlocutor. The discussing updating result in the behavior very similar to the original Axelrod model (discontinuous transition). In contrast, the accepting model leads to graded transition from the ordered to the fully disordered final states.

Additionally, we explore the Axelrod model with an extended conservativeness which incorporates not only similarity between individuals but also a preference to the last source of accepted information. The additional preference given to the last source of information increased the initial decay of the number of ideas in the system, changes the character of the phase transition between homogeneous and heterogeneous final states and could increase the number of stable regions (clusters) in the final state.

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# Majority vote model with independence on complex networks

Andrzej Krawiecki, Faculty of Physics, Warsaw University of Technology, Poland

One of the most popular models for the opinion formation is the majority vote model with agents represented by two-state spins located in the nodes and interacting via edges of a possibly complex network of social contacts. In the simplest version of this model the agents assume, with probability governed by a parameter q (0 < q < 1/2), the opinion in agreement with that of the majority of their neighbors. In a variant called the majority vote model with independence the agents obey the above-mentioned ferromagnetic update rule with certain probability 1 - p (0 ) while with probability p they make decisionrandomly. In this contribution the majority vote model with independence is investigated on complex networks, including random graphs and scale-free networks. It is shown that the parameters q and p/2 are equivalent and as one of them is decreased, with the other fixed, the model can exhibit transition to the ferromagnetic state at a critical value qc or pc which depends on the mean degree  $\langle k \rangle$  and on the moment  $\langle k^{3/2} \rangle$  of the distribution of the degrees of nodes p(k). The critical behavior of the magnetization M is determined in the mean-field approximation. The model on random regular or Erdos-Renyi graphs belongs to the universality class of the mean-field Ising model, with M scaling as  $(qc-q)^{\beta}$  or  $(2pc-2p)^{\beta}$ with  $\beta = 1/2$ . In the case of the model on scale-free networks with the degree distribution  $p(k) \sim k^{-\gamma}$  for  $5/2 < \gamma < 7/2$  the scaling behavior is non-universal, with  $\beta = 1/2(\gamma - 5/2)$ , while for  $\gamma > 7/2$  the mean-field scaling with  $\beta = 1/2$  occurs. These results are confirmed by Monte Carlo simulations.

# Opinion dynamics on complex networks: the role of model design

Janusz Szwabiński, Wrocław University of Science and Technology

From the physical point of view it is always an interesting question how the details of a model at the microscopic scale manifest at the macroscopic level. In the field of opinion dynamics such a macroscopic quantity is the opinion, defined in case of binary models as the magnetization.

Early models of opinion dynamics were usually put on 1D chains or 2D square lattices. Even in these simple geometries there was a certain freedom in designing a model. In particular, the form of the influence group exerting social pressure on individuals could differ significantly between models.

With the emergence of the network science in the last decades the 1D chains and square lattices are more and more often replaced by different kinds of complex networks as the underlying topology of social interactions. This is simply due to the fact that in many situations those networks capture the contact patterns among people in a more realistic way. However, although those networks allow for even more freedom to model designers, according to Macy and Willer "there was a little effort to provide analysis of how results differ depending on the model design".

I my talk I will use the q-voter model as an example of a binary opinion model and generalize it to complex networks. Different topologies of the influence group will be discussed together with their impact on the opinion dynamics. I will show, by making use of Monte Carlo simulations and simple probabilistic arguments that the differences between model designs may be either important or negligible depending on the average path lengths of the underlying networks.

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# Cellular automata motivated model of vehicle traffic in contemporary city center

Krzysztof Malarz, AGH University of Science and Technology

In this lecture the necessary improvements in Chowdhury–Schadschneider model [1] allowing for modelling bi-directional cars traffic will be presented. The modified model is applied for simulating traffic in real topology of streets in Kraków [2]. Also possible further model modifications [3] allowing for taking into account railway vehicles (trams) will be presented.

[1] D. Chowdhury, A. Schadschneider, Self-organization of traffic jams in cities: Effects of stochastic dynamics and signal periods, Phys. Rev. E 59 (1999) R1311

- [2] R. Socha, M.Sc. Thesis, AGH University of Science and Technology, Kraków, (2017)
- [3] K. Nowak, M.Sc. Thesis, AGH University of Science and Technology, Kraków, (2017)

# Wednesday, June 27, 2018

# Morning Session I: Innovative methods (9:00-11:00)

### Data integration: exploring the link between complex networks and neural networks

#### Pietro Lio', University of Cambridge

We are immersed in a Big Data ocean that contains many different data streams: molecular, images, clinical, social, behavioral, biometric, environmental, etc. Therefore data integration is nowadays one of the most important scientific and technological challenges. I will highlight similarities and differences among four useful methodologies in data integration. The first type of analysis we propose is a multilayer network approach. Another methodology is deep learning neural networks (supervise and unsupervised). The third approach is matrix factorisation and finally network regression. In particular I will show how cooupling between multilayer networks and deep learning could lead to cross modal and attention Networks. I will end with practical issues related to implementation and coding.

# Performance of cognitive agents' simple observational learning strategies in crossing a highway

Anna T. Lawniczak, University of Guelph

We study the performance of simple observational social learning strategies used by cognitive agents in making decisions while attempting to cross a cellular automaton based highway, when an incoming vehicle is suddenly observed. The cognitive agent could represent an autonomous vehicle, a robot, a driver, a pedestrian, or an animal. We assume that an agent faced with such situation has a knowledge about the types of decisions (and their consequences) made by other agents in similar situations in the past. In their decisionmaking, the cognitive agents use the simple strategy of mimicking what succeeded and avoiding what failed in the past. Our work focuses on simplicity of the learning algorithms and we investigate the learning performance of two decision-making processes. We consider homogeneous and heterogeneous (i.e., containing risk takers and risk avoiders) populations of cognitive agents operating under various highway traffic conditions. We discussed selected simulation results and provide their statistical analysis.

## The dedicated massively-parallel FPGA-based simulator for complex systems modeling

Krzysztof Hałagan, Lodz University of Technology Jaroslaw Jung, Lodz University of Technology

ARUZ (Analyzer of Real Complex Systems) [1,2] is a scalable, fully parallel data processing system equipped with low-latency communication channels, dedicated for simulations involving interactions among huge amount of relatively simple elements working in parallel. These elements can represent atoms, molecules or groups of atoms in molecular simulation of complex system. ARUZ was constructed in BioNanoPark in Lodz (Poland) using reconfigurable components – FPGAs (Field Programmable Gate Arrays) instead of common processors. Device is composed of almost 26 000 FPGAs interconnected in 3D network by 75 000 cables. The simulator architecture was inspired by the Dynamic Lattice Liquid (DLL) model [3] designed to simulate dynamics in complex liquid systems, like polymer melts, multi-phase systems, etc. [4,5]. The algorithm based on this model is executed in cycles representing discrete time steps. In each cycle, every element can be moved to the neighboring lattice node or/and have its properties updated. The algorithm requires global synchronization and is dominated by local data exchange and simple logical operations. ARUZ can simulate the system composed of several million of elements in milliseconds time scale with more than  $10^9$  algorithm steps performed per day.

Acknowledgment: The research was partially supported by Polish National Science Centre grant No. 2017/25/B/ST5/01970.

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EU patent applications by Jung, J., at al.: EP3079066, EP3079071, EP3079072, EP3079073
Pakula, T., Teichmann J.; J. Mol. Liq. 86, 109-121 (2000)

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# Morning Session II: Integrative approach (11:30-13:30)

# Autonomous vehicles simple learning strategies abstracted from collision avoidance decision-making algorithms

Bruno Di Stefano, Nuptek Systems Ltd.

No day passes that the media does not give us content about autonomous vehicles. The reality of large numbers of autonomous vehicles on the road is not a matter of "whether" but a matter of "when". Indeed, autonomous vehicles have already become a reality on our roads but they are still limited in number to experimental quantities. However, only the final part of the experiments is carried on with actual autonomous vehicles, as most of the work is carried on through modeling and simulation of the autonomous vehicle as a robot modeled as a cognitive agent. This vehicle agent must exhibit flawless self-operation in: (1) collision avoidance; (2) "programmed" and "adaptive" learning; (3) direction finding and following; (4) route planning and following; (5) user interaction.

The absolute highest priority is safety, represented by collision avoidance algorithms. All other goals, functionality, and performance are sacrificed (if necessary) to achieve safety. A certain number of algorithms are taught to the autonomous vehicle prior to any deployment (i.e. programmed learning), but the majorities of the other is learned after deployment (adaptive learning) and are specific to the road situation of the environment where the vehicle is expected to operate. This is no different from what a driver does: he/she learns basic driving rules and skills and later tailors them to the actual environment where he/she is driving. ) Direction finding and following, route planning and following, and user interaction are mostly technological problems for which there is already a lot of accumulated knowledge, and practical solutions already in use in conventional vehicles or in autonomous vehicles operating at levels 0, 1, 2, and 3 of the SAE classification.

In this talk we will present a short review of established algorithms for both collision avoidance and adaptive learning for safety augmentation and we will describe our research based on simple observational social learning strategy.

# Exact combinatorial approach to finite coagulating systems

Paweł Kukliński, Politechnika Warszawska

The work gives a brief introduction to coagulation systems. After revealing the shortcomings of the standard approach based on Smoluchowski's equation the need for another approach is emphasized. Thereafter, the work introduces an exact combinatorial approach to finite coalescing systems. In this formalism, cluster sizes and time are discrete, and the binary aggregation alone governs the time evolution of the systems. By considering the growth histories of all possible clusters, the exact expression for the probability of a coagulating system with an arbitrary kernel in a given cluster configuration is derived. Over the course of the work monodisperse initial conditions are applied. After stating the derived formulas, for the constant, multiplicative and additive kernel, comparisons of the theoretical predictions and simulations are performed with a very good result. At the end significant advantages and minor disadvantages of the approach are summarized.

### Q-voter model with independence on multiplex networks

Tomasz Gradowski, Faculty of Physics, Warsaw University of Technology

Q-voter model with independence is studied on multiplex networks with two layers (duplex networks) analytically using pair-approximation method and numerically by Monte Carlo simulations. The layers have a form of random regular, Erdős–Rényi and scale-free networks with identical degree distributions. In a usual q-voter model, each time step agent interacts with a group of q randomly chosen neighbours; if q-neighbourhood is homogeneous then the agent follows its opinion with probability 1-p and acts independently with probability p. In the q-voter model on multiplex networks two kinds of dynamics are considered, LO-CAL&AND and GLOBAL&AND [1]. In the case of LOCAL&AND dynamics agent changes opinion if the above-mentioned update rule applied separately to q-neighbourhoods on each layer suggests change; in the case of GLOBAL&AND dynamics the agent changes opinion if the above-mentioned rule applied to a neighborhood composed of all q-neighborhoods from all layers suggests change. Depending on the kind of dynamics and the parameter qcontinuous or discontinuous phase transition to a ferromagnetic state is observed as p is decreased. Qualitatively, this transition resembles that reported for the q-voter model with independence on a duplex network with fully connected layers [2]. Quantitatively, significant differences in comparison with the latter case are observed in Monte Carlo simulations, depending mainly on the relationship between q and the mean number of neighbours within each layer. These Monte Carlo results exhibit good quantitative agreement with the analytic predictions from the pair-approximation method.

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### Impact of limits in pathways between sinoatrial node and atrium on heart rhythm by timed automata model.

Danuta Makowiec, University of Gdansk

There are evidences that the human right atrium and sinoatrial node (SAN) are functionally separated except at discrete SAN-atrial electrical junctions, called SAN-exit-pathways. We hypothesize that this type anatomy is a source of re-entry around the SAN. A computationally efficient model will be presented which reconstructs human right atrium electrophysiology. Activity of a myocyte is simulated by a timed automaton with continuous and discrete transitions reproducing stages of cellular membrane. A stochastic 2D-network of timed automata is designed to model the right atrium architecture: SAN, atria-ventricular node (AVN), SAN-exit-pathways and heterogeneous atrial tissue.

Simulations were performed to measure effects of quantity of SAN-exit-pathways: all-, half-, few-cells connections, on development and propagation of normal versus arrhythmic excitations: SAN-re-entry or fibrillation. Additionally, two parameters were controlled to measure an influence of (1) atrial tissue fibrosis:  $p_{trans}$  - probability for transversal intercellular network connections, and (2) impairment of individual cells:  $p_{refuse}$  - probability of a cell to refuse to excite. Simulations provided a critical relationship between atrial anatomy and rhythm of heart excitations. A discrete model of cells and intercellular connections was found as efficient method for quantifying this relationship.

# List of Participants

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