NEW DIRECTIONS IN BIOCOMPUTATION

Dresden, Germany, September 12–13, 2017

Program, Abstracts and Participants

Dear Participant,

we are excited to welcome you to the Workshop "New Directions in Biocomputation". We are looking forward to exciting new science, stimulating discussions and new collaborations.

In this Booklet you find the program, poster and talk abstracts, and a participant list.

Best regards,

The organizing committee

Gerda Rentschler, Till Korten, Barbara Lindemann, Stefan Diez and Heiner Linke

Content

Program

September 12

8:30 – 9:30	Arrivals, registration (coffee available)
9.30 – 9:45	Welcome: **Stefan Diez** (B CUBE, TU Dresden) and **Heiner Linke** (Heiner Linke, NanoLund and Lund University, Coordinator of Bio4Comp)

Alternative parallel computation

9:45 – 10:15	**Yoshihisa Yamamoto** (Stanford University): Optical neural network at quantum limit for NP-hard Ising problems and NP-complete SAT problems
10:15 – 10:45	**Eric Lutz** (Univ. Erlangen-Nürnberg): The physics of information: from Maxwell's demon to Landauer
10:45 – 11:00	Coffee

Network-based biocomputation (NBC)

11.00 – 11:35	**Dan Nicolau Jr** (Molecular Sense, Oxford): Network-based biocomputation (NBC): mathematical basis and vision
11:35 – 12:10	**Heiner Linke** (Heiner Linke, NanoLund and Lund University, Coordinator of Bio4Comp): Status and technological challenges of NBC
12.10 – 12.30	**Dan Nicolau Sr.** (McGill, Montreal) Bacteria for network-based biocomputation
12:30 – 13:30	Lunch

Biological tools for computation

13:30 – 14:00 **Zev Bryant** (Stanford University): Engineering controllable biomolecular motors

14.00 – 14.30 **Beáta Bugyi** (University of Pécs): Activities of actin-binding proteins: principles and approaches

14.30 – 14:45 **Günther Woehlke** (TU Munich): Microtubule severing proteins

14:45 – 15:00 Coffee

15:00 – 16:30 Parallel workshops

(1) Biological agents and micro/nanofluidics: tagging and agent multiplication
(2) Architectural elements: tunnels, detectors, and gates
(3) Networks and real-life applications

16:30 – 17:00 Plenary session – conclusions from workshops

17:00 **Poster session**

18:30 **Dinner**

21:00 – 22:00 **Announcement of the first Bio4Comp Award and get together**

September 13

8:45 – 9:00 Coffee

Nanotools for biocomputation

9.00 – 9.30	**Irene Fernandez-Cuesta** (Univ. Hamburg): DNA Optical mapping: labelling and reading single molecules
9.30 – 10.00	**Adam Micolich** (UNSW, Sydney) Nanowire-based field-effect transistors for single-molecule detection
10.00 – 10:15	**Santiago Muiños Landin** (Univ. Leipzig): Reinforcement learning of Artificial Microswimmers
10.15 – 10:30	Coffee

Applications and theory of biocomputation

10.30 – 11.00	**Francis Woodhouse** (Univ. Cambridge): Active matter logic
11.00 – 11.30	**Boyan Yordanov** (Microsoft Research): topic: modelling and analysing biological systems and biological computation
11.00 – 11.20	**Benjamin Friedrich** (TU Dresden): Percolation in time-varying networks using renormalization group theory
11:20 – 11:40	**JunKyu Lee** (Queen's University of Belfast): Transprecision Computing Towards Energy Saving
11:40 – 12:00	**Carlo Vittorio Cannistraci** (TU Dresden): Brain active-matter bioinspired algorithms for prediction of self-organization and evolution in complex networks
12:00 – 12:15	Conclusions and next steps: **Heiner Linke** (Lund University)
12:15 – 14:00	Lunch and get together

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Talk abstracts

Quantum Neural Network for Cloud Service

Yoshihisa Yamamoto

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We will introduce a novel computing machine based on optical neural network operating at the quantum limit. The machine employs 2,000 degenerate optical parametric oscillator pulses as quantum neurons and a single homodyne measurement-feedback circuit to implement all-to all (4×10^6) quantum synaptic connections. The basic concept and quantum principle will be discussed, as well as the difference from gate-type and annealing-type quantum computers. The performance of this machine is evaluated against a quantum annealer by D-WAVE and various heuristics on CPU and supercomputers. The machine will be available online as a cloud server from November, 2017.

The physics of information: from Maxwell's demon to Landauer

Eric Lutz

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We will discuss the intimate connection existing between information theory and thermodynamics following its historical development. We will focus on two complementary aspects: 1) the gain of information which we will illustrate with Maxwell's famous demon and 2) the erasure of information summarized by Landauer's principle. We will further present a number of recent single-particle experiments that have for the first time realized the above gedanken experiments in the lab.
http://physicstoday.scitation.org/doi/10.1063/PT.3.2912
https://www.nature.com/doifinder/10.1038/nature10872

Status and technological challenges of NBC

Heiner Linke

NanoLund and Lund University, Coordinator of Bio4Comp;
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The EU project Bio4Comp (Parallel network-based biocomputation: technological baseline, scallop, and innovation ecosystem) aims to develop network-based biocomputation using nanofabrication and biological agents such as molecular motors. I will give an overview of the status of Bio4Comp, and will specifically identify technological challenges where a wider community of collaboration partners could make decisive contributions to the development of this technology. These challenges range from those related to nanofabrication via the modification of biological agents to the automatic and efficient detection of single molecules.

Activities of Actin-Binding Proteins: Principles and Approaches

Beáta Bugyi

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The eukaryotic actin cytoskeleton is one of the main intracellular polymer systems, which is a central scaffolding component and force generation machinery in many diverse cellular processes. Actin is an exquisitely conserved protein, yet its remarkable functional polymorphism is at the heart of the versatile cellular behavior. The fine tuning of the functioning of the actin biomolecular machine is orchestrated by the actions of geometrical and mechanical constrains as well as diverse actin-associated proteins and their isoforms. Despite its importance, the molecular mechanisms underlying the coupling of actin's functional diversity and the compositional pattern of proteins are unexplored in many cases. Understanding these processes at molecular level is an essential prerequisite for developing successful medical strategies, as well as can provide new concepts for the fabrication of biomimetic and nanodevices. In my talk, I introduce the biological principles governing the functional diversity of the actin machinery, focusing mainly on the activities of actin-associated proteins (assembly, disassembly and contractile machineries) in the regulation of actin dynamics.

Microtubule Severing Enzymes

Günther Woehlke, Ulrike Majdic, Stefan Müller, Frederik Schreiber

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Microtubules are cellular filaments that dynamically assemble and depolymerize in their cellular environments, giving rise to variable network structures. Microtubule dynamics is based on intrinsic, biochemical properties of tubulin, the action of end-binding and microtubule-severing enzymes. Severing enzymes are able to split existing filaments, thus doubling the number of filaments and generating new microtubule plus- and minus-ends. We have investigated the enzymatic and biophysical mechanism of severing, and derived a sequence of events that (i) starts with an electrostatic binding step that is (ii) followed by an ATP-dependent step, which occurs before the microscopically visible breakage (iii). We will present the evidence for this model, and discuss the implications for bio-computing applications.

Tripwire: Designing carbon nanotube transistors for electrical detection of passing actin filaments

Adam Micolich

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I will report progress on a carbon nanotube transistor design for electrically detecting actin filaments passing down nanochannels in on-chip in vitro motility assays. Such structures would be relevant for electrical read-out of results from biocomputation architectures or for control/actuation of actively switched junctions. I will focus on elements of the design related to the practicalities of working with actin/myosin, e.g., Debye length, simultaneous fluorescence microscopy, encapsulation, selectivity of active myosin binding, etc.

Reinforcement learning of Artificial Microswimmers

Santiago Muiños Landin[1], Keyan Ghazi-Zahedi[2], Frank Cichos[1]

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2 Max Planck Institute for Mathematics in the Sciences Information Theory of Cognitive Systems, Leipzig, Germany; e-mail: zahedi@mis.mpg.de

Living objects, like cells or bacteria are able to move actively in space and are also capable of responding to external sensory inputs through signal processing in a complex chemical network. Artificial microswimmer mimic the active motion of such biological systems, but are in general lacking the possibility to respond to their environment as such a chemical feedback system is not built in to a microswimmer.

We present a microswimmer control mechanism, which allows us to integrate algorithms of machine learning into the behavior of single and multiple self-thermophoretic microswimmers to study the emergence of collective behavior and solution of complex optimization problems with sparse signals in a simple model system. In particular we show the integration of a reinforcement learning (Q-learning) algorithm into the steering of microswimmers. It is shown, that despite the influence of Brownian noise, the swimmer is able to find the optimal path to a given target. Increasing the persistence of the microswimmers motion increases the learning speed. We also demonstrate first experiments for collective learning, where multiple swimmer share a common information. This allows an increased learning speed as well.

Overall, our experiments show, that a simple control of microswimmers provides a scalable micro robotic system, where adaption and collective behavior can be studied easily in a real world environment.

Active matter logic

Francis Woodhouse

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The ability of chemically or optically powered active matter to self-organise and spontaneously flow makes these systems increasingly attractive in smart microfluidics and materials design. Active matter has the potential to serve as the bedrock of customisable, controllable transport and processing systems, but to fully harness this potential, its intrinsic tendency toward turbulence must be tamed. Geometric confinement has recently emerged as an excellent stabilising scheme, allowing complex yet controllable behaviours to be engineered by careful design of the flow environment. Drawing on recent work showcasing a geometrically-realised bacterial analogue of the Ising model, I will describe a new model for incompressible active flow in networks before using this framework to introduce the theory of active matter logic. We will see how the synchronised self-organisation of individual network components across carefully chosen flow topologies could be harnessed to construct logic gates and to store data within SR latches, laying the foundation for autonomous microfluidic logic devices driven by bacterial fluids, active liquid crystals or chemically engineered motile colloids.

Modelling and Analysis of Biological Computation

Boyan Yordanov

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The Biological Computation Group at Microsoft Research is developing theory, methods, and software for understanding and programming information processing in biological systems. Our research focuses on three main areas. In the field of Molecular Programming we are developing approaches for designing molecular circuits made of DNA. In Synthetic Biology we are programming synthetic biological devices to perform complex functions. In Stem Cell Biology we aim to understand the computation performed by cells during development.

To make progress in these three areas, we are developing computational methods and software tools for modelling and analysis of biological computation. In this talk, I will present an overview of our computational approaches, focusing on the domain-specific programming languages we have used to describe and model different biological systems and several analysis methods from simulation to formal verification that we have utilized in a number of projects.

Percolation in time-varying networks using renormalization group theory

Jens Karschau, Marco Zimmerling, Benjamin M. Friedrich

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Keeping up with Moore's law in today's computing systems is only possible by connecting multiple processing nodes into a network;
likewise, distributed sensor systems prompt reliable message relay between nodes.
However, individual communication links are often unreliable, and, to make matters worse, failures tend to occur in temporal bursts.
To address reliable multi-hop routing in unreliable communication networks, we present a percolation theory for time-varying networks.
We introduce a minimal model, where network links switch stochastically between active and inactive states.
Using renormalization theory on these networks, we analytically show how the time-dependent probability to find a path of active links between two designated nodes converges to a Bernoulli process (i.e. without memory), as the hop distance between the nodes increases.
Our work extends classical percolation theory to the dynamic case, to elucidate temporal correlations of message losses, with implications for the design of communication protocols and control algorithms.

J. Karschau et al.: Renormalization group theory for percolation in time-varying networks. arXiv:1708.05704 (2017)

Transprecision Computing Towards Energy Saving

JunKyu Lee, Mahwish Arif, Hans Vandierendonck, Georgios Karakonstantis, Dimitrios Nikolopoulos

Centre for Data Science and Scalable Computing, Queen's University of Belfast, Northern Ireland, UK; e-mail junkyu.lee@qub.ac.uk

It is a challenge to maintain the power budget low for large-scale applications, since parallel computing obtains speedup, while requiring additional power according to the increased number of processors. In modern processors, lower precision arithmetic produces a result with a shorter runtime, engendering less energy consumption. In our research, we explore transprecision computing which utilizes various precision arithmetic for a dense linear system solver to reduce energy consumption by obtaining speedup without increasing number of processors.

Linear systems appear in many applications such as signal processing, electromagnetic simulation, quantum scattering, spectrophotometry, and scientific computation. The direct LU solver can solve linear systems, but is not always capable of producing a reliable solution for linear systems. To improve a solution accuracy, the iterative refinement algorithm was proposed in 1948. Since then, it was proposed to employ a lower precision for LU solver to achieve a speedup without losing accuracy. The speedup without increasing the number of cores resulted in energy saving. This method is referred to mixed precision method since it utilized two different precisions to represent matrix data.

To bring further energy saving to the mixed precision iterative refinement, we developed transprecision techniques which utilize various precision arithmetic according to numeric properties of algorithm and computational latencies depending on precisions. Our techniques were implemented on an Intel Xeon 2.4GHz core and brought around 3-4 X energy reduction to a previously proposed mixed precision iterative refinement when a double precision solution accuracy was required and a matrix size was ranged from 4K to 32K.

For our future work, we plan to explore transprecision techniques for machine learning applications and develop a software framework supporting energy-efficient transprecision techniques so that a user can utilize transprecision techniques with ease in the program to reduce energy.

Brain active-matter bioinspired algorithms for prediction of self-organization and evolution in complex networks

Carlo Vittorio Cannistraci

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The brain tissue, as active-matter, is not only inspiration for deep-learning artificial intelligence, but can suggest also other algorithms and paradigms of learning, which are related with its network topology and structural organization. I will discuss the *Local-Community-Paradigm (LCP)*, which is a recent theory we advanced, whose application on real data demonstrates that some basic rules of organization of brain network wiring resemble generalized principles of organization of complex systems to the extent that can be used to predict connectivity in social, economic and biological networks.

The ability to predict new interactions emerges from the structural organization of the complex network that is organized in many local communities inside which the likelihood that a new (or undiscovered) interaction emerges is higher than in the rest of the network. On the basis of this observation, a few years ago we developed the Local-Community-Paradigm (LCP) theory: it suggests that many real complex networks share with the brain a structural organization made by many local communities that favour local signalling activity and then development of new connections within the local communities. This idea was inspired by the famous assumption behind Hebbian learning, a hypothesis advanced by the psychologist Donald Olding Hebb during the late 40s: neurons that fire together wire together, giving rise to new local network connectivity able to implement a process of learning that we called *epitopological learning*. We proposed also that the identification of this form of learning in neuronal networks was only a special case. Hence, the epitopological learning and the associated local-community-paradigm (LCP) were respectively proposed as local rules of learning and organization, which were proven

to be valid in general for modelling link-growth and for topological link prediction in any complex network with LCP architecture.
To conclude, this talk promotes the power of bio-inspired computing, demonstrating that simple unsupervised rules inspired by principles of topological self-organization and adaptiveness arising during learning in living intelligent systems (like the brain) can efficiently equal perform complicated algorithms based on advanced, supervised and knowledge-based engineering.

References

[1] From link-prediction in brain connectomes and protein interactomes to the local-community-paradigm in complex networks. CV Cannistraci, G Alanis-Lobato, T Ravasi. Scientific reports 3, 2013.

[2] Common neighbours and the local-community-paradigm for topological link prediction in bipartite networks. S Daminelli, JM Thomas, C Durán and CV Cannistraci. New Journal of Physics 17 (11), 113037, 2015.

[3] Pioneering topological methods for network-based drug–target prediction by exploiting a brain-network self-organization theory. C Durán, S Daminelli, JM Thomas, VJ Haupt, M Schroeder and CV Cannistraci. Briefings in Bioinformatics, bbx041, 2016.

[4] Local-ring network automata and the impact of hyperbolic geometry in complex network link-prediction. Alessandro Muscoloni and Carlo Vittorio Cannistraci. https://arxiv.org/abs/1707.09496, 2017.

Poster abstracts

Fabrication and Operation of Kinesin-1-Powered Biocomputation Networks

Christoph Meinecke[1], Till Korten[2,3], Georg Heldt[1], Danny Reuter[1], Stefan Diez[2,3]

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Network-based biocomputation relies on accurate guiding of cytoskeletal filaments. Here we report on the fabrication and operation of a biocomputation network that encodes the specific instance {3, 5, 6, 10} of a classical nondeterministic-polynomial-time complete ("NP-complete") problem, the subset sum problem. The nanofabricated structures rely on a combination of physical and chemical guiding of the gliding of microtubules along channels. To achieve this the material stack is designed such that protein attachment to the walls of the nanochannels can be efficiently blocked such that only the bottom of the nanochannels is coated with the motor protein kinesin-1. Optimizations in the nanofabrication have greatly improved the smoothness of channel walls and floor, while optimizations in motor-protein expression and purification have improved the activity of the motor proteins. Together, these optimizations increased the longevity as well as the reliability of our devices. In the future, this will allow us to fabricate and operate large-scale networks that are able to solve substantial computational problems.

Pioneering topological methods for network-based drug-target prediction by exploiting a brain-network self-organization theory

Claudio Durán, Simone Daminelli, Josephine Thomas, Joachim Haupt, Michael Schroeder and Carlo Vittorio Cannistraci

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The bipartite network representation of the drug-target interactions (DTIs) in a biosystem enhances understanding of the drugs' multifaceted action modes, suggests therapeutic switching for approved drugs and unveils possible side effects. As experimental testing of DTIs is costly and time-consuming, computational predictors are of great aid. Here, for the first time, state-of-the-art DTI supervised predictors custom-made in network biology were compared-using standard and innovative validation frameworks-with unsupervised pure topological-based models designed for general-purpose link prediction in bipartite networks. Surprisingly, our results show that the bipartite topology alone, if adequately exploited by means of the recently proposed local-community-paradigm (LCP) theory-initially detected in brain-network topological self-organization and afterwards generalized to any complex network-is able to suggest highly reliable predictions, with comparable performance with the state-of-the-art-supervised methods that exploit additional (non-topological, for instance biochemical) DTI knowledge. Furthermore, a detailed analysis of the novel predictions revealed that each class of methods prioritizes distinct true interactions; hence, combining methodologies based on diverse principles represents a promising strategy to improve drug-target discovery. To conclude, this study promotes the power of bio-inspired computing, demonstrating that simple unsupervised rules inspired by principles of topological self-organization and adaptiveness arising during learning in living intelligent systems (like the brain) can efficiently equal perform complicated algorithms based on advanced, supervised and knowledge-based engineering.

MASH - a holistic software framework for simulation and analysis of dual channel single molecule microscopy videos

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A modular software designed for the analysis of single molecule (SM) videos will be presented in the context of current software and method developments in video-based singe molecule microscopy. The data analysis workflow and evalution of competing methods will be discussed. The focus will be camera-based two or three color single molecule Förster Resonance Energy Transfer (smFRET) (widefield/total internal reflection) microscopy, a wide-spread technique to study folding and un/binding of dye-labeled biomolecules like DNA and RNA. Single molecule localisation, intensity time trace creation and discretisation, and kinetic and thermodynamic modeling strategies are presented and compared using realistically simulated single molecule videos as ground truth for algorithm benchmarking to help users finding proper methods for their experimental data.

Neuromorphic memory and emulation of synaptic behavior by Si nanowire transistors

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The brain has remarkable memory and learning ability using parallel information processing in multiple synapses.[1] By mimicking the brain functionality, artificial synapses have been established using memristors [2] and transistors [3] based on synaptic plasticity of ionic or memristive film. However, to realize the feasible memory and learning for neurocomputing is still in challenge because of the low compatibility with conventional Si-based CMOS process and unintuitive memory function using the timing between pre- and post-synaptic signals.[4] Here, we report synaptic Si nanowire transistors which have ion-doped silicate dielectric film. A planar top gate can simultaneously modulate the conductivity of many post-synaptic nanowires through the film, that would be able to realize multiple neurotransmission in the brain. The synaptic transistor acts as a random access memory (RAM) cell due to the movement of doped metal ions in the film depending on the amplitude and frequency of pulse on the gate. Therefore, the short term potentiation (STP) is configured by the transfer characteristics of the FETs. In addition, synaptic learning is shown after rehearsed training, so that the synapse quickly reaches the same current level before the training. This study has achieved a breakthrough in the convenient interconnection between neuromorphic device and CMOS system with tunable memory mimicking the process of human brain.

[1] G. Neves et al., Nat. Rev. Neurosci., 9 (2008) 65-75
[2] D. S. Jeong et al., RSC Adv., 3 (2013) 3169-3183
[3] H. Tian et al., Adv.Mat., 28 (2016) 4991-4997
[4] T. Serrano-Gotarredona et al., Front Neurosci., 7 (2013) 1-15

Nanofabricated Bacterial Biocomputation Networks

Falco van Delft[1]; A. van Langen-Suurling[2]; Ch. de Boer[2]; F. Dirne[2]; A. Sudalaiyadum Perumal[3]; S. Kheireddine[3]; S. Roozbahani[3]; V. Tokárová[3]; O. Kašpar[3]; D. Nicolau[3]

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Parallel computation with motile biological agents has been proposed to tackle combinatorial mathematical problems, which will normally,-when using conventional, sequentially operating electronic computers -, place severe limitations on the problem sizes that can be solved. Previously, one of these problems, the 'sub-set sum' problem, has been encoded into a graphical, modular network, comprising so-called 'split junctions' and 'pass junctions'. A small instance of this problem has been embedded in a nano-fabricated planar device. This device has been explored in a parallel fashion, using a large number of actin filaments or microtubules in channels covered with motor proteins, to solve this particular instance of the 'sub-set sum' problem.

Autonomously moving bacteria are good alternatives to explore such channel devices, especially if cell division during exploration could be employed to increase the number of agents in a diverging network, keeping the agent density approximately constant during operation. Before constructing such bacterial computation networks, the efficiency and error rates of the junctions have to be optimized for bacteria, resulting in specific bacterial network design rules.

The purpose of the work presented here was to develop the steps needed for the successful fabrication of such bacterial devices. Although the channel widths (and depths) needed are typically larger than 1um, the accuracy of the channel widths, the sharpness of specific angles and corners, the aspect ratio of the channels and the controlled smoothness of other parts needed, demand nano-scale precision in order to fabricate successful devices. On the other hand, large area devices are needed for tackling useful problem sizes. Also the biological nature of the devices limits the number of materials that can be chosen for fabrication. Given all these constraints, a flowchart was constructed which contained (in short) the following steps:

1. Fabrication of a monolithic casting master on a 4-inch silicon wafer using electron beam lithography and Reactive Ion Etching
2. Casting of a PDMS replica from the monolithic Si master, and release
3. Sealing the replica with an oxygen permeable PDMS cover
4. Dicing network chips and filling them with bacteria containing fluids

The structures in the chips have been explored by E. coli HCB 437 bacteria. The bacterial behaviour was analyzed using ImageJ tracking software with trackmate & MtrackJ, and compilation of fluorescence micrographs. Analysis of these graphs for various modifications of the junctions resulted in a set of design rules, which has been successfully applied to fabricate biocomputation devices, as will be shown in this contribution.

Information Controlled Structure Formation in Artificial Microswimmer Systems

Utsab Khadka, Viktor Holubec, Haw Yang and Frank Cichos

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Self-organization is the generation of order out of local interactions in non-equilibrium. Its deeply connected to all fields of science from physics, chemistry to biology where functional living structures self-assemble and constantly evolve all based on physical interactions. The emergence of collective animal behavior, of society or language are the results of a self-organization processes as well though they involve abstract interactions arising from sensory inputs, information processing, storage and feedback resulting in collective behaviors as found for example in crowds of people, flocks of birds, school of fish or swarms of bacteria.

Here we introduce such information based interactions to the behavior of self-thermophoretic microswimmers. A real time feedback of other swimmer positions controls the swimming direction and speed. The emerging structures reveal frustrated geometries due to confinement to two dimensions. They diffuse like passive clusters of colloids but possess internal dynamical degrees of freedom that are determined by the feedback to the active particles. As the information processing in the feedback loops can be designed almost arbitrarily new perspectives for self-organization studies involving even machine learning and swarm intelligence arise.

What do we know about how researchers share data with each other? A presentation within the Scholarly Communication area

Madeleine Dutoit

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Scholarly Communication is a sub-area of Information Science studying "scholarly information, relationships among research areas and disciplines, comparisons of communication activities between fields, the information needs and uses of individual user groups, and the relationships among formal and informal aspects of communication." (Borgman, 2015). Within this area of Scholarly Communication, many things are changing rapidly today. The digitalization has for example changed the conditions for the systems used for dissemination of research results and data. The publication infrastructures are changing from within applying new models and the open access publishing sector has expoaded. Another of these changes concerns how research data is viewed and valued. Research data as new actors are predicted to become "recognized as significant scholarly contributions in their own right" (Hey et al., 2009). That is, the only end result of research does no longer have to consist of a scientific publication, but of archived research data, "seen as an end in itself" (Bowker, 2005).

As a study of the research data practices of scientists, I will present a few new findings in this area.

Neuronal Tracking using TRPO

Magda Dubois, Kai Arulkumaran, Anil A. Bharath

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A better understanding of the brain functionality requires a thorough un- derstanding of which neurons are connected with each other. Current imaging technique are able to provide precise scans of the cortex but because of a lack of available algorithms that are able to digitally trace neuronal structures despite breaks in the axon, studying the connectome requires a lot of time and cannot be done on a greater scale.
This project aims to test a new deep reinforcement learning method called Trust Region Policy Optimisation (TRPO) to the problem of tracing neuronal axons in artificial 2D data sets. This algorithm has recently provided high-quality results in robotics and game playing from images, and we hypothesize that it will also yield strong results in tracking axon branches.

Energetic cost reduction for parallel computation

Michael Konopik[1], Till Korten[2], Eric Lutz[1], Heiner Linke[3]

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[2] *B CUBE, Dresden University of Technology, Germany*
[3] *NanoLund and Lund University, Sweden*

The poster will cover the combination of two information theoretic concepts, Amdahl's law and Landauer's principle, to tackle the question of the influences of parallel computation on energy consumption in finite time.
Their combination results in the distinction between two sorts of energetic improvement; the overall improvement via reduction of the finite time energetic cost and via parallelization.
Amdahl's law describes the speedup via the usage of parallel computer, while Landauer's principle gives the fundamental cost to computation.

Recycling of molecular motor based bionano-devices

Mohammad Ashikur Rahman[1], C Reuther[2], M Mengoni[2], F Lindberg[3,4], H Linke[3,4], S Diez[2] and A Månsson[1,4]

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Biomolecular motors (myosin, kinesin etc.) have, over several years, been exploited for developments towards nanotechnological applications e.g. in biosensing 1. More recently, the efforts have been extended to the development of parallel biocomputation devices 2 for solving otherwise intractable mathematical problems. This requires using a device with an embedded nanofabricated network, which encodes a particular mathematical problem3 and where surface-adsorbed molecular motors (myosin and kinesin) propel their respective cytoskeletal filaments (actin and microtubules). However, producing such a device on a regular basis is expensive and time consuming. It is therefore crucial to develop a suitable method which will allow the use of such devices several times without disturbing either the embedded nanostructure or the surface chemistry. Here we show an effective method for regenerating biomolecular motors based nanodevices. We have used a small non-selective proteolytic enzyme, proteinase K, to cleave the surface adsorbed motor proteins. Effective cleavage of the motor proteins (e.g. myosin II) with diluted proteinase K (200μg/ml) was suggested by studying myosin induced actin filament sliding before proteinase K treatment (control experiment) and after such treatment followed by repeated incubation of the surface with the motor proteins. We found that actin filament sliding was maintained on surfaces re-used after proteinase K treatment (1-24 h) and new motor incubation. However, the sliding velocity was reduced to 56-68% of the control value. We hypothesized that the reason of not having 100% recovery of the velocity could be due to some remaining proteins or protein fragments on the surface after proteinase K treatment that prevented adsorption of new motors. This idea was supported by the finding that treatment of

the surface with SDS (5%, 5 min) upon proteinase K incubation (1 h) improved the surface regeneration dramatically, increasing the actin filament sliding velocity on the reused surface to 90% of the control value. Interestingly, this method was equally successful for regenerating surfaces for actin-myosin motility (trimethylchlorosilane derivatized glass) and microtubule-kinesin motility (glass). Moreover, we tested repeated (3 times) regeneration of both glass and trimethylchlorosilane derivatized SiO2 chip without any decrease in performance each time. Additionally, we found that Polyethylene glycol derivatized glass/SiO2 and ARP polymer resists on SiO2, used for motility inhibiting surface areas with microtubule-kinesin and actin-myosin, respectively, did not lose their motility inhibiting properties through the treatment. Finally, we observed effective regeneration of a nanostructured SiO2 chip for selective kinesin-1 propelled motility of microtubules on gold layers (pattern floor) with no motility in the surrounding areas. This method will be further exploited to regenerate biological agent based nanodevices with embedded nanoelectronics in the future.

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Activities of actin-binding proteins: principles and approaches

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Actin is a major contractile and structural protein present in the cytoplasm of most eukaryotic cells. In vertebrates, six actin isoforms can be differentiated and divided into two classes, muscle and non-muscle isoactins. Actin isoforms are highly conserved and play important roles in nearly all aspects of eukaryotic cell biology. Muscle actins (α-skeletal, α-cardiac, α- and γ-smooth muscle) are tissue specific and participate in muscle contraction as a component of myofibrils. β- and γ-cytoplasmic actins are ubiquitous and expressed in non-muscle cells, where they are involved in cell motility, cell shape determination, intracellular transport and mitosis. Isoactins cannot replace each other indicating that although actins have a very slight variation in sequence and have similar physicochemical properties, they play different physiological roles. Due to their specific biological functions, mutations in actin-coding genes may cause changes, incomplete operation or loss of related functions, which can lead to severe human diseases including deafness, cancer and developmental disorders.

In eukaryotic cells, actin exists in two forms: globular or G-actin and filamentous or F-actin. The 42 kDa globular actin monomer consist of four different subdomains and can assemble into fiber-like polymeric structures. The actin cytoskeleton undergoes continuous remodeling through interactions with a large repertoire of actin-binding proteins (ABPs).

There are numerous biophysical and biochemical techniques to study actin dynamics and how it is regulated by ABPs (e.g. fluorescence spectroscopy, total internal reflection fluorescence microscopy (TIRF), sedimentation assay etc).

This poster introduces the activities of actin-binding proteins in the regulation of actin dynamics, as well as presents examples how these activities can be resolved by using biophysical and biochemical approaches.

Enlightening discriminative network functional modules behind Principal Component Analysis separation in differential-omic science studies

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Omic science is rapidly growing and one of the most employed techniques to explore differential patterns in omic datasets is principal component analysis (PCA). However, a method to enlighten the network of omic features that mostly contribute to the sample separation obtained by PCA is missing. An alternative is to build correlation networks between univariately-selected significant omic features, but this neglects the multivariate unsupervised feature compression responsible for the PCA sample segregation. Biologists and medical researchers often prefer effective methods that offer an immediate interpretation to complicated algorithms that in principle promise an improvement but in practice are difficult to be applied and interpreted. Here we present PC-corr: a simple algorithm that associates to any PCA segregation a discriminative network of features. Such network can be inspected in search of functional modules useful in the definition of combinatorial and multiscale biomarkers from multifaceted omic data in systems and precision biomedicine. We offer proofs of PC-corr efficacy on lipidomic, metagenomic, developmental genomic, population genetic, cancer promoteromic and cancer stem-cell mechanomic data. Finally, PC-corr is a general functional network inference approach that can be easily adopted for big data exploration in computer science and analysis of complex systems in physics.

Aptamer conjugated actin filament for diagnostics

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Actin is the most abundant protein in eukaryotic cells and involved in diverse cellular functions such as muscle contraction, cell division, cytokinesis and intracellular transport. Gloublar (G)-actin self-assemble into filamentous actin (F-actin) of 8 nm diameter and several micrometers length. Actin together with the myosin motor (II) and microtubules together with kinesin motors have been utilized in nanobiotechnology for the development of miniaturized lab-on-a-chip and sensing devices. One of the most challenging parts for such developments device is the conjugation of biomolecules to F-actin. Previously, we have reported conjugation of monoclonal and polyclonal antibodies to actin filaments and subsequent transportation of captured analytes by myosin motor II fragments. Recently, it has been shown that DNA based aptamers can strongly and specifically bind to the human estrogen receptor (ERα), a key biomarker for breast cancer detection. We are here exploring bioconjugation strategies using heterobifunctional cross-linkers, for the covalent conjugation of amine-derivatized aptamers to actin filaments. The aptamer was covalently modified with photolinker and SFB heterobifunctional crosslinker. Subsequently, the modified aptamer was incubated with SANH modified actin filament at (RT; 30-35°C) for 3 h in the presence of a catalyst buffer 10 mM aniline. The degree of aptamer conjugation to actin filaments was quantified by measuring absorbance of signature peak in a spectrophotometer. Furthermore, the aptamer conjugated actin filament was found to binds specifically to ERα receptor giving rise to aggregation of the aptamer conjugated actin filament (cf. Mansson patented aggregation techniques). Further, capture and transportation of (ERα) on myosin motor (II) is underway.

Two-Photon Polymerization of hybrid polymers as a 3D printing technology on the micron-scale for applications in microoptics and microfluidics

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Additive manufacturing or 3D printing is one of the most hyped topics in the last years. It allows the fabrication of very complex geometries which are not feasible using other methods. Additionally, the shape of the target component can be modified without the necessity to redesign the production equipment. This makes 3D printing valuable for the production of highly customized products with small lot sizes Two-Photon Polymerization (2PP) is a femtosecond laser-induced process which enables 3D printing on a micrometer scale. This is achieved by focusing femtosecond laser pulses into a photoresist. As the underlying two-photon absorption is dependent on the applied light intensity, the photochemical process and as a direct consequence the solidification of the resist is confined to the tiny focal volume. The target geometry is then defined by 3D scanning of the focal volume and a subsequent rinsing for removal of the unexposed resist.

Favorable materials for application in 2PP as photoresists are so-called inorganic-organic hybrid polymers (ORMOCERs). This material class combines the advantages of inorganic or glass-like materials with the processing opportunities of polymers. ORMOCERs are synthesized from alcoxysilane precursors which undergo hydrolysis and polycondensation reactions and typically form a liquid resin. This resin consists of an inorganic [Si-O-Si]-network, which is responsible for high resistance against temperature and chemicals as well as for excellent mechanical and optical properties. The inorganic network is modified by organic groups that can on the one hand be used to further tailor chemical and physical properties. On the other hand these groups can be polymerizable by using UV light, femtosecond laser pulses and/or temperature.

The properties of ORMOCERs are of particular interest for applications in optics and life-sciences. Many ORMOCER modifications reveal excellent optical transmission, a customizable refractive index, and high stability against external influencing factors e.g. autoclaving or stressing with high-intensity UV light. Other

modifications are biocompatible or even degradable rendering them ideal materials for tissue engineering.
The application of ORMOCERs as photoresists for 2PP will be discussed in this contribution. One focus will be on aspheric refractive microlenses and on diffractive optical elements. In this example 2PP is an enabling technology for geometries that are not feasible using any other fabrication method. Furthermore, examples of microfluidic applications using ORMOCERs will be demonstrated. In this field, the microfluidic channel can be entirely written by 2PP or in another embodiment very small polymer microstructures can be integrated into classic microfluidic devices.

Scalable Fabrication of Carbon-Nanotube Field-Effect Transistors (CNT-FETs) Implementing Wafer-Level Electron-Beam Lithography and Dielectrophoretic CNT Assembly

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Since their discovery in 1998, Carbon Nanotube Field-Effect Transistors (CNT-FETs) have gained considerable interest as nanoelectronic components [1]. The nanoscopic quasi-one-dimensional geometry of single-walled carbon nanotubes (SWCNTs) and saturated bonds in their cylindrical molecular system allow a strong gate coupling, high charge carrier mobility, and low scattering figures in the CNT transistor channel. In the electronic sense, semiconducting SWCNTs represent 'the ultimate thin-body semiconductor system' waiving short-channel effects that typically occur in miniaturized of bulk semiconductor materials [2]. During the last decade, Fraunhofer ENAS and TU Chemnitz, Center for Microtechnologies have developed a comprehensive wafer-level nanotechnology platform offering engineering methods of nanopatterning and nano-micro integration for nanoelectronic components such as CNT-FETs. Application-wise, the CNT-FETs have been envisaged a novel key component for devices, circuits and systems in high-frequency domain [3] as well as sensor applications such as nanoelectromechanical (piezoresistive) [4], optical [5], biological or chemical detectors. For a scalable fabrication of such nanoelectronic and sensoric devices, the technological workflow needs high-level micro-nano patterning of appropriate transistor structures and advanced selection [6] and integration [7] concepts for the nanoelectronic materials, i.e. SWCNTs. We report on the sub-um structuring of electrode structures (patterned source-drain, embedded and structured gate) by means of conventional and electron-beam lithography (EBL), standard metallization, wafer-compatible dielectrophoretic SWCNT assembly and various consequent steps of post processing. We discuss especially the role of an effective contact formation between the nanomaterials and the electrodes for functional devices.

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SMART>SOS – implications to use cellular automata for bio-computing

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Sub-sub-Microbiological Art Research & Technology goes to Self-Organizing Synthesizer is one of the 10 winning projects of the new VERTIGO STARTS initiative supported by the European Commission's Horizon 2020 program. Together with Bio4Comp researchers from Dresden, Chemnitz, Würzburg (all Germany), Lund and Kalmar (both Sweden) we will develop a sound and video installation revealing the new paradigm of bio computation: a sub-sub-microbiological machinery based on microtubules.

SMART>SOS (Sub-sub-Microbiological Art Research & Technology goes to Self-Organizing Synthesizer) explores several novel approaches aesthetically, but also conceptually:

- On a microscopic scale, the researchers are used to working with light and colour, however, working with sound is a novelty.

- Above all, we intend to create a recursive network system with a kind of logic gates.

Here the simplest network topology is a ring of units interconnected by feedback loops using a combination of split and cross junctions. In phase one the logic gates are created by a simple split of channels, so the microtubules move either to the right or left neighbour. The result is a stochastic network: Slight variations of the probability in which direction the molecules are moving do result in changing distribution of molecules in the system.

In phase two this gate becomes a real logic gate computing the input: A XOR gate for instance passes only individual incoming molecules and blocks the molecules if they are coming from two sides.

Such a XOR-gate system resembles a 1d cellular automaton – functioning according to the additive "rule 90" (Stephen Wolfram). I have developed in the recent years a special method to sonify the dynamics of such systems – especially 1d cellular automata: Here I am analysing the activity of the units resulting in varying temporal

attractors. If one unit was more active the attractor respectively the pitch of a played tone rises, if a unit was less active the attractor /pitch is lowered by one step. In the best case, the result is a sound carpet woven by continuously pitches.

Extended simulations of various automata rules with varying numbers of 13-40 cell units revealed an interesting behaviour describing in a new way the dynamics of these automata. Each rule shows specific attractors, which can be linear or they reveal a chaotic oscillating pattern. It might have been expected that the system's behaviour with its ring like topology varies with even or odd number of units/cells. But it could be observed that the pattern also changes significantly with a series of rising odd numbers. I am happy to discuss with the Bio4Comp community these results and potential consequences for the design of a bio computing device.

Neural networks: computations and learning

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Deep neural networks (DNN) are the most common computational model in supervised learning and a major focus of artificial intelligence. Like biological computers, DNN are decentralized architectures that allow complex behavior to emerge from interactions of relatively simple units. We review the basic computational operations of neurons and the standard training procedure in deep networks.

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Notes

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Bio4Comp

Parallel network-based biocomputation: technological baseline, scale-up and innovation ecosystem

Combinatorial problems can be encoded into nanofabricated networks and solved by large numbers of molecular-motor-propelled protein filaments in so called Network-based biocomputation. In this workshop, experts of quantum- and DNA computing and molecular motor-powered, network-based computing will join forces to develop new directions in biocomputation.

This workshop is organized in the context of the 5-year EU Horizon 2020 project Bio4Comp that aims to develop network-based computing, and to build a strong research community around this challenge.

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Bio4Comp Partners

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