

SOE 9: Poster - Glasses / Stat. Phys. Bio. / Networks (joint session DY/BP/CP/PP/SOE)

In this poster session there are contribution from

- Focus Session: Slow Dynamics in Glasses and Granular Matter
- Focus Session: Feedback Control - Soft and Hard Matter
- Glasses
- Statistical Physics in Biological Systems
- Networks - Statistics and Dynamics

Time: Tuesday 9:30–12:30

Location: P1

SOE 9.1 Tue 9:30 P1

Investigation of the behavior of binary mixtures upon variation of the dynamic asymmetry — ●MARIE-LUISE BRAATZ¹, SEBASTIAN SCHRAMM¹, THOMAS BLOCHOWICZ¹, BERND STÜHN¹, and BERNHARD FRICK² — ¹Experimental Condensed Matter Physics, TU Darmstadt, Germany — ²Institut Laue Langevin, Grenoble, France

We study dynamically asymmetric binary mixtures comprised of polystyrene and the small molecule methyl tetrahydrofuran (MTHF). The blends are fully miscible on supercooling but still exhibit two glass transition temperatures. Between these two temperatures MTHF relaxes in a matrix of polystyrene, showing the signature of geometrical confinement on the nanoscale in its dynamic properties. Among the interesting characteristics observed, is a transition from fragile to strong behavior of the time constants and in some cases features of a type-A glass transition are found.

We study the behavior of these characteristics upon varying the molecular weight and thereby the dynamic asymmetry of the mixture as well as the concentration of the small molecules. Dielectric spectroscopy, depolarized dynamic light scattering and quasielastic neutron scattering are combined to cover a dynamic range of 1ps to 1000s.

Our results are compared to theoretical predictions that expect fragile-strong transitions and type-A glass transitions to be most pronounced at low concentrations of the small molecules and large dynamic asymmetries.

SOE 9.2 Tue 9:30 P1

Mesoscale modeling of aeolian sand transport — ●ANNE MEI-WALD, MARC LÄMMEL, and KLAUS KROY — Institut für Theoretische Physik, Leipzig, Germany

Aeolian transport of sand is one of the most important geological processes on Earth and other rocky planets, creating a wide range of self-organised dynamic structures, like ripples or sand dunes. To make the complex grain physics more amenable to analytical studies, it was proposed to coarse-grain the ensemble of grain trajectories by two types representing low-energetic reptating grains and high-energetic saltating grains [1]. We recently showed that our analytically tractable and numerically efficient continuum model reliably reproduces sand flux measurements obtained in various wind tunnel experiments [2].

Here, we scrutinize the potential of our approach to predict important grain-scale properties and find remarkable agreement with various experimental data. We also speculate about the reason for the success of the coarse-grained description, even in comparison to more detailed numerical models, despite its allegedly unfaithful representation of some of the grain-scale details [3]. Finally we conclude that the two-species continuum approach provides an appropriate starting point for analytical and efficient numerical modelling of seemingly complex aeolian saltation process and the structures it creates.

[1] Bagnold, *The physics of blown sand and desert dunes*. Dover Publ. (2005).

[2] Lämmel, Rings, and Kroy, *New J. Phys.* 14, 093037 (2012).

[3] Kok, and Renno, *J. Geophys. Res.* 114, D17204 (2009).

SOE 9.3 Tue 9:30 P1

Railway buckling safety: From Theory to application — ●JÁNOS TÖRÖK¹, LÁSZLÓ HALMA², and ISTVÁN FEJÉR² — ¹Department of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — ²Vasútépítők Kft, H-9023 Győr, Csaba utca 9

Using numerical simulation and mesoscopic theory we show that in granular materials the effective friction coefficient at walls depends heavily on the wall roughness. We show that it can be used in real application. In continuous welded rails the standard railbed in small radius curves are not able to resist the radial load arising from temperature and train movement. Today many different and expensive

methods are used to tackle this problem. We show that by making the bottom of the sleepers rough we can increase the buckling safety of the track.

SOE 9.4 Tue 9:30 P1

Continuum Mechanics Simulations of Nonlinear Deformation of Viscoplastic Solids — ●HELIANA CARDENAS¹ and THOMAS VOIGTMANN^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — ²Zukunftskolleg und Fachbereich Physik, Universität Konstanz, Konstanz, Germany

When amorphous solids are formed by solidification of dense liquids slow intrinsic relaxation plays a determining role on describing their behavior. Systems like this can be perturbed by external mechanical fields driving it to a non-equilibrium regime following then non-linear deformation laws. The mode-coupling theory of the glass transition (MCT) has been extended to describe the interplay between strong external forces and slow relaxation.

A non-linear extension of the Maxwell model of viscoelastic fluids is proposed. This model takes into account the relaxation time dependence on the shear rate and thereby mimics microscopic processes identified by MCT. Combining this constitutive equation with the Navier-Stokes equations we can describe the evolution of macroscopic flows. Attention will be focused on shear-thinning fluids where the fluid's viscosity decreases with an increasing rate of shear stress.

To solve non-linear integro-differential equations finite element modeling (FEM) is used through a computational fluid dynamics tool. The effect of different relaxation times for a pressure driven flow is studied by analyzing velocity profiles, among other measurable quantities.

SOE 9.5 Tue 9:30 P1

Mechanical Properties of Sheared Wet Granular Piles — ●SOMNATH KARMAKAR¹, MARC SCHABER¹, ANNA-LENA HIPPLER¹, MARTIN BRINKMANN², MARIO SCHEEL³, MARCO DI MICHIEL³, and RALF SEEMANN^{1,2} — ¹Experimental Physics, Saarland University, Saarbrücken, Germany — ²MPI for Dynamics and Self-Organization, Göttingen, Germany — ³European Synchrotron Radiation Facility, Grenoble, France

Adding small amount of wetting fluid to dry granulates typically leads to the granular stiffness which arises due the formation of minute liquid contacts between individual granules by the virtue of capillary forces. We experimentally study the mechanical properties of wet granulates, composed of monodisperse spherical glass or basalt beads. The glass microspheres are almost perfectly wetted by water whereas the basalt microspheres have a rather large contact angles with water. The different wettability causes a difference in the shape and volume distribution of the appeared liquid morphologies. We have investigated the shear strength, measured under cyclic shear deformation for various system parameters like liquid content, shear rate and absolute pressure. At large absolute pressures, the associated energy dissipation of a sheared wet granulate is considerably smaller than that of a completely dry bead assembly; where the wetting fluid might act as a 'liquid lubricant' by lowering the wet bead pile's shear stiffness. With time resolved X-ray microtomography, we could shed some light on the underlying microscopic mechanisms of the sheared wet granulates.

SOE 9.6 Tue 9:30 P1

Stability of Barchan Dune Fields — ●SVEN AUSCHRA, MARC LÄMMEL, and KLAUS KROY — Institut für theoretische Physik, Leipzig, Germany

Crescent-shaped barchan dunes are among the most impressive structures observed in arid regions on Earth and Mars. Although they are isolated from nearby dunes by bedrock, models suggests that truly isolated barchans would be unstable with respect to their mass balance

[1]. This suggests that some sort of interactions between the dunes in a dune field give rise to some size stabilization resulting in the empirically observed uniform size distribution along the dune field [2, 3].

To uncover the underlying mechanism, we perform a mass stability analysis for a pair of consecutive dunes in a barchan field. Sand supplied from the horn of the windward dune to its downwind neighbor initiates a complex response of its shape and mass. Based on a dimensionally reduced description justified by a closeby shape attractor, a one-dimensional fixed-point equation for the mass balance of the downwind dune is derived and analyzed for stable solutions.

[1] Fischer, Cates and Kroy, Phys. Rev. E 77, 031302, 2008.

[2] Hersen, Andersen, Elbelrhiti, Andreotti, Claudin and Douady, Phys. Rev. E 69, 011304, 2004.

[3] Duran, Schwämmle, Lind and Herrmann, Nonlin. Processes Geophys. 69, 455-467, 2001.

SOE 9.7 Tue 9:30 P1

Ab-initio MD parameter estimation for Na diffusion in glasses — ●LARS WINTERFELD and ERICH RUNGE — Institut für Physik, TU Ilmenau, 98693 Ilmenau

Molecular dynamics (MD) simulation provide a scalable method for the investigation of disordered systems like glasses. However, there is no generally accepted method for the determination of the MD model parameters. We present a new first-principle approach that allow us to self-consistently obtain such parameters by sampling an ensemble of representative configurations. We use MD to create these configurations and run ab-initio DFT calculations as basis for the subsequent fitting procedure. Results of this approach are compared for $(Na_2O)_x - SiO_2$ glass systems with those from the literature.

SOE 9.8 Tue 9:30 P1

Non-universal dielectric properties of glasses at very low temperatures — ●ANNINA LUCK, ANDREAS FLEISCHMANN, and CHRISTIAN ENNS — Kirchhoff-Institut für Physik, INF227, D-69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause specific material-dependent effects in magnetic fields.

To study the possible influence of nuclear electric quadrupoles connected with atomic tunneling systems on the low frequency dielectric properties of glasses down to a temperature of 10mK, we measured the multicomponent glass N-KZFS11, which contains 25 mass percent of tantalum oxide and a glass containing a similar amount of holmium oxide. As ^{181}Ta and ^{165}Ho carry very large nuclear electric quadrupole moments, these glasses seem to be ideal candidates to determine the influence of nuclear electric quadrupole moments on the physical properties of glasses at low temperatures.

Our measurements not only show a non-universal dielectric behaviour in the two glasses, but also differ significantly from various predictions of the standard tunneling model. We discuss these new findings in the framework of the tunneling model.

SOE 9.9 Tue 9:30 P1

Understanding the properties of two dimensional silica systems — ●PROJESHKUMAR ROY¹ and ANDREAS HEUER² — ¹Graduate school of chemistry, University of Muenster — ²Institute of physical chemistry, University of Muenster

Recently, STEM and SPM studies were performed by Lichtenstein et al, [1] in a virtually two dimensional silica bilayer; which was grown by depositing vaporised Si atoms on a [Ru(0001)] metal surface in an oxygen atmosphere. Silica bilayers were generated, which could be either amorphous or crystalline, depending on the preparation conditions. Under specific conditions even both states could be generated in the same layer, including a short-range transition between them. Remarkably, even in the amorphous case both layers were virtually identical. Due to the atomic resolution the ring statistics in the amorphous structure could be characterized in detail.

We report about computer simulations which have the aim to reproduce the properties of two-dimensional silica layers and, consequently, obtain an improved microscopic understanding of this system. In particular we want to learn, under which conditions crystalline and amorphous structures can be generated, respectively. For this purpose, an appropriate silica potential has to be developed which can be used in

the two-dimensional case and is able to generate the observed structural features.

[1] Lichtenstein L; Heyde M; Freund H.J.; J. Phys. Chem. C 2012, 116, 20426.

SOE 9.10 Tue 9:30 P1

Understanding the energy landscape of a simple water model — ●KATHARINA FERLING and ANDREAS HEUER — Institut für Physikalische Chemie, WWU Münster

Liquid water plays an important role not only in our everyday life but also in simulations and experiments where it serves as a solute with many applications. The understanding of the water behaviour, including its anomalies, can play an important role in improving the description of water. Here the emphasis lies on the property of building H-bonds which is believed to be one major factor for many anomalies such as the density change or the liquid-liquid phase transition at low temperatures. For the present investigation a simple model has been chosen which focuses on the distinction between a close-packed and an open structure. The one dimensional model - which was first introduced by Ben-Naim [1,2] - has now been extended with additional long range interactions in the underlying potential to get rid of the mean-field character of that model. First, simulations are performed in the NPT-ensemble with the aim to show water-like behaviour such as a high-density liquid and low-density liquid (HDL-LDL) transition. Second, from simulations in the NVT-ensemble for different volumes (lengths, resp.) a closer understanding of the possible anomalies can be reached, related to properties of the underlying potential energy landscape.

[1] Arieh Ben-Naim, J. Chem. Phys. 128, 024505 (2008)

[2] Lotta Heckmann and Barbara Drossel, J. Chem. Phys. 137, 064503 (2012)

SOE 9.11 Tue 9:30 P1

Compressed exponential decays in correlation experiments: The influence of temperature gradients and convection — ●JAN GABRIEL, THOMAS BLOCHOWICZ, and BERND STÜHN — Institut für Festkörperphysik, Darmstadt

In a wide range of correlation experiments using laser light or partially coherent X-rays so called compressed exponential correlation functions were reported [1] i.e. decays $c(\tau) \propto \exp(-(t/\tau)^\beta)$ with $\beta > 1$. The source of this phenomenon is still a point of discussion. For example for colloidal particles in supercooled liquid [2] it is claimed that near T_g hyperdiffusive behavior appears, which leads to compressed correlation functions.

We performed multispeckle-dynamic light scattering experiments in a temperature range from 230 K to 300 K with a sCMOS camera in a system of Polystyrene spheres in supercooled propanediol. At low temperatures compressed exponential decays are observed. At the same time, however, the speckle pattern shows indication for convection in the sample due to a slight temperature gradient, across the sample cuvette mounted on a cold finger cryostat. These effects increase with decreasing temperature and after a temperature jump and can be corrected for by assuming convective flow at constant velocity. Such corrections reduce or remove compressed exponential behavior.

[1] A Madsen, R. L. Leheny, H. Guo, M Sprun and Orsolyal, New J. Phys., 12, 055001 (2010)

[2] C. Caronna, Y. Chushkin, A. Madasen and A. Cupane, Phys. Rev. Lett., 100, 055702 (2008)

SOE 9.12 Tue 9:30 P1

Temperature and pressure dependence of the supramolecular structure of 2-ethyl-1-hexanol and 4-methyl-3-heptanol — ●THOMAS BÜNING¹, CHRISTIAN STERNEMANN¹, CATALIN GAINARU², MICHAEL PAULUS¹, KOLJA MENDE¹, FLORIAN WIRKERT¹, IRENA KIESEL¹, JOHANNES MÖLLER¹, JULIA NASE¹, STEFAN BAUER², ROLAND BÖHMER², and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund — ²Fakultät Physik/E3, Technische Universität Dortmund, D-44221 Dortmund

Hydrogen bonds are essential for structure and dynamics of e.g. alcohols, aqueous solutions and water. Due to their low tendency to crystallization and large variability in molecular configuration, monohydroxy alcohols are a typical system that is studied to learn about the impact of hydrogen-bonding on molecular liquids. Because of the hydrogen bonds alcohols form supramolecular structures in the liquid phase. Here, the molecular arrangements of monohydroxy alcohols such as 2-ethyl-1-hexanol (2E1H) and 4-methyl-3-heptanol (4M3H) strongly depend on the position of the OH group within the molecule.

Based on dielectric spectroscopy molecular arrangements in chain-like (2E1H) and, ring-like (4M3H) structures have been proposed. We present an x-ray diffraction study of 2E1H and 4M3H, providing new information regarding the supramolecular structure in pressure up to 4 kbar and temperature down to -110 °C.

SOE 9.13 Tue 9:30 P1

Molecular Order and Dynamics of Nanometric Thin Layers of Poly(styrene-*b*-1,4-isoprene) Diblock Copolymers — ●WYCLIFFE K. KIPNUSU¹, MAHDY M. ELMAHDY¹, MARTIN TRESS¹, EMMANUEL U. MAPESA¹, DETLEF-M. SMILGIES², JIANQI ZHANG³, CHRISTINE M. PAPADAKIS³, and FRIEDRICH KREMER¹ — ¹Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — ²CHESS, Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — ³Technische Universität München, Physik-Department, James-Frank-Straße 1, 85748 Garching, Germany

Order and dynamics of poly(styrene-block-1,4-isoprene), P(S-*b*-I) diblock copolymers in nanometer thin layers with different isoprene volume fraction (fPI) and identical molecular weight of the styrene blocks are studied by a combination of Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). GISAXS and AFM reveal randomly oriented lamellar structures in the films and a parallel orientation at the top surface, respectively. Using BDS, three well separated relaxation processes are detected, (i) and (ii) the dynamic glass transitions (segmental mode) in the styrene and isoprene blocks respectively and (iii) the normal mode relaxation representing fluctuations of the isoprene chain as a whole or parts of it. While the two former do not show any thickness dependence in their spectral positions, the latter becomes faster with decreasing sample thickness. This reflects the difference in the length-scale on which the molecular fluctuations take place.

SOE 9.14 Tue 9:30 P1

Intra- and inter-molecular dynamics in the course of vitrification in organic glasses — LUDWIG POPP, BENJAMIN SUTNER, ●WILHELM KOSSAK, and FRIEDRICH KREMER — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Linnestr. 5, 04103 Leipzig

FTIR and BDS are utilized to study the vitrification of various well known glass formers in a wide temperature range around the calorimetric glass transition temperature, T_g. Measurements on Propylene glycol, Glycerol, Salol, Benzophenone, Sorbitol, Xylitol, etc. are compared and the sub-molecular specificity of the different moieties in their contribution to thermally activated processes including the dynamic glass transition are discussed. By that the necessity of atomistic models of the glass transition beyond coarse grained models is revealed.

SOE 9.15 Tue 9:30 P1

The potential energy landscape of sheared glass-forming systems — ●MARKUS BLANK-BURIAN and ANDREAS HEUER — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small supercooled binary Lennard-Jones mixtures ($65 \leq N \leq 1040$) under a constant shear rate. The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system. The potential energy landscape (PEL) is most informative for small systems. However, we also study the influence of finite size effects on our results.

In previous work, it was shown, that the finite size effects in un-sheared systems is quite small for thermodynamic observables and for the diffusivity. The dynamics of these systems can be described by a continuous time random walk (CTRW) between minima in the potential energy landscape. Our focus now lies on comparing these results with the constantly sheared system.

In the sheared system, we test for finite size effects in general properties like the velocity profile or the shear viscosity. Since the potential energy landscape is now time-dependent, we use affine transformations to understand the temporal evolution of its minima. With this insight, we can use the same continuous time random walk analysis as with the un-sheared system.

SOE 9.16 Tue 9:30 P1

Self-stabilizing Learning Rules in Neural Models driven by Objective Functions — ●RODRIGO ECHEVESTE and CLAUDIUS GROS — Institut für Theoretische Physik, Johann Wolfgang Goethe Universität, Max-von-Laue-Str. 1, Frankfurt am Main, Germany

In the present work, learning rules for a neuronal model are derived from two objective functions. On the one hand, the neuron's firing bias is adjusted by minimizing the Kullback-Leibler divergence with respect to an exponential output distribution. On the other hand, learning rules for the synaptic weights are obtained by minimizing a Fisher information that measures the sensitivity of the input distribution with respect to the growth of the synaptic weights. In this way, we obtain rules that both account for Hebbian/anti-Hebbian learning and stabilize the system to avoid unbounded weight growth. As a by-product of the derivation, a sliding threshold, similar to the one found in BCM models, is obtained for the learning rules.

As a first application of these rules, the single neuron case is studied in the context of principal component analysis and linear discrimination. We observe that the weight vector aligns to the principal component when the input distribution has a single direction of maximal variance but, when presented with two directions of equal variance, the neuron tends to pick the one with larger negative Kurtosis. In particular, this fact allows the neuron to linearly separate bimodal inputs. Robustness to large input sizes (> 1000 inputs) is also studied, observing that the neuron is still able to find the principal component in a distribution under these conditions.

SOE 9.17 Tue 9:30 P1

Fluctuations of Probe Particles Coupled to Molecular Motors — ●PATRICK PIETZONKA, EVA ZIMMERMANN, and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart

In recent years, many experiments have been carried out in which the motion of molecular motors is probed by the observation of attached colloidal particles. For the experimental determination of the torque exerted by the rotational motor F₁-ATPase onto such a particle, the application of a fluctuation theorem (FT) for the motion of the colloid has been proposed [1].

However, we show that this approach is generally valid only in the limit of fluctuations on short timescales. The statistics of fluctuations during larger time-intervals depends significantly on the intrinsic behavior of the motor and the linker, which is not observable in experiments. In particular, we investigate a simple model characterized by discrete motor jumps and harmonic coupling between the motor and the colloid [2]. Using the framework of the theory of large deviations, we calculate the distribution of fluctuations of the colloid in the long-time limit. This result implies a refined formulation of the FT-like relation observed in experiments. Moreover, we gain general insight into the properties of stochastic processes with hidden degrees of freedom.

[1] K. Hayashi *et al.*, Phys. Rev. Lett. **104**, 218103 (2010)

[2] E. Zimmermann and U. Seifert, New J. Phys. **14**, 103023 (2012)

SOE 9.18 Tue 9:30 P1

Detention time of a model microswimmer at a plane surface: importance of hydrodynamic interactions — ●KONSTANTIN SCHAAR, ANDREAS ZÖTTL, and HOLGER STARK — TU Berlin, Institut für Theoretische Physik

We discuss the detention time of a microswimmer at a plane no-slip surface taking into account hydrodynamic interactions of the swimmer with the surface and rotational diffusion. To evaluate the detention time, we use the formalism of the mean first-passage time (MFPT) based on an appropriate Smoluchowski equation. The microswimmer operates in 'squirmers' mode and can easily be tuned between a 'pusher' and a 'puller'. The hydrodynamic interactions with the surface are described by lubrication theory.

We examine the MFPT and also the distribution of first passage times at the surface and achieve good agreement of our results with direct simulations of the squirmers motion close to the no-slip surface using the method of multi-particle collision dynamics. The detention time of the squirmers is clearly determined by hydrodynamic interactions with the surface. They rotate the squirmers away from the surface and therefore reduce the detention time considerably compared to pure rotational diffusion. We find that pushers have a larger detention time than pullers.

SOE 9.19 Tue 9:30 P1

Thermodynamically consistent coarse graining of molecular motor models — ●EVA ZIMMERMANN and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart

In many single molecule experiments probe particles that are attached to molecular motors are used to infer properties of the motor protein from the analysis of the particle's trajectory and to manipulate the

system by exerting external forces on the motor protein via the probe particle. Theoretical modelling used to describe such assays should comprise at least two coupled degrees of freedom. However, many simple theoretical models applied to molecular motor experiments contain only one degree of freedom representing the motor.

We use a simple illustrative model consisting of two coupled degrees of freedom for the molecular motor and the probe particle to introduce a coarse graining method that allows to eliminate the explicit dynamics of the probe particle in a dynamically and thermodynamically consistent way. We discuss under which conditions the coarse grained model reduces to the widely-used one-particle models.

SOE 9.20 Tue 9:30 P1

Active Turing Systems — ●SILKE BERGELER, FLORIAN THÜROFF, and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Active Turing systems combine the ideas of active matter and reaction diffusion systems showing Turing patterns. We investigate such systems analytically and numerically starting within the framework of Boltzmann-like equations. Adapting previous analytical approaches for active systems we derive a set of hydrodynamic equations and perform a linear stability analysis of the isotropic uniform steady state. We find that the stability against homogeneous perturbations switches from unstable to stable by crossing a threshold noise from below. From direct simulations of the Boltzmann equation we observe that activity changes the form of the Turing patterns and broadens the parameter range for which patterns emerge. Analytical investigations on the stability of the isotropic homogeneous steady state are confirmed by numerical analysis.

SOE 9.21 Tue 9:30 P1

Application of a random fitness landscape model to a long term evolution experiment — ●MARES BAREKZAI¹, SU-CHAN PARK², and JOACHIM KRUG³ — ¹Department of Physics, University of Cologne, Germany — ²Department of Physics, Catholic University of Korea, Bucheon, South Korea — ³Department of Physics, University of Cologne, Germany

Since 1988, a long term microbial evolution experiment has attracted attention in the scientific community. In the experiment 12 populations of *Escherichia coli* are propagated in a daily refreshed minimal medium for more than 50000 generations. One of many results are the fitness trajectories of these asexually evolving populations, where fitness is measured as relative growth rate compared to the founding population. Is there a simple model to interpret the observed microbial evolution? We approached this question using the House of Cards Model introduced in 1978 by Kingman, which models the evolution of an asexual population on an uncorrelated random fitness landscape in the limit of infinite genome size. This limit implies that all mutations generate new fitness values drawn from a fixed probability distribution. The model produces fitness trajectories that are in qualitative agreement with the experimental data. Based on an analytical solution for the long term behavior of the model, we estimate the model parameters from the experimental data and provide a biological interpretation of our results.

SOE 9.22 Tue 9:30 P1

Event chain simulations of polymer bundles — ●TOBIAS ALEXANDER KAMPMANN and JAN KIERFELD — TU Dortmund, Germany, NRW

We study simulation methods for large polymer systems forming locally dense structures such as polymer or filament bundles. In order to simulate such systems effectively using Monte-Carlo methods, we propose a novel event chain algorithm adapted from hard sphere systems [E. P. Bernard, W. Krauth, Phys. Rev. E, 80: 056704 (2009)]. The algorithm works rejection-free and reduces autocorrelation and equilibration times significantly.

We demonstrate the advantages of the algorithm by investigating the diffusive behaviour of bundle structures. Using the event chain algorithm a polymer bundle exhibits the correct scaling of diffusion constants with bundle size, which is not obtained using simple local displacement moves. We apply the algorithm to bundle networks formed by semiflexible filaments with short-range attractive interactions.

SOE 9.23 Tue 9:30 P1

Estimation of sleep stages and sleep depth dynamics by neural clustering — ●STEPHAN VOLKLAND¹ and JENS CHRIS-

TIAN CLAUSSEN^{2,1} — ¹INB, Universität zu Lübeck, Germany — ²Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The quantitative analysis of sleep from polysomnographic data (i.e., simultaneous recording of EEG, EMG and EOG) is practically limited by the final step of sleep scoring, i.e. extensive manual inspection of data according to the Rechtschaffen and Kales rules or the recent AASM counterpart, leading to a manually classified time series of sleep stages on a discrete scale of six values (wake, REM, S1, S2, S3, S4). Starting from the observation that the stages S2, S3, and S4 are merely defined by spectral properties, namely by activity in the delta and sigma band, here we present a neural clustering approach to assess sleep stages automatically by unsupervised neural clustering and a posteriori assignment of sleep stages. One particular goal is to provide a finer resolution in time as well as a finer interpolation in sleep depth than obtainable from manual scoring. We find that EOG and EMG data are still needed to improve classification of wake and REM states, and still an interpolation of states at the borders of wake, REM and S1 is difficult. In the range between the NonREM stages S1–S4 an interpolation with higher resolution is feasible, as expected.

SOE 9.24 Tue 9:30 P1

Extended diffusion model of sleep depth dynamics — ●ANNA BARKENTIEN¹ and JENS CHRISTIAN CLAUSSEN^{2,1} — ¹INB, Universität zu Lübeck, Germany — ²Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The duration of wake bouts during sleep has puzzled complex systems scientists since a decade since [1], as these distributions eventually resemble a power-law. The theoretical understanding is incomplete, biologically plausible models still are not available. A pure Markov analysis [2] assuming random switching however ignores any deterministic components in the dynamics which are manifest in time correlations. The phenomenological model proposed in [1] describes sleep depth by a one-dimensional diffusion process with a reflecting border for sleep and a restoring force for wake. We extend this model in [3] to account for the REM state and modify the restoring force law to account for deviations to the power law that are observed in data from some (but not all) labs and obtain a better fit to data [3]. We conclude that a refined model as [3] is necessary to account for the different experimental results, but significantly larger cohorts of sleep studies would be needed to distinguish between the two-regime and the one-regime distributions. This concerns only the wake → sleep transition, the sleep → wake transition remains consistent with a random process homogeneous in time.

[1] C.C. Lo et al, EPL 57, 631, 2002. [2] J.W. Kim et al, PRL 102, 2009. [3] A. Barkentien and J.C. Clausen (in preparation).

SOE 9.25 Tue 9:30 P1

Multidimensional epistasis and the transitory advantage of sex — ●JOHANNES NEIDHART, STEFAN NOWAK, IVAN G. SZENDRO, and JOACHIM KRUG — THP, Universität zu Köln, Deutschland

The benefit of sex and recombination is a long standing problem. We numerically study evolutionary dynamics on high dimensional epistatic fitness landscapes, with focus on the temporal development of the evolutionary advantage of recombination. We show that the adaptive advantage of recombination on static landscapes is strictly transitory. These findings are explained by means of well established results for a setup with two loci. It is further shown that the transitory advantage can be prolonged indefinitely in fluctuating environments.

SOE 9.26 Tue 9:30 P1

Adaptive walks in Kauffman's NK-Landscape — ●STEFAN NOWAK and JOACHIM KRUG — Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study evolutionary dynamics in a high-dimensional genotype space in the limit of rare mutations and strong selection. In this regime the population performs an uphill walk which terminates at local fitness optima. We analyze the length and attained fitness of such walks with our focus on the influence of different genetic interaction patterns.

SOE 9.27 Tue 9:30 P1

Coexisting autocatalysts generate increasing complexity — ●EMANUEL GREGOR WORST¹, PHILIPP ZIMMER², EVA WOLLRAB¹, KARSTEN KRUSE², and ALBRECHT OTT¹ — ¹Biologische Experimentalphysik, Universität des Saarlandes, Deutschland — ²Theoretische Biologische Physik, Universität des Saarlandes, Deutschland

The evolution towards more complex structures from the earliest building blocks of life remains poorly understood. Here we present an experimental realization that exhibits evolutionary properties in one dimension and generates multiple coexisting species. Molecular chains of a certain length (identified as a species) are autocatalytically reproducing, and new species form randomly by spontaneous concatenation. We use DNA strands and DNA ligase, covalently linking single-stranded DNA, as an experimental model system. Reproduction occurs by template-directed ligation. Spontaneous and random generation of new species is a consequence of thermal fluctuations. We show that the system evolves towards more complex structures in a non-trivial way if the ratio between autocatalytic reproduction and spontaneous generation of new species exceeds a critical value. An outstanding characteristic of this system is the iterated production of more complex species while coexistence is maintained.

SOE 9.28 Tue 9:30 P1

Identifying molecular expression dynamics in practice - how to distinguish between noise regulation and direct deterministic control using experimental data — ●MARTIN HOFFMANN¹ and JÖRG GALLE² — ¹Fraunhofer ITEM, Project Group Personalized Tumor Therapy, Biopark I, Josef-Engert-Strasse 9, 93053 Regensburg, Germany — ²Interdisciplinary Centre for Bioinformatics, University of Leipzig, Haertelstr. 16-18, 04107 Leipzig, Germany

Biological noise plays an important role in generating phenotypic diversity and contributes to unspecific environmental adaptation. However, the classical pathway view of cell biology focusing on deterministic stimulus-response relationships may well accommodate the majority of biological phenomena. It is thus necessary to develop combined theoretical and experimental approaches that can dissect the relative contribution of noise regulation and direct deterministic control. Accordingly, we define molecular level conditions for noise-driven and deterministic dynamics and compare corresponding modeling results to published experimental data. We show that both models can fit the FACS data for the toggle switch system equally well while simulated dynamic mRNA labeling results in distinct observations for both models. Using synthetic time course data we demonstrate that complete system identification can be achieved based on single cell tracking. As demonstrated, noise regulation can be an effective second layer of cell regulation that may be associated with active short term search processes.

SOE 9.29 Tue 9:30 P1

Propagation and propagation failure of waves on excitable tree networks — NIKOS KOUVARIS¹, ●THOMAS ISELE², ALEXANDER MIKHAILOV³, and ECKEHARD SCHÖLL² — ¹Department of Physics, University of Barcelona, Martí i Franques 1, 08028, Barcelona, Spain — ²Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — ³Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

We study the properties of pulse solutions on excitable tree networks by means of numerical (simulation and continuation) as well as analytical methods. We focus on the dependence of the propagation velocity and the change of stability properties with respect to the branching ratio (i.e. degree) of the nodes. But we also consider different coupling strengths and the continuous (thermodynamic) limit of our model.

SOE 9.30 Tue 9:30 P1

Dynamics of neural networks with transient synaptic plasticity rules — ●BULCSÚ SÁNDOR and CLAUDIUS GROS — Institut für Theoretische Physik, Goethe Universität, Frankfurt am Main, Deutschland

Working memory makes it possible to hold information temporarily for processing purposes; as such it has an important role in the execution of cognitive tasks. Its operation may possibly be mediated via short-term or transient synaptic plasticity effects. Thus the standard Tsodyks-Markram model for transient synaptic dynamics, built upon short-term synaptic plasticity effects, is a promising candidate to investigate the underlying dynamical behavior of these systems.

In our work we propose a simplified continuous time model for pre-synaptic plasticity rules, called full depletion model, which may allow a stricter control of the dynamics. The model is implemented for clique encoding recurrent networks with a Mexican-hat connection profile of synaptic weights. These systems show a wide variety of dynamical states as a function of the control parameters. We study the different types of behaviour emerging from transient synaptic plasticity rules

from a dynamical system's point of view.

SOE 9.31 Tue 9:30 P1

Optimization of complex network for minimizing traffic congestion: case study for a popular internet based service in Serbia — ●IGOR STANKOVIĆ¹, VLADICA TINOTOR², and JOVAN RADUNOVIĆ³ — ¹Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — ²Republic Agency for Electronic Communications, Višnjićeva 8, 11000 Belgrade, Serbia — ³School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia

We present a case study of network parameter optimization for a popular internet based service in Serbia. The physical layer of the network consists of two existing nation-wide optical networks, i.e., a commercial telecommunication network and a network of public power grid operator. The second network is build for synchronization and control of the power grid and is not currently used commercially. Information traffic is directed by standard Open Shortest Path First routing protocol and in our case initial link weights are assigned according to the link costs [1]. We apply optimization algorithm aimed at avoiding, if possible, link overload by a judicious link weight tuning. The output characteristics which enter into quality of service function are link utilization and total cost of the service. The input parameters of the optimization algorithm are network topology, relevant protocol, link costs and capacities.

[1] J. Smiljanic, I. Stankovic, "Efficient Routing on Small Complex Networks Without Buffers", *Physica A* **392**, (2013) 2294.

SOE 9.32 Tue 9:30 P1

Motifs in Triadic Random Graphs Based on Steiner Triple Systems — ●MARCO WINKLER and JÖRG REICHARDT — Institute for Theoretical Physics, University of Würzburg, Germany

Conventionally, pairwise relationships between nodes are considered to be the fundamental building blocks of complex networks. However, over the last decade so-called motifs have attracted much attention. It has been hypothesized that these motifs, rather than links, serve as the building blocks of network structures. Although the relation between a network's topology and its function, its robustness against perturbations, or its efficiency in spreading information, is the central theme of network science, there is still a lack of sound generative models needed for testing the functional role of subgraph motifs. Our work aims to overcome this limitation. We employ the framework of exponential random graph models (ERGMs) to define models based on triadic substructures. The fact that only a small portion of triads can actually be set independently poses a challenge for the formulation of such models. To overcome this obstacle, we use Steiner triple systems (STSs). These are partitions of sets of nodes into pair-disjoint triads, which thus can be specified independently. Combining the concepts of ERGMs and STSs, we suggest generative models capable of generating ensembles of networks with nontrivial triadic Z-score profiles. Further, we discover inevitable correlations between the abundance of triad patterns, which occur solely for statistical reasons and need to be taken into account when discussing the functional implications of motif statistics.

SOE 9.33 Tue 9:30 P1

Architecture of biologically inspired adaptive transport networks — ●JOHANNES GRÄWER¹, CARL MODES², MARCELO O. MAGNASCO², and ELENI KATIFORI¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Laboratory of Mathematical Physics, The Rockefeller University, New York, NY, USA

We study self-organized adaptation mechanisms of biologically inspired transport networks (e.g. plasmodial veins of slime moulds). Therefore, evolving network architectures are simulated using a generic dynamical system and weighted graphs. The graphs' edges represent tubes with Hagen-Poiseuille flow, connected through junctions, represented by their nodes. A local update rule, that changes the conductivity of the tubes (edge weights) according to the flow through them, is used as a self-organizing adaptation principle. We model these interrelated transportation and adaptation processes on paradigmatic complex network topologies (e.g. Watts-Strogatz, Barabási-Albert, Erdős-Rényi) with random initial edge weights. We examine the adaptation dynamics and find, that it exhibits discrete, cascade reorganization events until the network reaches a hierarchically organized state.

SOE 9.34 Tue 9:30 P1

Quantum walks on 1D and 2D quasi-crystals — ●CHI-HUNG WENG and OLIVER MÜLKEN — Institute of Physics, University of Freiburg, Germany

We study the dynamics of quantum walks on a quasi-crystals modelled by the tight-binding Aubry-André-Harper (AAH) equation. We numerically solved both the diagonal/off-diagonal AAH in both 1D and 2D cases. It is known that the 2D diagonal AAH can also be regarded as a model for the Integer Quantum Hall Effect (IQHE), a phenomena when a 2D electron gas is subjected to strong magnetic fields at a low temperature. As a consequence we also observe the edge states which are responsible for carrying the current. Those states can be changed from localized to de-localized, as a topological phase within the aperiodic modulated on-site potential varies. In order to identify how localized the states are, as well as how fast the transport is, the Inverse Participation Ratio (IPR) and Mean Squared Displacement (MSD) are calculated, respectively. Moreover, we also study the impact of disorder and non-Hermitian settings (i.e. system with absorbers or Parity-Time (PT) symmetric modulated aperiodicity) on the dynamics.

SOE 9.35 Tue 9:30 P1

Transport efficiency in complex networks — ●MARCO TABARELLI and OLIVER MÜLKEN — Albert-Ludwigs-Universität, Freiburg, Germany

We examine complex networks of two-level quantum systems regarding their efficiency to transport excitons through the network. Our model uses the so-called Quantum Stochastic Walk (QSW), a version of a quantum master equation in Lindblad form (LME) which allows to parametrize the classical-quantum mechanical crossover. To describe a circular probability current an external node is coupled to two "ends" of the network acting as a source to an entrance node and a trap to an exit node. These links are directed and their effect is realized with additional Lindblad operators in the dissipative term of the LME. Comparing stationary solutions of node populations sheds light on the probability current through the network. In addition to the geometry of the network, parameters varied include the internal coupling constant, source- and trap strength and the ratio of coherent and de-coherent transitions. Networks studied include modified linear chains and networks with self-similarity properties.

SOE 9.36 Tue 9:30 P1

Feedback control of vorticity in a Newtonian fluid — ●MARIA ZEITZ and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Our goal is to explore feedback control strategies to stabilize novel dynamic flow patterns in microfluidic model systems. As an example, we investigate a Couette flow geometry without the inner cylinder filled with a Newtonian fluid. Its vorticity satisfies a diffusion equation. To stabilize a mean vortex strength in the flow field, we use feedback control with hysteresis. We either set the angular velocity of the outer cylinder or apply a torque at the boundary and switch velocity or

torque value in a hysteretic fashion depending on the actual mean vortex strength. Since the boundary condition changes with time, the system does not reach a stationary state. In this setup, we explore the possibility of time-periodic solutions and spatial flow patterns. In a second step, we will also implement time-delayed feedback in our system.

SOE 9.37 Tue 9:30 P1

Fractal distributions in a cyclic information-engine with optimal feedback — ●MICHAEL BAUER, ANDRE C. BARATO, and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

It is known that information obtained by measurements can be converted into work, the paradigmatic example being Szilard's engine. For a two level system coupled to a heat bath and a work reservoir we obtain the optimal protocol corresponding to the maximal work extraction. Moreover, we consider a controller performing cyclic measurements and changing the protocol accordingly. Analyzing this optimal cyclic machine we find a recursion relation for the initial occupation probability of the level with higher energy, which depends on the measurement error. Through the numerical analysis of this relation we obtain a fractal histogram, which is a strange attractor (common in chaos theory). This fractal structure can be explained with a simplified model leading to the Cantor set.

SOE 9.38 Tue 9:30 P1

Feedback control of non-equilibrium dynamics of a multi-layer system of confined colloidal particles in planar shear flow — ●SASCHA GERLOFF, TARLAN A. VEZIROV, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We perform computer simulations of charged colloidal particles in planar shear flow combined with feedback control. The particles interact via a combined Yukawa- and soft-sphere-potential. The system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate [1]. The parameters are set to suit experimental data for Ludox silica particles, which were previously studied [2, 3].

We employ overdamped Brownian dynamics simulations to investigate the structure and the rheological behavior of the considered system. We then supplement our equations of motion by an additional dynamical equation, which corresponds to a feedback control mechanism for the shear rate via the shear stress. This enables the system to select between steady states dependent on the control parameters. Furthermore we present an approximation which estimates the transition between steady states in the control parameter space analytically.

[1] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. E **88**, 5 (2013).

[2] S. Grandner and S. H. L. Klapp, J. Chem. Phys. **129**, 244703 (2008).

[3] S. H. L. Klapp, Y. Zeng, D. Qu and R. v. Klitzing, Phys. Rev. Lett. **100**, 118303 (2008).