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Author, Institution: E-Mail:	Jordi Mas, BSC jordi.mascastella@bsc.es
Other contributors	Géza Ódor, HPC-Europa3 visitor

ABSTRACT:
This document describes the HPC-Europa3 visit of Dr. Géza Ódor, Centre for Energy Research, Institute for Technical Physics and Materials Science of the Hungarian Academy of Sciences (Budapest, Hungary), to Dr. Gustavo Deco, Pompeu Fabra University (UPF, Barcelona, Spain), and their subsequent ongoing collaboration. The study of universal scaling behaviour in statistical physics can be applied to the study of brain science with the help of HPC. The emerging collaboration between the two groups shows the benefits of the transnational access program.

KEYWORD LIST:
Statistical physics, critical phase transitions, neuroscience, brain, connectome

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Executive summary

This document describes the HPC-Europa3 visit of Dr. Geza Odor, Centre for Energy Research, Institute for Technical Physics and Materials Science of the Hungarian Academy of Sciences (Budapest, Hungary), to Dr. Gustavo Deco, Pompeu Fabra University (UPF, Barcelona, Spain), and their subsequent ongoing collaboration.

Prof. Ódor has a huge expertise and a long career in the research of universal scaling behaviour in statistical physics, which can be applied, with the help of HPC to the study of other different fields such as neuroscience.

Prof. Ódor has limited computing resources available in his department in Hungary and the national HPC infrastructure is overloaded. BSC provided access to the power9+V100 system within the HPC-Europa3 programme that covered his computational needs. Moreover, he had started a collaboration with Prof. Deco from the Computational Neuroscience Group in the Center for Brain and Cognition at the Pompeu Fabra University in Barcelona. The expertise and feedback from Prof. Deco's world leading brain science group has been very beneficial and opened up new directions in whole brain modelling.

An extensive use of the HPC resources available have been carried out at BSC (around 100.000 core hours). Typically, jobs were run 2-3 times at a duration of 6-12 hours/job per day within a maximum array of 100 CPUs, using their GPU optimized Kuramoto model solver codes.

This emerging collaboration between the two groups shows the benefits of the transnational access program.

1 Introduction

Prof. Géza Ódor is Hungarian, born in Budapest (1960). He studied electrical engineering and graduated from Technical University of Budapest (1984) with his diploma thesis about “Band structure calculation of non-metallic complex materials”. He took his first PhD at Eötvös Loránd University (ELTE), the oldest and largest university in Hungary. His doctoral thesis in 1989 was about “Renormalization group studies in real and momentum space”. He visited the United States where he took a Master in Science degree in Physics (1991-1993) at the University of Illinois Chicago (UIC). His second PhD from Eötvös Loránd University (ELTE) was in 1996 about Statistical Physics. In 2004, he became Doctor of the Hungarian Academy of Sciences with his thesis entitled “Universality classes in non-equilibrium systems”.

Photo of Prof. Géza Ódor

His current research interests are theory of phase transitions, non-equilibrium critical systems, surface growth phenomena, and parallel computing. More detailed information is available in his webpage: https://public.ek-cer.hu/~odor/; and the Google Scholar link: https://scholar.google.com/citations?user=SjsdoOoAAAAJ&hl=en

Prof. Géza Ódor participated in previous editions of the HPC Europa program. He was an awardee of HPC-Europa2 program and carried out collaborative visits in Barcelona during the years 2009, 2011, and 2012.

During the edition of HPC-Europa3 program he has applied three times under the calls #4 (2018), #8 (2019), and #12 (2020). He has been granted two visits:

- 1st project: Call #8 (HPC17MYDRL), with visit from 1 to 15 September 2019, title: Synchronization in whole brain models to study heterogeneity effects
- 2nd project: Call #12 (HPC17NVCHF), with visit from 5 to 19 September 2021, title: Synchronization behavior and scaling in the fruit-fly brain

For both visits, the host has been Prof. Gustavo Deco, Pompeu Fabra University (UPF, Barcelona). He is Research Professor at the Institució Catalana de Recerca i Estudis Avançats (ICREA) and Full Professor at the Pompeu Fabra University (UPF) where he leads the Computational Neuroscience group. He is also Director of the Center of Brain and Cognition (UPF). In 1987, he received his first PhD in Physics for his thesis on Relativistic Atomic Collisions. In 2001, he received his second PhD in Psychology at the Ludwig-Maximilians-University of Munich.

2 Scientific background

Theoretical and experimental research provides many signals for the brain to operate in a critical state. Critical systems exhibit optimal computational properties, suggesting why the nervous system would benefit from such mode. Whole-brain models were able to demonstrate that resting-state organization conforms to a state of 'criticality' that promotes responsiveness to external stimulation and optimal provides computational properties, suggesting why the nervous system would benefit from such mode. For criticality, certain control parameters need to be tuned, leading to the obvious question: why and how is this achieved?

Real systems, however, are highly inhomogeneous and one must consider whether heterogeneity is weak enough to use homogeneous models. Heterogeneity is also called disorder in statistical physics and can lead to such rare-region (RR) effects that smear the phase transitions. RRs can have various effects depending on their relevancy. They can change discontinuous transition to a continuous one or can generate so-called Griffiths phases (GPs). In the case of GPs, critical-like power-law dynamics appears over an extended region around the critical point, causing slowly decaying autocorrelations and burstiness. This behaviour was proposed to be the reason for the working memory in the brain. Furthermore, in GPs the susceptibility is infinite for an entire range of control parameters near the critical point, providing high sensitivity to stimuli, beneficial for information processing. Therefore, studying the effects of heterogeneity is a very important issue in models of real systems, in particular in neuroscience.

2.1 *Previous scientific research by the visitor*

Prof. Ódor started this kind of research on synthetic (Ódor et al. 2015) and real neural networks (Gastner and Ódor, 2016; Ódor, 2016; 2019) some years ago. They have showed that if the heterogeneity is not too large, one can find critical behaviour and GP in these models using large human connectome graphs, generated by the Openconnectome project from DTI images (see Fig.1).

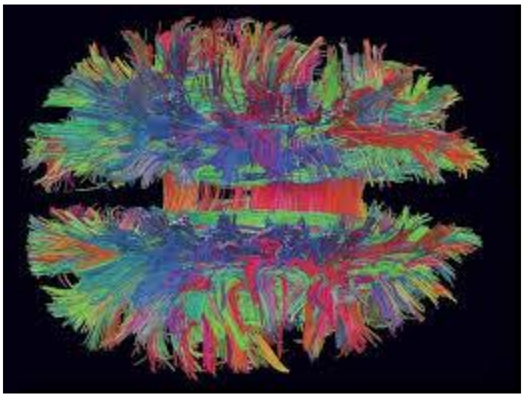


Fig.1 Picture of a human connectome obtained by diffusion tensor imaging (DTI) technique.

A very recent experimental study has provided confirmation for the applied connectome generation methods (Delettre et al., 2019). It has also been showed that if the kind of equalization of the network sensitivity that the visitor proposed (Ódor, 2016) is applied, the simulated and experimentally measured, critical behaviour agrees well on human subjects (Rocha et al., 2018).

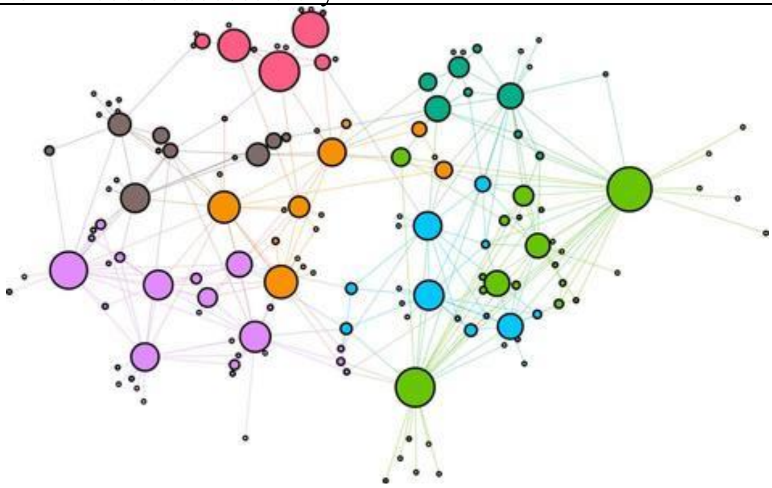


Fig.2 Modules of the "KKI-18" connectome graph, obtained from the Openconnectome project to be used.

It is also known, that individual neurons emit periodic signals, thus criticality may emerge by the collective behaviour of oscillators at the phase synchronization transition point. However, not much is known about the dynamics of the synchronization process in these models. Very recently theoretical analysis of the homogeneous Ginzburg-Landau type equations arrived at the conclusion that empirically reported scale-invariant avalanches can possibly arise if the cortex is operated at the edge of a synchronization phase transition, where neuronal avalanches and incipient oscillations coexist (Di Santo et al, 2018). The hypothesis, that cortical dynamics operates near criticality also suggests, that it exhibits universal critical exponents which marks the Kuramoto equation, a fundamental model for synchronization, as a prime candidate for an underlying universal model.

3 Rationale of the HPC Europa3 project. Overview

3.1 First project

However, solving the Kuramoto equation on connectomes of sizes, that allow measuring critical exponents without suffering from strong size effects requires supercomputing power on present day hardware. Jeffrey Kelling –one of the visitor's collaborators- developed a parallel code, which uses the Runge-Kutta-4 method for this problem with a speedup of ~100 on GeForce GTX TITAN Black GPU cards with respect to i7-4930K CPU @ 3.40GHz CPU cores, permitting them to integrate the equation on large graphs. This made it possible to determine dynamical critical exponents of the Kuramoto model on large lattices with unprecedented accuracy (Juhasz et al. 2021).

This code also permitted Ódor's team to locate a transition between partially phase synchronized and desynchronized states. At this crossover point we observed power-law-tailed phase synchronization durations, characterized by the exponent $\tau = 1.2(1)$, away from activity avalanche duration experimental values for the brain. However, mimicking a network with inhibitory interactions by flipping the signs of the outgoing weights of a randomly selected 20% of nodes, we found $\tau = 1.9(2)$, which is in the range of human brain experiments (Ódor and Kelling, 2019).

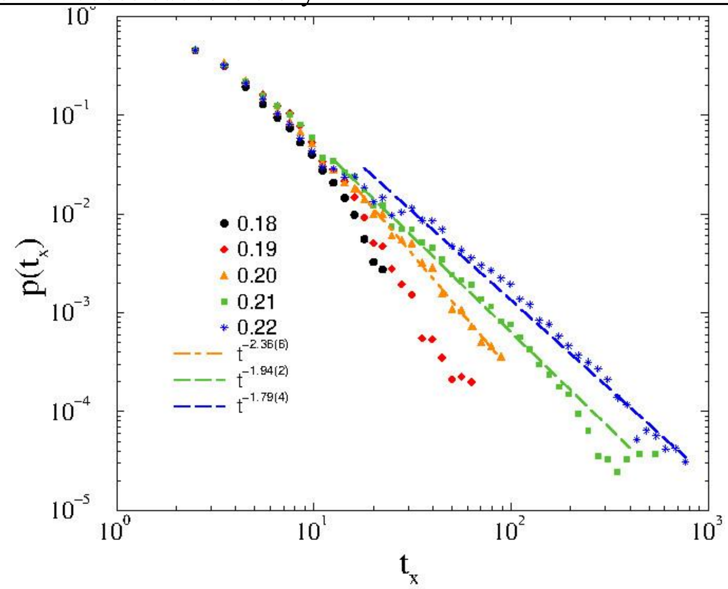


Fig.3 Duration distribution of t x on the KKI-18-I model for growth K = 0.18 (bullets), 0.19 (diamonds), 0.2 (up triangles), 0.21 (boxes), 0.22 (stars). The dashed line shows a PL fits to the tail region: t x > 10.

This implies that inhibitory interactions in brain models are necessary to describe experimental values. We also obtained results on a large two-dimensional lattice, having additional random, long-range links, finding a critical exponent $\tau = 1.6(1)$ for comparison. The details of this algorithm were presented at the NVIDIA's GPU Technology Conference (GTC2019) in San José (US).

Until then Ódor's team was dealing with the phase synchronization in the Kuramoto model. This is known to have a lower critical dimension of d = 4 (Hong et al., 2005) that is above the topological dimension of the human connectome they used. Note, that the human brain has ~10^{11} neurons, thus one can think if coming close to the thermodynamic limit. Without real phases it is not correct to speak about critical point or possible Griffiths effects. On the other hand, considering frequency synchronization of this model we can arrive to more interesting results. The frequency synchronization has a lower critical dimension d = 2 (Hong et al. 2005), thus we may expect to find real critical dynamical exponents which can be compared with the universality class values of basic models. In the case of Griffiths effects, we may see non-universal values to be compared with whole brain experiments.

Furthermore, G Ódor planned to investigate the effects of noise by the addition of a Gaussian distributed term to the Kuramoto equation, which is has also been considered in other brain models by altering the scaling behaviour. Together with the host Prof. Deco other more neuro-science related models, which exhibit synchronization behaviour, other connectome graphs were explored (Deco et al. 2017).

A specific aim of the visit was to run numerical studies by solving the Kuramoto equation, using the Runge-Kutta algorithm, to determine time dependent frequency synchronization behaviour on large human connectomes. These contain almost one million nodes, organized in a hierarchical modular structure (Gastner and Ódor, 2016). Note that this connectome size is still 10^4 times smaller than the number of neurons in the human brain! These runs have to be repeated and averaged over several initial disorder and/or noise realizations. The initial (quenched) disorder corresponds to the intrinsic frequencies (omega_i) of the oscillators. Furthermore, the whole procedure should be repeated at different control parameters near the critical point.

3.2 Second project

The first visit and collaboration at the fall of 2019 on whole brain modelling was successful, which leaded to a publication in the *Journal of Neuroscience* (Ódor et al., 2021). This was about critical behaviour simulations on a large human connectome network, containing ~ 850K nodes. They investigated the effects of stochastic noise on the desynchronization power-laws. Later, the largest precise connectome of a fruit fly became available and the applicability of the previous method to detect possible differences and similarities appeared as a good opportunity. The second visit extended a new branch towards the analysis of steady-state susceptibility.

The availability of the connectome graph of a fruit fly (Xu et al. 2020) was a great chance to apply their analyses. It contains ~22.000 neurons; it is large enough and it does not suffer from the approximations made by generating human connectomes using DTI technique. See Fig. 4.

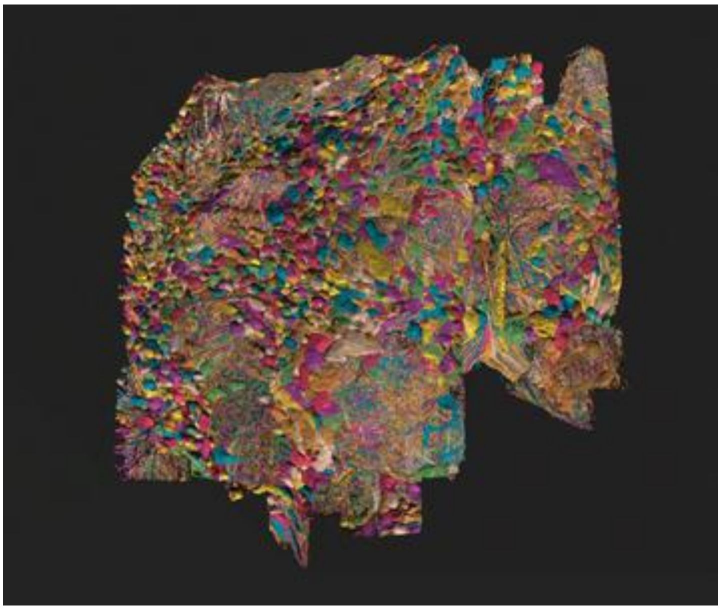
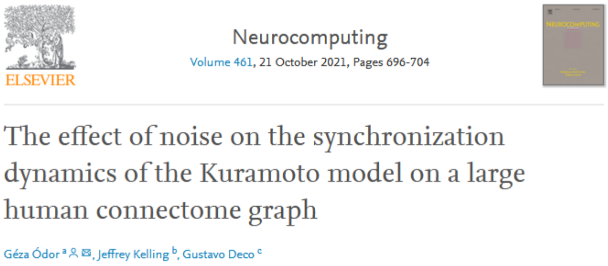


Fig 4. The hemibrain connectome offers a complete picture of neurons in certain parts of the fruit fly brain and details the way they connect to other parts of the brain. Credit: FlyEM/Janelia Research Campus

In this second visit the aim was also to run numerical studies by solving the Kuramoto equation, using the Runge-Kutta algorithm, to determine time dependent phase and frequency synchronization behaviour on the fruit fly connectome. This contains ~22.000 nodes, organized in a hierarchical modular structure (Kuramoto, 1984) and 3413161 weighted edges.

4 Achievement of the collaboration

The main achievements of scientific collaborations are the outputs in the form of scientific publications. In this case, a paper has been already published after the first visit of Prof. Ódor with the host Prof. Deco. Other papers are in preparation may appear in the future.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Neurocomputing
Volume 461, 21 October 2021, Pages 696-704
The effect of noise on the synchronization dynamics of the Kuramoto model on a large human connectome graph
Géza Ódor [a], Jeffrey Kelling [b], Gustavo Deco [c]

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(https://www.sciencedirect.com/science/article/pii/S0925231221007712)

Further achievmement of the collaboration is an invited review article on the topic:
Geza Odor, M. T. Gastner, J. Kelling, G. Deco,
Modelling on the very large-scale connectome,
J. Phys. Complex. 2 (2021) 045002.

Abstract
We have extended the study of the Kuramoto model with additive Gaussian noise running on the KKI-18 large human connectome graph. We determined the dynamical behavior of this model by solving it numerically in an assumed homeostatic state, below the synchronization crossover point we determined previously. The de-synchronization duration distributions exhibit power-law tails, characterized by the exponent in the range $1.1<\tau_t<2$, overlapping the in vivo human brain activity experiments by Palva et al. We show that these scaling results remain valid, by a transformation of the ultra-slow eigen-frequencies to Gaussian with unit variance. We also compare the connectome results with those, obtained on a regular cube with $N=10^6$ nodes, related to the embedding space, and show that the quenched internal frequencies themselves can cause frustrated synchronization scaling in an extended coupling space.

Keywords:
Frustrated synchronization; Human connectome; Chimera states; Noisy Kuramoto; Criticality in resting state

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5 Conclusion

In the scientific sphere, the most important challenge of this research has been to provide numerical evidence for the existence of chimera states and frustrated synchronization phenomena in a real biological, structural neural network. Regarding the programme outcomes, HPC-Europa3 serves as a transnational platform to promote the use of HPC in international research collaborations and, within this project, successfully builds bridges from statistical physics towards neuroscience.

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