SOE 20: Networks: From Topology to Dynamics IV (joint session DY/SOE)

Time: Friday 9:30–11:45 Location: ZEU 250

SOE 20.1 Fri 9:30 ZEU 250

Efficient integration of short-range models on complex networks — •Jeffrey Kelling[1,2], Géza Ódor[3], Lilla Barancsuk[3], Shengfeng Deng[3], Bálint Hartmann[3], and Sibylle Gemming[2] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [3]Centre for Energy Research, Budapest, Hunguary

Complex, hierarchical or random network topolgies can give rise to unique behavior in many physical models. We study dynamical synchronization behavior in Kuramoto models on power grids and brain connectomes with millons of connections and $\mathcal{O}(100k)$ nodes. At these scales it is crucial to use the sparsity when computing derivatives, which, due to the random network structure, makes employing modern parallel hardware tricky. Here, we present our approach to numerically solving large systems ordinary differential equations on random directed graphs, where we focus on the computationally expensive task of computing derivatives and leave the common integration step to the `boost::odeint` library. Our application can utilize both parallel CPUs and GPUs. We also provide an overview of our results on human and fly brain connectomes as well as failure cascades in power grids and provide a measure of the advantage gained from our computational optimization efforts.

SOE 20.2 Fri 9:45 ZEU 250

Discovering hidden layers in quantum graphs — Łukasz Gajewski, •Julian Sienkiewicz, and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Warsaw, Poland

Finding hidden layers in complex networks is an important and nontrivial problem in modern science. We explore the framework of quantum graphs to determine whether concealed parts of a multilayer system exist and, if so, their extent, i.e., how many unknown layers are there. Assuming that the only information available is the time evolution of wave propagation on a single layer of a network, it is indeed possible to uncover that which is hidden by merely observing the dynamics. We present evidence on both synthetic and real-world networks that the frequency spectrum of the wave dynamics can express distinct features in the form of additional frequency peaks. These peaks exhibit dependence on the number of layers taking part in the propagation and thus allowing for the extraction of said number. We show that, in fact, with sufficient observation time, one can fully reconstruct the row-normalized adjacency matrix spectrum. We compare our propositions to a machine learning approach using a wave packet signature method modified for the purposes of multilayer systems.

SOE 20.3 Fri 10:00 ZEU 250

Dynamic network modelling of tumor disease and sepsis — •Eckehard Schöll[1,2,3], Jakub Sawicki[1,2], Rico Berner[1,4], Fenja Drauschke[1], Moritz Alkofer[1], Eckhardt Schneider[5], and Thomas Löser[5] — [1]Institut für Theoretische Physik, TU Berlin — [2]Potsdam Institute for Climate Impact Research — [3]Bernstein Center for Computational Neuroscience Berlin — [4]Institut für Physik, HU Berlin — [5]Institut LOESER, Wettiner Straße 6, 04105 Leipzig

We introduce a novel functional model for tumor disease and sepsis within the framework of complex networks [1,2]. Both diseases are treated in a unified way centered on their effect on the innate immune system. We propose an adaptively coupled two-layer network model of phase oscillators based upon the interaction of parenchymal cells (organ tissue) and immune cells, respectively, and the co-evolutionary dynamics of parenchymal, immune cells, and cytokines. The interaction and information exchange via cytokines between the cells of the parenchyma and the innate immune system is modeled by adaptive coupling weights. The emergent complex collective dynamics is represented with a few fundamental control parameters. Concepts and methods of nonlinear dynamical systems and networks theory, such as partial synchronization and clustering, as well as numerical and statistical methods are applied to describe physiological and pathological states. [1] Sawicki, J., Berner, R., Löser, T., and Schöll, E., Front. Netw. Physiol. 1, 730385 (2022). [2] Berner, R., Sawicki, J., Thiele, M., Löser, T. and Schöll, E., Front. Netw. Physiol. 2, 904480 (2022).

SOE 20.4 Fri 10:15 ZEU 250

Automated chemical reaction network discovery for the simulation of long-timescale degradation of materials — •Joe Gilkes[1], Mark Storr[2], Reinhard J. Maurer[1], and Scott Habershon[1] — [1]University of Warwick, United Kingdom — [2]AWE plc, United Kingdom

Degradation of organic materials such as polymers occurs over time scales of years and involves rare reaction events over an expansive network of elementary processes. Building such networks in order to predict the degradation pathways of these materials requires tackling combinatorially large chemical spaces, and propagating these networks in time becomes considerably more difficult as network size increases. Predicting overall rates by which materials break down requires accurate calculations of the energetic barriers of thousands of elementary reaction steps, which also comes with a substantial computational cost. We present a software framework written in the Julia language for automatically traversing chemical reaction space with an approach that iteratively expands the reaction network through successive re-evaluation of degradation products. We couple this with a machine learning model to predict activation energies. The result is a workflow that can swiftly sample reaction space to create computationally efficient molecular breakdown networks, and then run simulations to predict the long-term stability of these species under a range of environmental conditions. We demonstrate this approach for the example of polyethylene degradation.
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15 min. break

SOE 20.5 Fri 10:45 ZEU 250

Exact statistical mechanics of spin models on networks — •Konstantin Klemm — IFISC (CSIC-UIB), Mallorca, Spain

Biological, social, and technical systems are modeled as discrete entities interacting through a network. Predicting these systems' behaviour thus involves the computationally difficult task of solving dynamics on a given complex network. Although networks of interest typically have an abundance of short cycles influencing dynamics, existing computational methods build on the assumption that short cycles are small structural corrections, thus making a *locally tree-like* approximation. Here we show that exact and efficient prediction, exemplified by the Ising and spin glass models, is possible for many networks. We exploit *globally tree-like* structure in the sense of small tree-width. The full manuscript is available at https://arxiv.org/abs/2111.04766 .

SOE 20.6 Fri 11:00 ZEU 250

Network meta-analysis: A statistical physics perpective — Annabel L. Davies[1] and •Tobias Galla[2] — [1]Bristol Medical School, University of Bristol, Bristol BS8 2PS, UK — [2]IFISC, Instituto de Física Interdisciplinar y Sistemas Complejos (CSIC-UIB), Campus Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain

Network meta-analysis (NMA) is a technique used in medical statistics to combine evidence from multiple medical trials. In particular it allows one to compare treatments that have not been tested directly against each other in a trial. NMA defines an inference and information processing problem on a network of treatment options and trials connecting the treatments. In this talk I will briefly outline the 'NMA problem', and I will then describe how statistical physics can offer useful ideas and tools for this area, including from the theory of complex networks, stochastic modelling and simulation techniques [1]. In particular I will present an analogy we recently established between NMA and random walks on networks [2], and which improves existing algorithms for the estimation of 'proportion contributions' – that is the importance of any one element in the network for the comparison of any two given treatment options. One main aim of the talk is to attract physicists to this timely, interesting and worthwhile area of research.

[1] Annabel L Davies and Tobias Galla, J. Stat. Mech. (2022) 11R001

[2] Annabel L Davies, Theodoros Papakonstantinou, Adriani Nikolakopoulou, Gerta Rücker, Tobias Galla, Statistics in Medicine, 41 (2022) 2091

SOE 20.7 Fri 11:15 ZEU 250

Controlling the coarsening dynamics of ferrogranular networks by means of a vertical magnetic field — •Oksana

Bilous[1], Pedro Sánchez[1], Matthias Biersack[2], Ali Lakkis[2], Reinhard Richter[2], and Sofia Kantorovich[1] — [1]University of Vienna — [2]University of Bayreuth

In nature, phase transitions of various nature are significant and often lead to abrupt changes in the macroscopic properties of the material. Here, we address the question if a viscoelastic phase separation (VPS), proposed in 2000 by Hajime Tanaka for dynamically asymmetric mixtures, scales up for a shaken mixture of steel and glass spheres, i.e. for a so-called ferrogranulate when an external magnetic field is applied perpendicular to the plane in which the system is confined. In this contribution we focus on computer simulation. We calculated magnetization, dipolar and steric energies, radial distribution functions, the average number of neighbours and the efficiency of the emerging networks as functions of the simulation time and the values of the external vertical magnetic fields. Our results demonstrate that the network formation can be inhibited by the field perpendicular to the sample via dipole-dipole repulsion the field. These results are qualitatively confirmed by the experimental data.

SOE 20.8 Fri 11:30 ZEU 250

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