Symposium
New Directions in Natural Sciences:
Complexity, Machine Learning and Algorithms

March 6st, 2020
Venue: Kardinal Schwarzenberg Haus,
Kapitelplatz 3, 5020 Salzburg

The main purpose of this meeting is the gathering of the EASA class "Natural Sciences" in order to foster scientific contacts among its members, to discuss essential past achievements in the areas it comprises (mathematics, physics, chemistry, biology etc.), and to look into important as well as promising future issues. This time the latter predominantly focus on machine learning and algorithms not only with regard to big data but also relating to methods to treat problems of complexity in natural sciences.

Scientific organisers:
Prof. Dr. Klaus Mainzer (Dean Class IV "Natural Sciences" of EASA)
Prof. Dr. Willibald Plessas (University of Graz)
Prof. Dr. Marko Robnik (University of Maribor)

ABSTRACTS

Klaus Mainzer: *Complexity, Machine Learning, and Algorithms*
(Technical University of Munich and University of Tübingen)

Recent developments in natural sciences are challenged by increasing complexity of big data, machine learning, and algorithms. What is the state of the art? What are the foundations? What can be done? Where are possible limitations?

Innovation and research in mathematics, physics, chemistry, and biology more and more depend on complex data and applications of algorithms and computer technology. Although highly specialized, natural sciences are also growing together by common computational methods. This development of the natural sciences is embedded in a world-wide trend of digitalization of our civilization. Therefore, our meeting aims at interdisciplinary information and communication between highly specialized disciplines in the Class of Natural Sciences, and also in the European Academy of Sciences and Arts.

Mirjam Cvetic: *Unification of Fundamental Forces of Nature by Modern String Theory*
University of Pennsylvania, Philadelphia

We outline the key features of the Standard Model of particle physics comprising electromagnetic, strong, and weak forces. It represents a consistent and experimentally confirmed quantum field theory of these elementary interactions. On the other hand, in this concept gravitational forces still resist a consistent description as a quantum theory.

With regard to the latter, we focus on the key features of String Theory, which is a consistent quantum theory of extended objects – strings. We elucidate, how it can unify the established quantum field theories of elementary particles with quantum gravity. We review, how String Theory sheds light on important fundamental questions of theoretical physics, such as the quantum structure of black holes or the geometric background of the Standard Model. We highlight recent developments in the geometric domain of String Theory, where the string coupling constant can be large, i.e. the so-called F-theory. We outline the key geometric features of F-theory that lead to a consistent construction of the Standard Model with three families of quarks and leptons, as confirmed by collider experiments. We also highlight subsequent systematic explorations of the landscape of three-family Standard Models as well as future directions for studies of such constructions via machine learning algorithms.

Felicitas Pauss: *Science Without Borders: From Infinitely Small to Infinitely Large*
ETH Zürich

Particle accelerators such as the Large Hadron Collider (LHC) at CERN, located at the Swiss-French boarder close to Geneva, are super-microscopes that allow us to explore the microcosm by studying in-depth the interactions between the basic building blocks of matter. On the other hand, the LHC is also a "time machine" that enables us to investigate the physical laws from the very first moments of the universe.

We shall address fundamental questions regarding the structure and evolution of the universe by linking the infinitely small with the infinitely large. On this journey through space and time, major technical challenges (accelerator, experiment, and computing) will be exemplified.

The lecture will shed light on the current status and future prospects of this fascinating research. The connection between challenges in basic research and innovation plays just as important a role as the dynamics of managing big projects in very large international teams.

Tomaz Prosen: *Dynamical Complexity and Chaos in Quantum Many-Body Systems*
University of Ljubljana

The question of characterising the complexity of dynamics of quantum systems with many interacting particles is, at the same time, very attractive and extremely illusive. Although a generalisation of the notion of Kolmogorov's complexity to (non-commutative) quantum dynamical systems has existed for a long time, it does not provide a very useful measure of complexity. For example, it assigns positive complexity even to quasi-free or non-interacting evolutions in the so-called thermodynamic limit.

Within a recent intense burst of studies on dynamical chaos in many-body systems, which were largely motivated by the proposals of Kitaev, Maldacena, Stanford and others on holographic models of black holes, new, more intuitive and more useful, measures of complexity have been proposed. Amongst the most promising one is the concept of the so-called "operator spreading" with a complexity indicator given by "operator entanglement". Most recently, even non-trivial, exactly solvable models of many-body dynamical chaos appeared, where measures of operator spreading can be computed and the transitions from "regularity to chaos" analytically shown. These models are particularly topical, as they provide physical examples that may be used to demonstrate quantum supremacy of the currently emerging quantum computers.

Ferenc Krausz: *Attosecond Science: From Basic Research to Cancer Detection*
MPI for Quantum Optics Munich

Born around the turn of the new millennium, attosecond meteorology has provided real-time insight into atomic-scale electron motions and light-field oscillations, previously inaccessible by human observation. Until recently, this capability has relied on attosecond extreme ultraviolet pulses, generated and measured in complex vacuum systems. Next-generation attosecond meteorology is now about to change this state of matters profoundly. Sub-femtosecond current injection into wide-gap materials can directly probe ultrafast electron phenomena in condensed matter systems and can also be used for sampling the electric field of light up to ultraviolet frequencies. Peta-Hertz field sampling draws on a robust solid-state circuitry and routine few-cycle laser technology, opening the door for complete characterizations of electromagnetic fields all the way from the far infrared to the vacuum ultraviolet. These fields, with accurately measured temporal evolution, serve as a unique probe for the polarization response of matter. Field-resolved spectroscopy will access valence electronic as well as nuclear motions in all forms of matter and constitutes a generalization of pump-probe approaches. Its implementation with a solid-state instrumentation opens the door for real-world applications, such as early cancer detection by measuring miniscule changes of the molecular composition of blood via field-resolved vibrational molecular fingerprinting.

Kurt Wüthrich: *Biophysics and Structural Biology*
Scripps Research, La Jolla, and ETH Zürich and iHuman Institute, ShanghaiTech University

We focus on present work in structural biology regarding G-protein-coupled receptors (GPCRs), which are represented by 826 different proteins in the human proteome and are the targets for more than 30% of all prescription drugs approved by the Food and Drug Administration (FDA). The current structural biology of this class of membrane proteins is characterized by integrative use of multiple experimental techniques, with X-ray crystallography, cryo-electron microscopy (cryo-EM), nuclear magnetic resonance spectroscopy (NMR) and single-molecule spectroscopy. The mutual complementarity of the results obtained will be discussed, with an outlook to the impact of these results on the human well-being in the 21st century.

Marc Thorsten Hütt: *How Patterns in Data Help Us to Understand Biological Complexity*
Jacobs University Bremen

One of the biggest challenges in the Life Sciences is the interpretation of high-throughput ('omics') data. Using the example of bacterial gene regulation, we illustrate, how patterns in 'omics' data arise from the interplay of distinct logical categories. We show that two types of control – 'digital' (operating based on essentially binary logic) and 'analog' (operating based on gradual changes) – shape gene expression patterns. Our analysis of this interplay of control types employs concepts from network science, machine learning, and mathematical modelling. In this way, it illuminates the full complexity of this biological system.

Gisbert Wüstholz: *Computability, Complexity, and Effectivity in Number Theory*
ETH and University of Zürich

Finding solutions of algebraic equations in rational numbers is a central question in number theory with applications also in other parts of natural sciences. This already begins with linear equations like the famous abc-conjecture.

One of the very significant areas in mathematics is cryptography, which uses the full strength of mathematical research. The well-known Rivest–Shamir–Adleman (RSA) cryptosystem is conceptually an almost trivial application of elementary number theory. However, in reality a big amount of highly non-trivial number theory comes together. Conceptually much less trivial are the elliptic cryptosystems, where non-linear equations, so-called elliptic curves, play the key role. They depend on parameters and consequently have much higher flexibility. Here, very deep concepts of arithmetic have to be used and have led to very difficult problems of the existence and computability of solutions of relatively simply looking algebraic equations. This has an enormous impact in particular on cryptography. We shall try to give a glance onto the beautiful parts of modern arithmetic with emphasis on computability and complexity. Of course, in the background one finds everywhere algorithms.

Dusan Repovs: *Topologically-Based Machine-Learning Methods*
University of Ljubljana

We shall discuss some new approaches and applications of machine learning architectures, based on tools from topological data analysis and used in conjunction with conventional machine learning methods. Topological data analysis is based on algebraic topology and can identify significant global mathematical structures that are beyond the reach of other approaches. When applying topology one benefits from generality, whereas when applying conventional methods one benefits from specificity.

Dirk Inzé: *Solving the Complexity of Biological Systems*
Ghent University

A long-term goal of biology is to understand, how the genome of an organism determines its phenotype and interaction with the environment. In the last decades, the functions of numerous individual genes were identified that, for example, affect human health or determine seed numbers in crops. However, how all genes of the genome act together in networks to form complex organs and organisms is still poorly understood. One of the challenges is that the translation of the genome information into a phenotype is subject to many layers of regulation

acting at the level of DNA, RNA, proteins, and metabolites. Whereas we learned to measure and analyze many of these regulatory processes, we still are far from mastering this complexity. Biologists are now starting to apply machine learning and artificial intelligence approaches to biological systems at multiple scales. I shall present my views on future directions on the analysis of complex biological systems and I shall illustrate this with examples of our research on genetic networks that govern organ sizes in plants.

Markus Hengstschläger: *Medical Genetics in Digital Transformation*
Medical University of Vienna

Predictive analytics and artificial intelligence applied for the interpretation of whole human genome data obtained via next generation sequencing offer a tremendous chance for the development of new therapeutic strategies. However, this current merger between biotechnology and information technology also calls for biological as well as ethical discussions regarding the definition of health and disease. We all are genetic individuals, and the vast majority of that, what defines an individual human being, is the result of nature and nurture.