YRS 2018

YOUNG RESEARCHERS SYMPOSIUM 2018

22nd June, 2018 • Fraunhofer-Zentrum Kaiserslautern

ABSTRACT BOOK

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TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

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Welcome Message from the Patrons

Dear colleagues

It is our pleasure to welcome you to Kaiserslautern's Young Researchers Symposium 2018!

For the fourth time since 2011, this symposium will take place - and, as in 2016, will be carried out jointly by the TU-Nachwuchsring and the High Performance Center for Simulation- and Software-Based Innovation. Thus, the Young Researchers Symposium (YRS) once again offers young scientists from Kaiserslautern a truly interdisciplinary platform to present their research work as well as for informal exchange and networking.

In order to attract young scientists from all TUK's disciplines and to make the YRS even more attractive for doctoral students, in particular, the concept of the YRS was adapted this year; among other things, the application procedure was simplified to a one step process and thus more readily accessible for scientists from various scientific disciplines. Our measures seem to have been successful: compared to 2016, over 60% more abstracts have been submitted and reviewed this year. PhD students from nine departments of the TUK as well as of the Institutes DFKI, IVW, and Fraunhofer ITWM and IESE have applied to present their research work in a talk or poster.

As in the previous Young Researchers Symposia, the best contributions will be awarded attractive prizes at the end of the event. For this, all contributions will be judged by both, the scientific committee and the YRS audience. For the first time this year, the scientific committee is entirely made up of young scientists from TUK and scientists of the Fraunhofer Institutes ITWM and IESE, representing all disciplines of the University and the participating Institutes. This has become possible due to the very good cooperation between TUK and the High Performance Center and thanks to the dedicated and important engagement of the TU-Nachwuchsring board. Like the many other activities of TU-Nachwuchsring, the organization of this year's YRS follows the spirit of "By young scientists for young scientists."

We would like to thank all authors for their many interesting contributions and all attendees for taking part in the YRS making the symposium a lively networking platform through their questions and discussions.

We wish all participants a successful and interesting YRS 2018!

Prof. Dr. Arnd Poetzsch-Heffter,
Vice President for Research and Technology
Technische Universität Kaiserslautern

Dr. Konrad Steiner
Managing Director
High Performance Center Simulation and Software Based Innovation

Patrons of YRS 2018

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Catching Fog:
how fog thrives undiscovered cryptic life in the Atacama Desert

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***Abstract*— The Atacama Desert represents the driest place on Earth and probably the oldest desert, with an hyperarid core highly adverse to the development of vegetation [1]. Besides high solar radiation and a broad temperature amplitude almost down till freezing, access to water is the most critical point for life. Whereas precipitation is stated as less than 1 mm per year, fog is a daily event promoted by the close vicinity to the Coastal Range. Cryptic organisms such as cyanobacteria, green algae and lichens as extremophiles are among a group of organisms that are known to withstand with different strategies. As an assemblage called biological soil crusts (BSCs; fig. 1a) they intermingle and concatenate the first millimeters of soil as a protection against erosion where they conquer up to 12 % of the Earths' terrestrial surface [2]. Besides being part of BSCs lichens growing attached on cacti (epiphytic; fig. 1b) can be partners catching fog water that is dripping and accessible for cacti. Additionally translucent quartz stones combines perfect conditions for vivid cyanobacterial communities (hypolithic; fig. 1c) being the bottom of primary production in these habitats. The establishment of climate stations, drone flights, photosynthesis measurements, microscopic and molecular approaches such as sequencing helped to discover and describe a novel and unexpected diversity hotspot and how the different life forms interact with fog. The results presented are part of ongoing research in the frame of the EarthShape Project, describing three different microhabitats (BSCs, epiphytic lichens, hypolithic cyanobacteria) of cryptic organisms at the hyperarid core of the Atacama Desert.**

Keywords—biological soil crust, Atacama, cyanobacteria, lichens, hypolithic

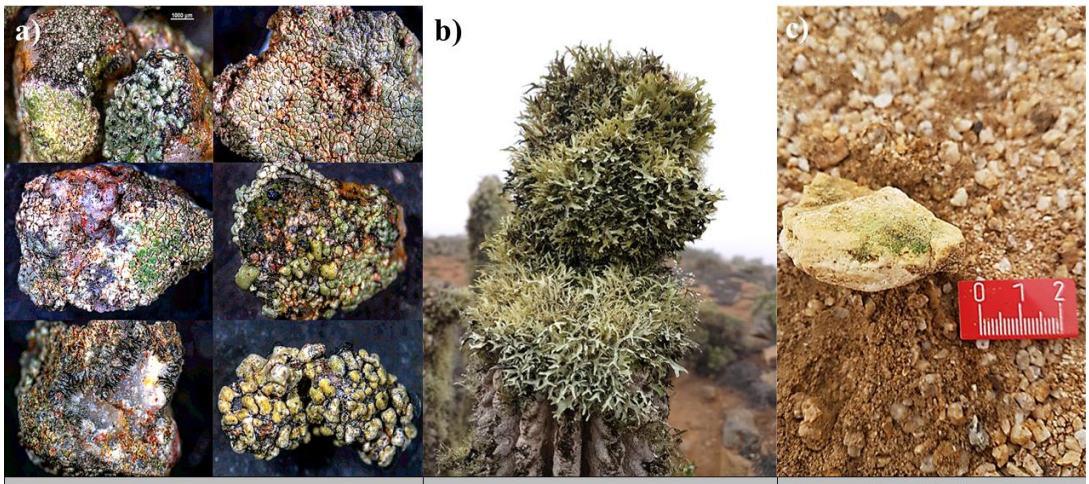

Fig. 1: Different life habitats in the Atacama Desert

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3D characterization of aggregates for concrete based on computed tomography

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***Abstract*— Aggregates are an important part of concrete and have a strong influence on its properties. Currently the European standards specify time-consuming and manual methods for the geometrical classification of aggregates. Most methods cannot be used for fine fractions. A method based on data gained from computed tomography (CT) images of aggregates intends to complement the traditional methods and provides a novel opportunity for the 3D characterization even for fine fractions.**

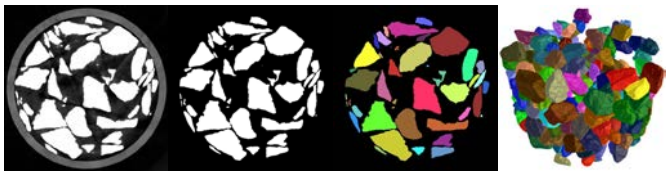
Keywords*— *aggregates; computed tomography (CT); three-dimensional characterization; geometrical parameters

I. Introduction

As 70 % of the ingredients of concrete are aggregates, they have a strong influence on the properties in the fresh as well as in the hardened state. The increasing usage of high performance concrete requires a more precise characterization of the source materials. At the moment it is not possible to give a precise three dimensional description of the shape of aggregates. The standard methods only classify the shapes of aggregates to be spherical or cuboid. As the high performance concrete used for filigree structures only contains fine fractions (mostly < 4 mm), it is also of great interest to have a more detailed characterization of these fractions.

II. Samples and Methods

A selection of aggregate samples with strong varying properties in shape, size and material have been examined to ensure the method is applicable to all kinds of aggregates. In a first step a manual examination of the samples, according to the European standards, regarding the size and shape properties has been carried out. Subsequently these samples have been examined by means of computed tomography (CT). To validate the CT-method, the CT-results have been compared to the manual results.

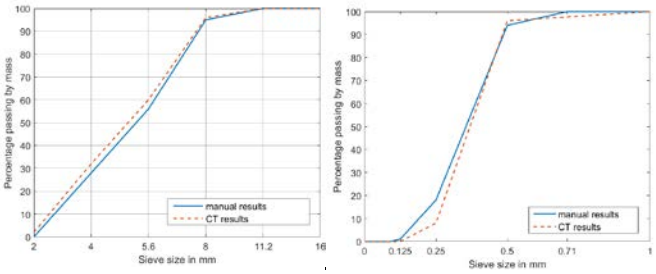


Process of Image processing [1]

A main focus for the validation is the determination of the particle size distribution of the samples. In Fig. 1 the process of the image processing for the analysis of the CT data is illustrated.

III. Results and Discussion

Fig. 2 shows the comparison of the particle size distributions of two different aggregates determined by means of CT (solid lines) and manual method (dashed lines). In the left part the results of a gravel sample (4-8 mm) are presented and in the right part the results of a fine sand (0.25-0.5 mm). It can be seen that the CT-results achieve a good accordance with the manual results.



Comparison of the results (CT: solid lines-manual: dashed lines) for particle size distributions – left: gravel 4-8 mm, right: sand 0.25-0.5 mm [2]

Acknowledgment

The author would like to acknowledge the cooperation with the department for image processing of the Fraunhofer-Institute for Industrial Mathematics (ITWM), P+T Technische Mörtel GmbH & Co. KG and ProCon X-Ray GmbH.

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Self-Adaptation for the Resilience of Automated Systems

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***Abstract*—Automated systems acting in open environments can encounter unknown situations of unknown risk. Resilience is the ability of a system to remain dependable when facing such situations. Self-adaption is a way to achieve this resilience. In this short paper, I present the concepts of how to use self-adaption for achieving the resilience of automated system. I present the existing work of my department in this context and show how the contribution of my doctorate thesis fits in.**

Keywords—Self-Adaption; Resilience; Automated Systems; Dynamic Risk Assessment; Dynamic Risk Management

The automation of technical systems gives the possibility to remove the most common source of accidents: human mistakes. For closed environments, this automation is done for many years now. Not so much with the goal of saving human lives in mind but with the goal of saving money. Currently we can see high investments in robotics and self-driving vehicles towards achieving automation in open environments. This automation in open environments puts significant challenges on the engineering and assurance procedures involved in the production of such technical systems. The main challenge is the high amount of uncertainties in open environments. Change is the natural state of any system operating in an open environment. *The persistence of dependability when facing changes* has been defined as resilience [1] and is of the upmost importance for any automated system in an open environment.

Self-Adaptation is a way to achieve resilience [2]. Figure 1 illustrates this concept. The technical system is transitioning through a space of states classified as safe states, warning states, hazard states and catastrophic states. In a catastrophic state an accidents has happened and the system has caused harm to its environment. For safe states it is guaranteed that a transition to any catastrophic state is not possible. This guarantee cannot be given for a hazard state. It is common practice to establish a space of warning states that shall serve as a buffer between the safe and hazard state space to allow the execution of certain actions to return the system to a safe state, e.g. maintenance work. The case in which this is possible is illustrated in the upper part of figure 1. However, this is not always possible. In such cases, we still need to guarantee that a transition to a catastrophic state is unlikely enough that the system can be considered as safe. This can be achieved by self-adaptation. By changing the system to a more robust but probably less performant configuration, a state classified as hazard state before can become a safe state.

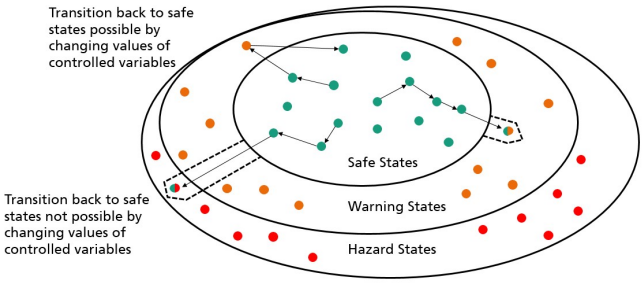

Figure 1 Self-Adaptation for Resilience

In earlier work, we have developed a language to model adaptation behavior [3] and techniques to prove certain properties of such a modeled behavior [4]. As automated systems in open environments will have to communicate with each other, we developed conditional safety certificates as a contract-based approach to allow safe self-adaptation in system collaborations [5]. In the context of my doctorate thesis, I investigate the subject of Dynamic Risk Assessment: How can a technical system know its current position within the state space illustrated in figure 1. In my thesis, I investigate this subject for the case of self-driving vehicles and present the Safety Supervisor solution with the novelties of mission-oriented, connected, situation-dependent, integrity-aware and fail operational calculation of collision risk metrics. Under the term of Dynamic Risk Management, it is our intention to bring these works together

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Influence of crystal orientation on crack initiation behaviour in polycrystalline turbine materials

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Abstract - Germany is phasing out nuclear power by 2023. This will undoubtedly result in further increased utilization of renewable energy sources for power generation (solar, wind), but also potential issues in managing fluctuations in the energy grid during adverse weather conditions. Gas turbines have an important role to play as buffers to compensate for any volatility in the difference between supply and demand of electrical energy because they can be ramped up to peak load in a very short time. While coal fired or nuclear based steam power plants need several hours up to days to become fully operational, current gas turbines only need about 30 minutes for a cold start do maximum power. For this reason, they can react far more quickly to address shortages in the electricity network. The associated rapid changes in operation place particularly high demands on the turbine materials because start-stop processes and load changes result in significant thermally induced stresses exceeding by far the loadings which occur in constant operation.

Classic deterministic material models, used to describe fatigue behaviour in coarse grained polycrystalline turbine blade material, consider the typical large scatter in fatigue lifetimes by high safety factors. One main reason for the scatter in fatigue lifetime is the microstructure of cast Nickel base alloys frequently used as turbine blade materials. During the casting process, a small number of large randomly orientated grains are formed in the component cross section. The orientation of the grains has a great influence on mechanical behavior and thus on crack initiation during cyclic loading: Elastic stiffness differs by a factor 3 depending on grain orientation, which also strongly influences plastic deformation processes. Hence, very high safety factors are used to exclude failure in operation.

To fully utilize the material's strength in turbine blade design, new models for better lifetime prediction are necessary. Probabilistic models, based on statistics, require more parameters than deterministic approaches. Therefore, a detailed understanding of grain orientation influence on fatigue processes, especially crack initiation within the microstructure is necessary. In the present work, Monte Carlo simulations are used to investigate the influence of random grain orientations on material properties in case of uniaxial and multiaxial stress states. To simulate the mechanical behaviour of a polycrystal, Voronoi tessellations were used to generate random grain shapes and sizes for a given sample geometry. The grain models (fig. 1) were integrated into finite element simulations, and near-operating loads were simulated.

Figure 1: Vornoi Tesselation for Finite Element Simulation to investigate grain size and oriantation influence on the mechanical behaviour of polycystalline turbine blade material .

It turns out, the consideration of significantly more influence parameters, like grain orientation, grain size and stress state, leads to a better understanding of the crack initiation and fatigue behaviour and can lead to an improvement of the turbine blade design and finally to higher effencies.

Plasmonic Hurricanes on the Nanoscale

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Modern computing devices are usually composed of electronic semiconductor circuits. In the near future, the processing speed which can be achieved with these components will reach a fundamental limit. This will impede advances in both science and the development of new technologies. A potential solution is the replacement of electronic signals with light, which enables a much faster data transmission. However, a major problem with the use of electromagnetic waves is the so-called diffraction limit: light cannot be focused down to lengthscales much smaller than its wavelength. Due to this restriction, optical signal processing and data transmission devices cannot be miniaturized as much as their electronic counterparts [1].
One way to circumvent the diffraction limit and to focus electromagnetic signals down to the nanoscale is the use of plasmons. In physics, they describe the coherent oscillation of the electron gas in a metal. Plasmons can be local or propagating. The latter could be used for highly efficient information transport on the nanoscale. Plasmons are a field of current research, so before they can be used for applications in modern technologies, their fundamental properties must be understood.

So-called propagating surface plasmons can be created with a slit in a metal surface and laser light. The light sets the electrons of the metal close to the slit into motion. They start to oscillate and create an electromagnetic wave which propagates along the metal surface. If the sample is placed in a vacuum, this can be imaged with a photoemission electron microscope (PEEM) [2]. The technique utilizes the photoelectric effect: when light hits a metal surface, a part of its energy is passed on to the metals' electrons and they are emitted into the vacuum. The positively charged extractor of the PEEM accelerates the negatively charged electrons into the microscope. Unlike light, electrons cannot be focused with glass lenses, so a PEEM uses an electrostatic lens system to create a magnified image.
The goal of our experiments was to image the propagation of the plasmon wave in realtime. This can be realized in a pump-probe experiment with two ultrashort femtosecond laser pulses, which are delayed relatively to each other. The first pulse creates the plasmons, while the second one monitors their evolution by emitting electrons from the surface and creates an image. In this way, the second pulse acts like a stroboscope lamp which reveals the position of the wave at a fixed time delay after the first pulse. For the creation of a movie of plasmons moving with almost the speed of light, the pulse delay was varied and each 0,1 femtoseconds an image was taken.
We manipulated the plasmons' propagation direction with help of a special excitation structure, a so called plasmonic vortex lens (PVL), which gives the plasmons an orbital angular momentum. For this, multiple slits in a gold surface are arranged to a spiral-like structure. The plasmons form a rotating vortex, similar to a swirl in water or a hurricane, see Fig. 1. It exhibits a characteristic number of lobes which indicates the plasmonic angular momentum. With our time resolution, additional properties like for example the vortex rotation speed can be investigated [3].

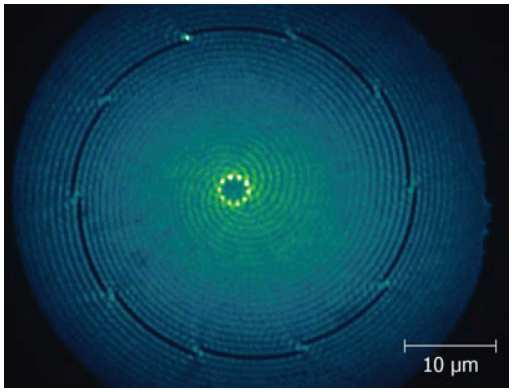

Fig. 1. PEEM image of a plasmonic vortex lens, measured at a pulse delay of 60 femtoseconds. The black lines correspond to slits in the gold surface, while a plasmonic vortex can be seen at the center of the structure.

Our observations of plasmon dynamics at a femtosecond time scale offer progress towards the understanding of fundamental plasmonic properties. This paves the way towards the application of plasmonics in future information technology devices.

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Social Desirability Bias in Attitudinal Measures

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I. INTRODUCTION

This doctoral project examines the to date ignored topic of heterogeneous trait desirabilities (also: 'desirability beliefs') in attitudinal measures and attempts to account for the conflicting empirical results in the field of research on social desirability (SD) bias.

Social desirability describes a bias that results when survey respondents present themselves in a more positive light than is actually accurate. It is one of the central concerns in survey research, particularly in surveys in which respondents are asked to divulge 'sensitive' information. Sensitive topics are traditionally considered those that are a) intrusive (i.e. income, sexual preferences), b) sanctionable (tax evasion, under the table work) or c) have to do with social norms (recycling, donating to charity) [1].

'Trait desirability' and 'desirability beliefs' describe the perceived social norms surrounding a survey item [2]. The stronger and clearer the social norm is surrounding a survey item, the more it should be susceptible to SD bias. Many studies, typically examining the reporting of sensitive *behaviours* such as drug use, sexual practices, theft, traffic violations etc., often either implicitly assume homogeneous desirability at topic-level or ignore the direction and extent of trait desirability. Studies looking at the effect of SD on reported *attitudes* are much sparser [3] but often make the same untested assumptions concerning the desirability of individual attitudinal survey items.

II. METHOD

A preliminary study was conducted in the Spring of 2017 in Kaiserslautern (n=387) which focused on attitudes towards various out- and minority-groups (women, homosexuals, Muslims and poor people). Confirmatory factor analyses (CFAs) were estimated to establish the construct validity of the attitudinal measures. The results showed a second-order latent construct structure fit the model well which was in line with current findings on patterns of generalized prejudice [4,5].

In a second step, multilevel analyses were conducted to explain respondent scores on the 17 attitudinal items with random effects to account for respondent- and item-level variance. Fixed effects were specified to attempt to explain the variance at the second-level.

III. INITIAL RESULTS

The results of the preliminary study show that the trait desirability of individual items significantly influences item scores (0.340, $p<0.1$) and explains substantial amounts of variance in terms of average per-item scores [5]. Fig. 1 shows the variance of the individual attitudinal items before and after controlling for item-level trait desirability. After controlling, the differences between the prevalence of various attitude expressions become much less pronounced (see Fig 1.).

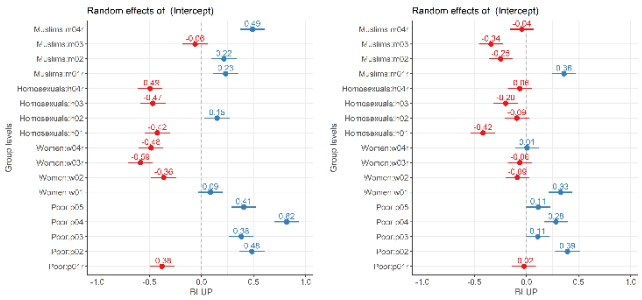

Fig. 1 Random effects, uncontrolled (left) and controlled (right) for item trait desirability.

IV. CONCLUSION & OUTLOOK

The doctoral project draws attention to the importance of closely examining the desirability of individual survey items. It may not be wise to assume, for example, that homophobia is uniformly undesirable: some expressions of the prejudice are more acceptable than others. Failure to examine desirability at an item-level will lead to a 'cancelling out' of conflicting effects and confound empirical analyses. For some attitudinal items, the socially desirable response would be to actually exaggerate prejudice rather than hide it.

In Summer 2018 a random probability sample of the German population (n=3,000) will be conducted test the hypotheses and preliminary findings. With this new, robust sample, we will attempt to replicate the results of the initial analyses. Furthermore, the interaction between respondent-, topic- and item-related characteristics will be more closely examined.

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Boundary conditions for the thermal simulation of tribological testing devices

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I. Introduction

Efficiency, in regard to both energy and materials, is becoming an ever more important requirement in the design of technical products. One major cause for energy and material losses are friction and wear of contacting surfaces in relative motion. These contacts are referred to as tribological systems. A thorough understanding of their behavior is necessary to improve the efficiency of machines.

Polymer-based materials provide a set of properties that are beneficial for the use in tribological systems. Also, the processing of polymer materials is energy efficient and cost-effective. Furthermore, they can be modified using a wide variety of filler materials to taylor their properties to the demands of specific applications. However, a major challenge in the design of polymer-based tribological systems is that their material properties are strongly temperature-dependent. Frictional heat causes an increase in temperature, which greatly influences the system's behavior. As a result, the same material may exhibit a strongly divergent behavior in applications with dissimilar heat balances. Tribological properties of a material may not even be reproducible on different testing devices.

One approach to overcome these difficulties is the thermal simulation of tribological systems. Simulations can provide a three-dimensional temperature distribution of the system. The temperature dependent material properties can then be inferred. To achieve an accurate simulation, a suitable choice of boundary conditions is important. In the case of thermal simulations, this concerns the heat transfer at the outer limits of the model.

II. EXPERIMENTAL

To gain a better understanding of the influence of different boundary conditions, a Pin-on-Disc testing device was analyzed. In this device, a rectangular plastic specimen is sliding against a steel disc. The temperature distribution inside the specimen was determined numerically using two different modeling approaches. Firstly, a highly simplified model was set up. In this model, only the geometry of the specimen was included, while the rest of the testing device was modeled using thermal boundary conditions on the specimen's surfaces. Secondly, a more comprehensive model was built, which included several surrounding parts of the testing device (Fig. 1).

Simulations of the same tribological experiments were conducted using both models. The results were then compared to measurement data, which was collected during the actual lab experiments using contact-free temperature measurement and thermal imaging. The results obtained from the two different numerical models were compared in order to understand the influence of the models' level of detail on the quality of the results.

III. RESULTS

The results obtained from the comprehensive model show that the temperature of the specimen holder is close to the ambient temperature. This behavior is also observed in the simplified model. However, temperatures close to the contact surface deviate between the two models, due to the different modeling approaches. The steel disc and the adjacent shaft reach temperatures, which are considerably above the ambient temperature and thus cannot be modeled using isothermal boundary conditions.

IV. CONCLUSION

A more accurate temperature distribution can be achieved by using a more complex geometrical model. The increase in accuracy justifies both the additional effort required to establish the model and the increased computational cost.

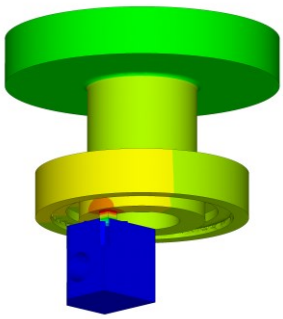

Fig. 1. Thermal simulation of a Pin-on-Disc test setup.

Magnetostrictive materials - modeling, simulation and applications

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Each one of us has already seen them or, perhaps, even experienced them in action: the tiny Electronic Article Surveillance (EAS) tags fixed on merchandise to prevent shoplifting. A common type of these tags are the so-called *acoustomagnetic* or *magnetostrictive* tags, which, if active, cause a penetrant sound produced by detectors at the exit of the shop. These tags take advantage of the *magnetoelastic coupling*, an effect that makes it possible for them to convert magnetic energy into mechanical energy and vice versa, finally causing an acoustic signal. The tiny snitch in the tag that helps to convict the shoplifter is a thin magnetostrictive metal strip (see Fig. 1). This special type of a material experiences a deformation under the influence of a magnetic field and, in turn, changes its magnetization when subjected to mechanical stress.

Magnetostrictive materials belong to the large class of Smart Materials, which experience a change in their shape, dimensions, stiffness and viscosity due to the influence of an external field, such as a temperature, pressure or an electromagnetic field. Among prominent Smart Materials are *piezoelectric* materials that induce a voltage due to elastic deformation (applied e.g. in headphones or speakers), *photo- or thermochrome* materials that change their colors due to temperature or ultraviolet light (used in sunglasses) or *shape memory alloys* which "remember" their original shape after the deformation (applied in modern medicine). These remarkable properties offer wide application areas for such "intelligent" materials: Magnetostrictive materials, for example, are used as sensors or actuators, as robots, artificial muscles or oscillators in sonar systems. The magnetostrictive effect is also responsible for the "electric hum", the special noise that can be heard in the vicinity of electrical devices and machines such as transformers.

In the meantime, magnetostrictive materials are an inherent part of our everyday life. Yet, their application requires a profound understanding of their properties, behavior and characteristics. How can we mathematically describe the coupling between the mechanical and magnetic fields? Can we predict their behavior on the basis of mathematical formulas? How can we derive these formulas from the laws of Physics? These are some of the questions that will be addressed during the talk. The aim of the talk is to provide an insight into the mathematical modeling and analysis of magnetostrictive materials. We will focus on the derivation of the coupled system of equations using well-known energy principles, as well as on the subsequent analysis in a mathematical framework. Various numerical simulations will confirm the theoretical results and illustrate the coupling effect.

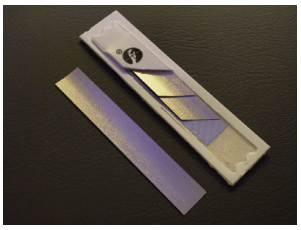

Fig. 1. Structure of an EAS tag (source: Wikipedia commons)

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Homogenization and Design Optimization for Shells with a Periodic Frame Structure

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The design optimization of cylindrical shells arises in many different fields of application. In particular we have a special interest in minimizing the deflection of a shell caused by concentrated loads, also called twitching, or achieving a desired stress profile throughout our shell structures. Such a structural optimization problem arises in different applications dealing with thin shells made of periodically distributed thin beams. Examples of such periodic shell structures are textiles, thin shells used in dry shavers and different filters, see Fig. 1 (left). All stated examples have to fulfill high requirements in their daily uses and should be optimized for their specific purpose. The underlying shells are of thickness ε and made of a periodic pattern of the same size, i.e. small compared to the full shell length. Our analysis exploits this periodicity by a multi-scale homogenization method and we show explicitly for the problem of shell twitching how our research can benefit in finding better designs. We outline the different research steps. First we have to find a macroscopic model for the shell twitch. For homogeneous shells with constant effective bending and torsion properties, the analysis for the dimension reduction w.r.t. the thickness was considered in [1] and simplified for linear elasticity in [2]. The analytic solution for cylindric shells under 2 symmetric point loads was given in [3]. We found an analytic solution for the shell configuration shown on Fig. 1 (left) and corresponding boundary conditions with the help of Fourier transformation and series.

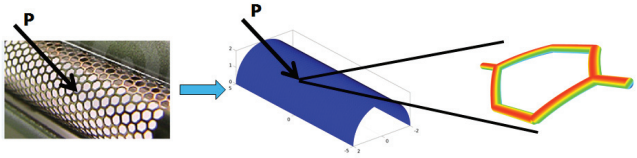

Fig. 1. Homogenization scheme.

The step from a heterogeneous shell made of beams to a homogeneous one is obtained by classical homogenization techniques presented in [4] and was summarized in [5]. This computation yields an equivalent homogeneous shell while the effective coefficients are computed from appropriate auxiliary problems on the periodicity cell of the microscopic structure, see Fig. 1 (right). The principal idea to obtain these properties is to reduce the cell problem on the 3-D structure to beam equations on a 1-D network structure. This simplification reduces the complexity tremendously.

The last step is the structure optimization. This requires a parametrization of the periodic structure. Due to the dimension reduction the equations are living on a graph or network, which drastically reduces the number of parameters. To find a better design it is crucial to restrict our admissible design parameter g to some compact set $U_g \subset \mathbb{R}^2$ as it is shown on Fig. 2 (left), s.t. we attain an admissible minimizer. The choice of U_g depends on constraints, depending on the application of the shell. We can arbitrarily choose a point g inside the blue box and we get the full periodicity cell, Fig. 2 (middle), by reflecting the initial structure across the orange and the black line. We are able to calculate the effective bending properties symbolically, using the advantages of computer algebra, such that the results are exact and visible. It provides analytic formulas, where the influence of the applied elastic properties and cross-section of the beams are given explicitly. This application is new for homogenization.

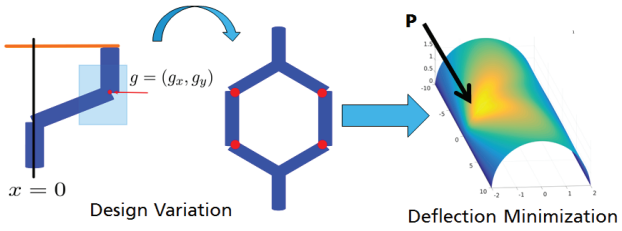

Fig. 2. Design is varied by shift of the node in the blue square.

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Mass transfer during droplet formation

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In liquid-liquid extraction processes, both mass transfer and coalescence are the key factors. The present study deals with techniques for the measurement of mass transfer during droplet formation. Interfacial tension measurements, LIF measurements and confocal Raman spectroscopy measurements are applied and compared. It could be shown that Marangoni effects significantly influence mass transfer, which is half done already after 5 seconds.

Keywords—droplet formation, mass transfer, Marangoni

I. Introduction

Liquid-liquid extraction is used in many technical processes, e.g. in the biochemical, petrochemical or chemical industries, but the basic fundamentals are still not fully understood. For fast and reliable interpretation of extraction methods, process models are needed which take droplet interactions (e.g., droplet coalescence and breakage) into account. At high concentrations, mass transfer is influenced by Marangoni convection, arising from a surface tension gradient which induce fluctuations affecting droplet interactions. This already starts with droplet formation followed by rise, breakage and/or coalescence. Local and temporal highly resolved measurements were performed during droplet formation to capture mass transfer induced by Marangoni convection. A deeper insight on the local phenomena, which are experimentally difficult to explore, can be gained with the aid of Computational Fluid Dynamics (CFD) simulations.

II. Experimental and Results

Using a newly constructed measuring cell and a confocal Raman spectroscope (type torus 532, software LabSpec6), the mass transfer was investigated during the formation of toluene droplets with acetonitrile (disperse phase) in water (continuous phase), with an initial solute concentration of $c_{ACN,0}$ = 10 wt%. The concentration was measured at different positions in the droplet. In the middle of the droplet, the concentration has already halved after 5 seconds, which also confirmed parallel interfacial tension measurements (PCA 15; Dataphysics) [1]. As a basis for the interfacial tension measurement as well as for the Raman spectroscopy, the equilibria for different solute concentrations have been determined. For the mass transfer visualization during droplet formation (s. Fig. 1), rhodamine 6G was added to the dispersed phase (toluene + acetone or acetonitrile). The fluorescence of the rhodamine makes it possible to visualize the mass transfer during the LIF measurement. It can be seen that the Marangoni convection causes strong fluctuations in the concentration at the phase interface, which also leads to large concentration fluctuations in the interior of the droplet (Fig. 1).

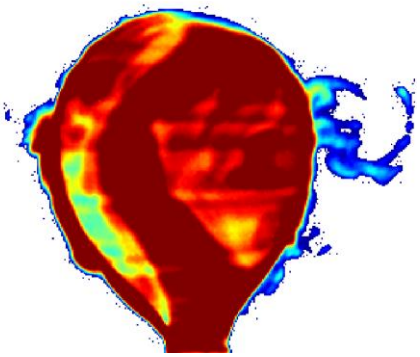

Figure 1: LIF measurement during droplet formation of a toluene droplet (solute: acetone and rhodamine 6G)

III. Conclusion and Outlook

A study on the influence of the Marangoni effect on mass transfer at single droplets during droplet formation was carried out. With two independent methods, the local high resolution measurement inside the droplet (Raman spectroscopy) and the integral surface measurement of the interfacial tension, a rapid decrease of the concentration could be determined in the first seconds after the droplet formation. In both cases, more than half of the mass transfer was done after 5 seconds. Furthermore, the Marangoni influence on local concentrations could be visualized by LIF measurements.

In further studies, detailed numerical volume-of-fluid (VOF) based simulations will help to determine surface and bulk droplet concentrations with high temporal resolution, thus allowing a better understanding of the droplet formation and a comparison with existing experimental data.

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The spin-wave majority gate for data processing

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In the last 40-50 years the number of transistors in integrated circuits has doubled approximately every two years. But in recent years it was observed that this behavior, also known as Moore's law, is coming to an end due to limit of the downscaling in CMOS circuits. Therefore people all around the world are searching for a new technology, which is able to be the next step in the evolution of data processing. One promising candidate is Magnonics, in which spin waves are used to perform logic operations. In this contribution we show the advantages of a spin-wave based technology compared to the CMOS technology and we give an example of an already existing magnonic prototype: the macroscopic spin-wave majority gate.

Magnonics is based on magnons - the quanta of spin waves, which are collective excitations of a magnetic material. These spin waves can be used for a new type of data processing: spin-wave logic, which has a few advantages compared to a CMOS-based logic. The transport of information by using spin waves can provide low power operation and future devices can be fabricated with sizes down to sub-10 nm. One of the biggest advantages lies in the wave nature of spin waves. For logic operation one can use not only the amplitude but also the phase of spin-waves. In addition a parallel data processing by using different frequencies is possible. Spin waves can also be used in a wide frequency range, from the important GHz regime up to the promising THz regime. Due to its wave character it's possible to create a large set of different logic devices, which can open the way to a non-Boolean data processing.
An example is the majority operation, in which the output state is given by the majority of the input states. In Magnonics, one can realize the majority operation by using a spin-wave majority gate, which consists of an odd number of inputs and one output. In such a device the information is encoded in the phase of the spin waves and the operation itself is performed by using the interference of the input signals. Majority gates have the potential of building very efficient circuits and are able to reduce the footprint of logic circuits drastically.
Together with our collaborators we have fabricated a prototype of a spin-wave majority gate (Fig. 1). It is a macroscopic device made from a micrometer thick Yittrium Iron Garnet (YIG) film. YIG is a magnetic insulator material which features a large spin-wave propagation length. The prototype (Fig. 1) consist of the Ψ-shaped majority gate structure itself, three input antennas, used for the excitation of spin waves in each input waveguide, and one output antenna to detect the interference signal. The investigation of the logic operation of the device was realized by using microwave technique: we variably adjust the phase of the input signals. A phase of $\Phi = 0$ correspond to a logic 0 and a phase of $\Phi = \pi$ to a logic 1. The operation of the macroscopic device as a majority gate is proven - the output phase of the signal is determined by the majority of the input phases [1]. The achievable clock speed is determined to be $f = 88\,\mathrm{MHz}$.
The miniaturization of the device is naturally the next step and in this contribution we will also report on the recent progress towards a microstructured spin-wave majority gate.

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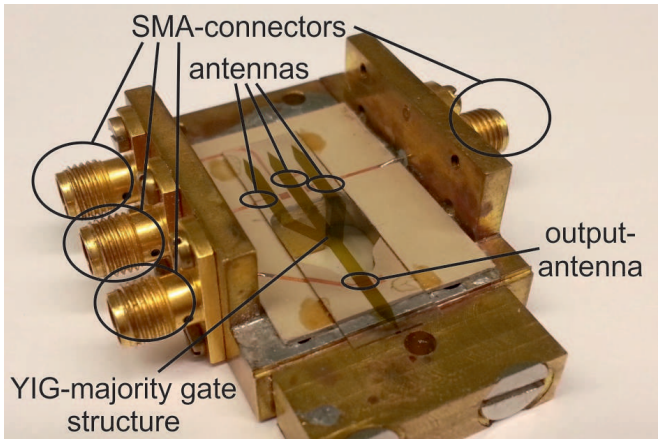

Fig. 1. Picture of a the macroscopic spin-wave majority gate. The Ψ-shaped structure is the majority gate itself made from the magnetic material Yittrium Iron Garnet. The antennas are used to excite and to detect spin-waves.

How to Make Brittle Polymeric Composites Tough

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***Abstract*—Brittle polymers are used as matrices for fibre reinforced composites and are systematically blended with rubbery, particle-like phases to increase their resistance to crack formation and propagation. This study shows that even small amounts of *toughening agents* can drastically increase material properties such as the fracture toughness of polymeric fibre composites. Thereby, it is possible to specifically make use of various energy dissipating mechanisms in the material.**

I. Introduction

Polymeric fibre composites are of major importance for a cleaner and more sustainable future. Due to their low specific weight and simultaneously high strength, these materials are an essential part in manufacturing lightweight structures and thus reducing energy consumption in automotive, aerospace and engineering applications. However, a main drawback coming along such polymers that are e.g. required to protect the embedded fibres from environmental influences, is their brittleness. These polymers are about 10 to 100 times more brittle than steels and alloys and suffer from a poor resistance to crack propagation [1]. One approach to overcome this shortcoming is to blend them with a second phase, e.g. rubber. This study focusses on the single and synergistic effects of *block copolymers* (BCP) that thermodynamically driven, self-assemble and self-organize in the polymeric network structure and their combination with *preformed core-shell rubber particles* (CSR). Both toughening agents are easily processed and provide a resistance to crack propagation on the nano-scale.

II. Materials and Experimental

The polymer system used was a Bisphenol-A-based epoxy resin. To examine the influence of the rubber modifiers on the toughness of the composite material, the BCP and CSR modifier concentrations were varied in between 0 to 17 vol.-%. Samples were manufactured and tested as bulk and as carbon fibre reinforced composites. For the latter, carbon fibre mats were systematically impregnated by the modified resin systems. To evaluate the impact of the modifiers on the crack propagation behaviour, fracture toughness tests according ASTM 5045 (bulk) and DIN EN 6033 (fibre composite) as well as an in-depth Scanning Electron Microscopy analysis of the fracture mechanisms were performed.

III. Results

Fig. 1 shows the normalized crack driving force G_{Ic}, a measure of the resistance to crack propagation of a material, as a function of the BCP and CSR concentration in a carbon fibre reinforced polymer. The resistance to a propagating crack strongly increases with both types of modifiers. Different mechanisms are induced by the toughening agents on the micro and nano scale and hinder the crack to easily pass through the material [2]. Thereby, one important mechanism is *localized plastic deformation* of the polymer itself. A change of the stress conditions allows the brittle polymer to plastically deform. However, after increasing the modifier concentration

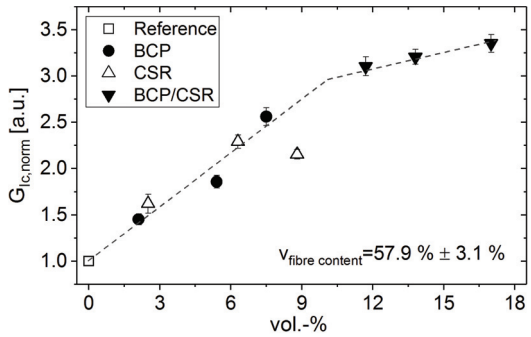

Fig. 1. Crack driving force G_{Ic} of a differently modified carbon fibre reinforced polymer

above 10 vol.-%, the toughening effect diminishes and the previously increasing trend bottoms out. In this scenario, the densely packed carbon fibres start hindering the plastic deformation capability of the polymer and restrict a further toughening of the composite.

IV. Conclusion

The data obtained in this study reveals that the resistance to crack propagation of polymeric fibre composites can be increased more than threefold by a modification of BCP and CSR. Both toughening agents show a similar effect on the crack driving force in a composite. Furthermore, increasing G_{Ic} beyond 10 vol.-% is restricted by the presence of carbon fibres.

Acknowledgment

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Decision Support for Smart Ecosystem Evolution

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***Abstract*—We observe the trend towards complex systems of systems, so-called smart ecosystems. The evolution of such an ecosystem is characterized by the challenge of gaining insights into the ecosystem for the purpose of deriving requirements. In our research we work on the creation of an understanding of information needs in the context of smart ecosystems to build dedicated representations, which support the ecosystem evolution.**

***Keywords—software engineering, requirements engineering, smart ecosystem*.**

I. Introduction

Digital systems emerge more and more, catching even industries so far traditionally not yet affected by IT, so that in future they will hardly work without relying on intelligent or smart systems [1]. Typically, it is not pure software or one individual system, that provides the desired innovative services, but rather an interconnection of various technical systems including hardware as well as software parts. Commonly, we distinguish between information systems and embedded systems as two separate classes of systems [2]. However, in the ages of the digital transformation, we observer a dissolution of the previously clear separation of classes and experience a trend towards interconnecting *smart ecosystems* [2]. Such a system is characterized through "the software and actor interaction in relation to a common technological infrastructure, that results in a set of contributions and influences directly or indirectly the ecosystem [3]." This means, while we integrate various non-trivial information systems and embedded systems into a smart ecosystem [2], the functioning as one unit remains one of the central aspects. To achieve this in practice, the systems of various organizations potentially originating from different domains are orchestrated on a central platform connecting all the systems in a meaningful way.

II. Research Challenge

Requirements engineering as a key phase in software engineering has the purpose of eliciting, analyzing, documenting and managing the properties, i.e., requirements, of a software system [4]. While the development of traditional software systems is well established, the creation and evolution of smart ecosystems up to now imposes challenges that arise due to the complexity of the systems as well as the heterogeneity of the involved partners [5]. To make sound decisions about the future evolution of such a smart ecosystem, i.e., to derive requirements, it is necessary to have deep insights into the current state of the ecosystem as well as the partners contributing to it. However, in practice, the concrete information needs are still unknown.

III. Solution Idea

The cornerstone for supporting the derivation of requirements is the knowledge about the information needs w.r.t. smart ecosystems that are specific for such systems and go beyond the ones of traditional software systems. For this purpose, we perform a series of interviews with researchers and practitioners in this field along with a systematic literature review to gather and understand the information needs. We classify these information needs into a taxonomy indicating which roles, e.g. business responsible, technical responsible etc., need which information for which purpose. Furthermore, the taxonomy is enriched with information about the underlying data which is required to fulfill the information needs. On this basis, we develop a data acquisition strategy, which is particularly relevant since data might not be accessible directly due to the distribution of the system and the involvement of various organizations. Therefore, the consequences of not having certain data available on the possibility of fulfilling information needs is investigated. Finally, the contribution encompasses the development of representations for the data. The complexity of smart ecosystems requires the usage of dedicated representations to make the information accessible and create the required insights into the ecosystem. Hereby, we aim at generating views from the acquired data and combining them with manually created ones if automation is impossible.

IV. Conclusion

Our research aims at supporting decision making process w.r.t. requirements in the context of smart ecosystems by understanding information needs to ultimately provide representation of such ecosystems. Hereby, automation does not replace requirements engineers, but supports their work with respect to the future development of smart ecosystems.

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Numerical and experimental studies on bubble breakage and coalescence in a slurry bubble column

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Keywords—slurry bubble column, breakage, coalescence, turbulence

Heterogeneously catalyzed reactions, e.g., the hydrogenation of carbon monoxide in the production process of hydrocarbons (e.g., Fischer-Tropsch or methanol synthesis) are carried out in slurry bubble columns on a technical scale. Slurry bubble columns are of rather simple design (regarding geometries, internals etc.) where the gaseous educt is fed at the bottom of the column and rises in a slurry solid–liquid mixture where the solid represents the catalyst. However, mathematical description and modeling of slurry bubble columns is tedious due to the complex phase interactions and simple process models fail. Decisive influences on the conversion in the reactors are the distribution and interactions of the gas and solid phase as well as the gas–liquid interface, which is limiting local mass transfer and thereby reactor yield.

In order to gain insights into these influencing factors, computational fluid dynamics (CFD) are applied in which especially the complex interactions between bubbles, particles and the continuous phase have to be considered [1, 2]. Particles with diameters in the sub-millimeter range (microparticles) increase the coalescence probability with an increasing particle loading. This causes a change of the slurry properties (i.e., carrier density and viscosity) as well as the flow characteristics and reduces the total gas holdup in the system [3]. The mutual influences in the calculations are depicted in Fig 1. By contrast, larger particles in the millimeter range can directly cause the breakage of bubbles (cf. dashed arrow in Fig. 1) and thus increase the total gas holdup in the system [4].

To simulate bubbly flows, a solver has been developed based on a particle simulation approach, the so-called Euler-Lagrange approach, using the open source software package OpenFOAM [5]. Phenomena such as bubble break-up and coalescence and the external forces acting between the phases (i.e., gravity/buoyancy, drag force, virtual mass force, lift force, wall lubrication force) are taken into account. To model continuous phase turbulence, the standard k-ε turbulence model is applied. The multiphase solver was extended to take the presence of solid particles into account.

Experiments were carried out in a rectangular duct made of paraglass wherein both the holdup of the gas phase and the particle fraction in several height segments of the column were measured. The rising bubbles were recorded using a high-speed camera and the local bubble size distributions (BSD) were analyzed. Both the particle volume fraction and the particle size distribution (in the sub-millimeter range) were varied.

To validate and compare the simulation results with the experimental data (e.g., local BSDs), boundary conditions were deduced from the experiments. In addition to a validation of global quantities such as the gas holdup at different particle loadings, an examination of the calculated local variables such as the bubble diameters and the particle concentrations depending on the axial position has been made. The deviations between the simulations and the measurements are discussed and improvements of the modeling are proposed where the modeling resp. modification of the dissipation rate of the turbulent kinetic energy plays a decisive role.

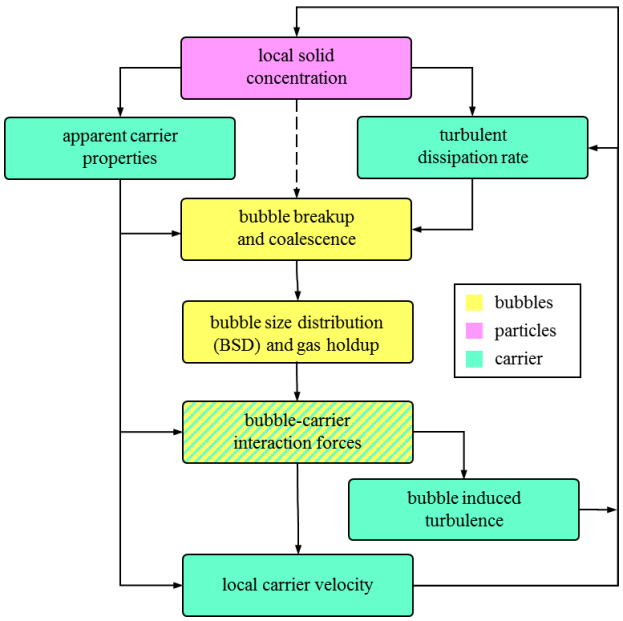

Fig. 1. Schematic of the effects in a slurry bubble column influencing BSD and gas holdup

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Simulating Direct Metal Laser Writing

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Direct laser writing (DLW) enables the creation of (sub-)millimeter sized polymer structures and allows feature sizes of less than a micrometer. Therefore, the polymerization of a photoresist is triggered locally via two-photon absorption within the focal volume of a laser beam. As in conventional laser additive manufacturing (LAM), the focus is moved along a path hereby filling the part to be produced.

Fields of use include photonics, rapid prototyping, microfluidics and biomimetics. However, often electrically conductive or metallic parts are desired. This requires additional steps to either coat the surface or obtain massive metallic parts, which for the latter restricts feasible geometries. Thus, direct laser writing of such structures is subject of ongoing research.

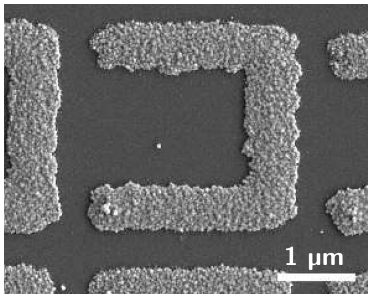

Fig. 1. Split-ring-resonators written by *AG Optische Technologien und Photonik* at TU Kaiserslautern via reduction of AgCl.

A downscaling of powder bed based LAM is prohibitive, particles that allow the above mentioned feature sizes are of approximately 10 nm size and can practically only be handled when suspended in liquids. Instead, one uses aqueous metal salt solutions as initial agent, while the laser triggers the precipitation of the pure metal. Other approaches [2] aim at confining metal particles in conventionally written polymer structures.

From the surface features and texture of first parts (Fig. 1), we conclude that the chemical reaction "instantly" (i.e. on time scales much smaller than the writing process itself) yields nano-particles that then aggregate on the substrate.

It remains difficult to produce structures which substantially protrude the substrate in vertical direction or consist of multiple layers. This is not only due to the sensitivity of the chemical process to various parameters (age of chemical agents etc.), but also to the free diffusion and a plume of particle laden solvent rising from the focus location. As countermeasure, an additional so called trapping laser may be used; when illuminated with light, nano particles will experience a force along the intensity gradient [3], which can be exploited to restrain particle diffusion and has been employed for similar purposes [4].

With our simulations we can determine, whether the observed plume has its root causes in buoyancy and could be eliminated with an additional trapping laser. We exclude the involved chemistry from our modeling and take a cloud of 10 nm-particles as starting point. On the liquid domain, we solve the Navier-Stokes equations employing the Boussinesq-approximation, and the heat equation. For the latter, source locations are identified with particle positions, as the solvent is transparent for the laser. Findings that describe strongly heterogeneous heating of particle arrays due to plasmonic effects [1] are not included into the modeling. The resulting buoyancy-driven velocity field is coupled to the particle motion, i.e. for the i^{th} particle, we integrate its trajectory

$$m^i \ddot{\vec{r}}^i = \sum_{j \neq i} \vec{F}^{ij} + \vec{F}^i_{\text{random}} + \vec{F}^i_{\text{liq}} + \vec{F}_{\text{trap}}, \qquad (1)$$

where $\vec{F}^{ij}$ is the particle-particle interaction force, $\vec{F}^i_{\text{liq}}$ denotes the force exerted by the surrounding liquid on the particle and $\vec{F}_{\text{random}}$ is the Brownian random force.

Future research is targeted at clustering mechanisms under these process conditions, in order to obtain a criterion to be used in computationally cheaper continuum-level simulations.

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SQMOM simulations of complex bubble size distributions

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Keywords—bubble column, CFD, moments, classes, bubble size distribution

In the chemical industry bubble columns, from a purely constructive point of view, seem like simple apparatus. The column, mainly a cylindrical tube with diameters up to 20 meters, itself has no moving parts and only internals like dispersers, baffles etc. Main purpose of these apparatuses is to enable absorption, a mass transfer between gas bubbles into the liquid phase. In addition, a chemical reaction in the liquid phase may be used to generate chemical products such as phenol. This mass transfer is one of the crucial limiting factors of the reaction, which depends primarily on the interfacial area between the phases and with that on the bubble size distribution (BSD). The main difficulty in apparatus design is the tradeoff between maximum interface area between the phases, which means very small bubble sizes and the maximum throughput, which favors larger bubbles instead. Today the design of even those seemingly simple apparatus is still done by using empirically gathered coefficients. [1]

An efficient computational fluid dynamics (CFD)-simulation would be a huge improvement for apparatus design. The simulation of larger apparatuses in CFD can be achieved with two different approaches, the Euler-Lagrange and the Euler-Euler method. The first approach is computationally more expensive and with that only feasible for smaller apparatuses. For larger production scale the common approaches in Euler-Euler simulations to calculate the change in the BSD are the moment based method (e.g. Quadrature Method of Moments) and the classes method. The moment-based methods are computational inexpensive, but have the drawback, that since the moments are the integral of the distribution only the total change in the whole distribution is calculated and with that the shape of the BSD is lost. For complex BSD, which are commonly found in bubble columns like bimodal distributions, this is not feasible. The class method allows tracking of the change in the shape of the BSD, but at a much higher computational cost and with the need of many classes. For an efficient apparatus design of modern bubble columns there is a need for a better method to calculate the BSD in CFD-simulations.

This is the reason for the in this work used Sectional Quadrature Method of Moments (SQMoM) [2], a combination of both approaches to overcome these drawbacks and enable the simulation of BSD with difficult shapes, like bimodal distributions. The change of the distribution moments are calculated section wise. This enables to track the shape of the distribution with fewer classes than a common classes method, due to the fact that the moments conserve more information about the BSD. The SQMoM is implemented into the OpenFOAM solver multiphaseEulerFoam, which allows the usage of multiple phases and with that classes in the CFD-simulation. To validate the SQMoM solver a laboratory scaled bubble column is investigated. Here the BSD is analyzed locally in different zones of the bubble column using a fully automated camera system, with an automated evaluation approach for the large amount of data. In addition, the velocity of the dispersed phase is measured using the camera system combined with an optical flow evaluation. The SQMoM simulation and the laboratory scale experiments show good agreement. The next step is to implement mass transfer and reactions into the solver to account for chemical reactions. The in this work implemented SQMoM solver enables a more detailed tracking of the bubble size distribution in multiphase flows at low computational cost, which enables a better description of chemical processes for example inside bubble columns.

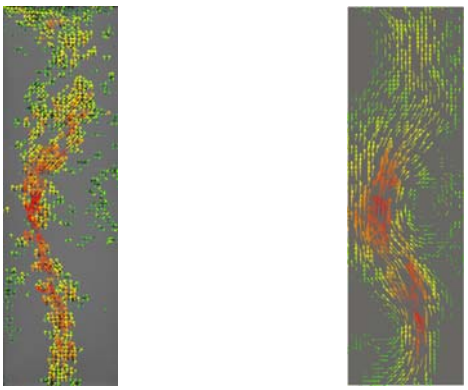

Fig 1: Optical flow analysis (Experiment left) vector plot (simulation right).

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A New Approach to Hierarchically Structured Zeolite ZSM-11

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***Abstract*—Hierarchically structured zeolite ZSM-11 was obtained by steam assisted crystallization of the zeolite in the presence of mesoporous silica spheres to induce the formation of macropores in the zeolite crystallites.**

Zeolites (crystalline microporous aluminium silicates) are widely used in ion exchange, adsorption or as versatile catalysts for many reactions in the refining and petrochemical industry. The first synthetic zeolites were introduced in the 1950s. While for many applications, the microporous nature of zeolites with pore sizes below 2 nm is very well suited and can create special catalytic effects, e.g., shape selective catalysis, the relatively narrow pores could be less advantageous if proceed very fast, i.e., where the reaction rate may become limited by mass transport effects, in particular through a slow diffusion of reactant or product molecules through the micropore system [1,2].

In this context, the possibilities to create larger pores, which could act as "highways" to the micropore system of zeolites, are currently intensively explored by many groups. Several methods to achieve hierarchially structured zeolites have been reported so far. In this contribution, we report on a new method to induce the formation of a hierarchically structured ZSM-11-type material containing both, the micropore system typical for zeolites and a system of larger meso- or even macropores which could serve as transport pores to and from the micropores [3].

Our method is based on formation of zeolite ZSM-11 by steam assisted crystallization. For this purpose, mesoporous silica spheres were converted into zeolitic macropores with the addition of an organic template.

Scanning electron microscopy (cf. Fig. 1) together with nitrogen adsorption studies (determination of pore size distribution) reveal that this method produces large mesopores inside a zeolite crystallite. The consequences of these additional large pores on the adsorptive and catalytic properties of zeolite ZSM-11 will be demonstrated with pertinent experimental data.

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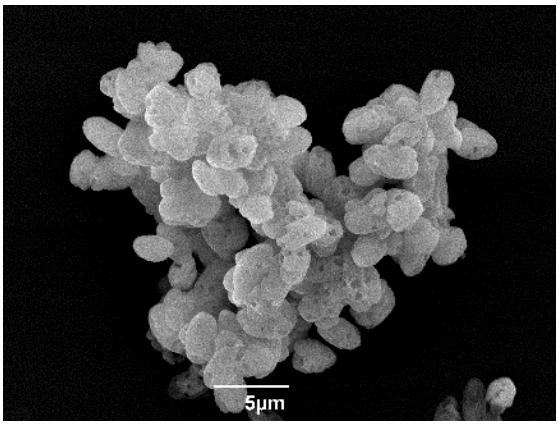

Fig. 1: Scanning electron micrograph of hierarchical ZSM-11 with a magnification of 3000.

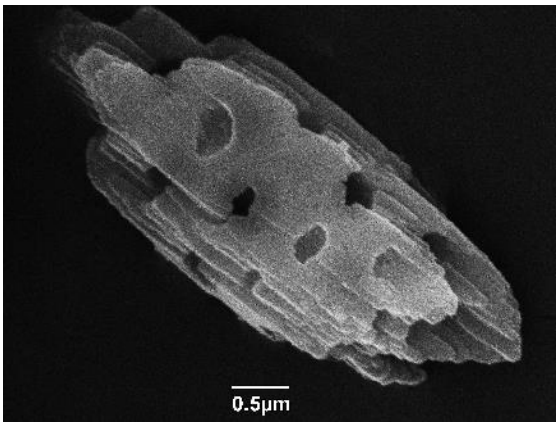

Fig. 2: Scanning electron micrograph of hierarchical ZSM-11 with a magnification of 10000.

Multinuclear Catalysts Inspired by Bioinorganic Chemistry

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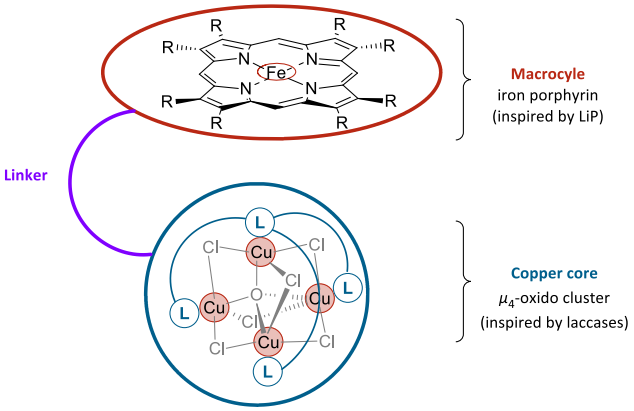
Keywords: catalysis, metal ions, enzymes, redox reactions

Catalysis is defined as the increase of a chemical reaction rate with the use of an additional substance, a so called catalyst, which is not consumed during the conversion of different substances and speeds up the reaction.[1]
We encounter catalysis in each day of our life. Our life-style is based on industrial products such as plastics that are produced via industrial catalysis. The alcoholic fermentation of sugar to alcohol proceeds via enzymatic catalysis in yeast. Also, the enzymatic browning of freshly cut fruits is based on the catalytic activation of oxygen by tyrosinase.
Many of these natural as well as industrial catalysts take advantage of the catalytic activity of metal ions, which are therefore incorporated in their active center. Organic frameworks can be used to tune their catalytic properties. Among such catalysts, multinuclear compounds are of special interest because first, they lead to a higher yield with regard to catalyst loading, and second, they enable an efficient electron transfer of multiple electrons at once, which is required for complex redox reactions. The latter concept is used by nature in various multinuclear metalloenzymes such as laccases, e.g., that obtain a tetranuclear copper center in their active site.

Figure **1**: White rot fungi that enzymatically degrade old wood.

Due to the combination of four copper ions in their active center they are able to catalyze four electron redox reactions such as water oxidation. Also, together with lignin peroxidases (LiP), they play an important role in lignin formation as well as degradation (Figure **1**). Lignin is one of the largest natural biopolymers with plants usually containing around 10-30 % of lignin. It is responsible for the rigidity of plants, protects cellulose and hemicellulose against hydrolysis and is rather hard to degenerate.[2] It is one of the largest renewable resources and a waste component in the paper industry which is mostly incinerated due to a lack of possible applications and industrial degeneration methods. Therefore, the catalytic degradation of lignin to small organic compounds that can be used in industrial processes is highly desirable.
Inspired by these biocatalysts we seek to combine the active centers of the two enzymes involved in the natural degradation, laccase and LiP, in a model system to create a similarly efficient reactivity. Tetranuclear copper clusters of the type $[Cu_4OX_6L_4]$ (X = halogen, L = ligand or X) are useful catalytic systems and are able to activate H_2O_2 for subsequent substrate oxidation.[3,4] Thus, such clusters are to be used as a model system for laccases. They are to be combined with iron porphyrin complexes, known model systems for peroxidases. The overall catalyst design is depicted schematically in Scheme **1**. In this presentation, the syntheses of the copper cluster and the encapsulating ligand that is used as organic framework to tune the catalytic properties are presented.



Scheme **1**: Schematic representation of the multinuclear catalyst

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Individual Atoms in a Quantum Bath

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***Abstract*—We report on the interfacing of a Bose-Einstein condensate (BEC) with individual neutral impurity atoms. We show, that the impurity atoms can be used as a probe to extract information about the BEC. Our results pave the way for the local probing and manipulation of complex quantum systems.**

***Index Terms*—spin-impurities, quantum physics, ultracold quantum gases, model system, spin-exchange**

I. Introduction

The understanding of quantum mechanics has revolutionized technology, enabling applications such as the vast use of semiconductors for information technology to the control and detection of quantum mechanical angular momentum by nuclear magnetic resonance (NMR) in medicine [1]. For most of these devices, constructed from bulk material, the physical description is founded on macroscopic models rather than a microscopic, single-atom based understanding of the system. Nevertheless, this understanding is necessary, when approaching long-standing technological challenges such as the realization of high temperature superconductivity [2].

Ultracold quantum gases are excellent testbeds to engineer and study complex quantum systems at such a fundamental level: Since the behavior of ultracold matter at temperatures just above absolute zero (typically 100 nK) is dominated by quantum mechanics and the interaction properties between atoms at these temperatures are well understood, it is possible to theoretically model and experimentally control the behavior of quantum systems. A quantum physicist's equivalent of a *Drosophila melanogaster* are Bose-Einstein condensates - a quantum effect, where thousands of particles accumulate into exactly the same quantum mechanical wavefunction - a phenomenon that cannot be explained by the laws of classical physics and, once prepared and tweaked at will, can be studied under a microscope.

II. Results

In our experiment, we have achieved to interface a Bose-Einstein condensate with neutral atoms of a different atomic species, so-called impurities, for the first time [3]. The knowledge of microscopic interaction properties between atoms of the Bose-Einstein condensate and the impurity atoms enables us to extract information about the condensate from measuring the impurity atoms only. This makes each impurity a single atom sensor, e.g. a single-atom thermometer [4]. A particular advantage of our combination of Bose-Einstein condensate and individual impurity atoms is that the angular momentum of each impurity atom is a degree of freedom: It can be prepared and read out during the interaction with the Bose-Einstein condensate. This enables us to study a unique scenario: By observing the exchange of angular momenta between condensate atoms and impurities, we can count individual collisional events of the atoms involved in the interaction. Besides the intriguing beauty of this collision sensing ability for quantum physicists, the detection collision by collision allows inferring the quantum state of the condensate, demonstrating the application of single-atom aided sensing of a quantum many-body system.

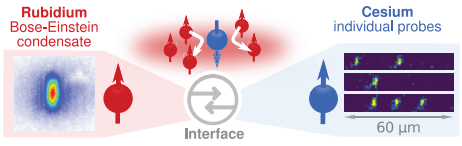

Fig. 1. **Experiment overview**. Rubidium (Rb) Bose-Einstein condensate (red) and individual Cesium (Cs) atom probes (blue) are prepared independently. Interaction is initialized by transporting Cs into the Rb bath. After the interaction, position and state of Cs is read out (right).

III. Outlook

We have shown that the interfacing of a Bose-Einstein condensate with individual neutral atoms of a different atomic species allows for the local probing and manipulation of a quantum system. In the future, we will address fundamental questions of quantum physics such as the thermalization of the Bose-Einstein condensate, after being driven away from its thermal equilibrium. Secondly, the impurities can not only be used as local sensors, but as local and controllable disrupters of the quantum bath. By such a doping, the behavior of the complete system can be strongly modified as known from the effect of doping in semiconductor technology - however in the limit of a single impurity.

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Crack growth simulation for materials with anisotropic fracture resistance using a phase field model

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***Abstract*—The integration of anisotorpic material behavior in approaches for crack growth simulations is required for materials showing a directionality of the fracture resistance. A phase field (PF) model for brittle fracture is enhanced in order to account for this behavior. Accurate simulation results are obtained.**

***Index Terms*—Phase field, Fracture, Directional fracture resistance, Finite elements**

I. Introduction

Manufacturing processes like e.g. hot rolling or extruding can cause a directional fracture resistance of materials. The directionality is a consequence of an elongated micro structure, as illustrated in Fig. 1, which leads to favorable directions for crack extension. While elastic anisotropy effects the reaction of a material to a certain load, anisotropy of the fracture resistance influences the direction of crack extension. Two

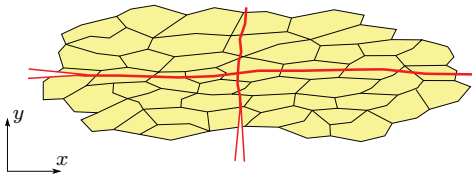

Fig. 1. Schematic illustraton of crack paths.

crack paths resulting from loading in different spatial directions are indicated in Fig. 1. The horizontal crack requires less energy per crack length than the vertical crack, since less grain boundaries have to be passed, which in terms of the fracture resistance can be expressed with $K^x_{th} < K^y_{th}$.

One approach providing several benefits for the numerical simulation of crack paths is the phase field method. To approximate sharp cracks an additional field variable $s(x,t)$ is introduced to represent cracks as continuous transition between 1 (intact material) and 0 (broken material). Within this work a phase field fracture model is enhanced in order to capture the effect of a directional fracture resistance.

We greatfully acknowledge funding from DFG through IRTG 2057.

II. PF Model for Anisotropic Crack Growth

The basic phase field fracture model used for this work was proposed by Kuhn and Müller (see [1]). The core of this model is the formulation of the total internal energy:

$$E = \int_V U(\nabla \boldsymbol{u}, s)\,\mathrm{d}V + \int_V \Gamma(s, \nabla s)\,\mathrm{d}V, \qquad (1)$$

of a body under certain displacement and traction boundary conditions, which may also contain cracks. In (1) U is the linear elastic strain energy density and Γ is the crack energy density, which depends on the phase field variable $s(\boldsymbol{x},t)$ and its spacial gradient. The evolution equation for s is found by a variational principle, which is in line with Griffith's theory. To account for an anisotropic behavior regarding the crack extension, the gradient ∇s is weighted by appropriate factors Φ_{ij}, which depend on the orientation of the material and the intensity of the anisotropy in the following denoted by θ and α, respectively.

III. Numerical Example

The coupled nonlinear system of equations is solved by means of the finite element method. The numerical example shown in Fig. 2 is a plate with a sharp notch under quasi static mode I loading. As expected the crack growth in horizontal direction for the isotropic case. Using parameters accounting for a material with anisotropic fracture resistance the crack extends under a deflection angle φ w.r.t the horizontal axis.

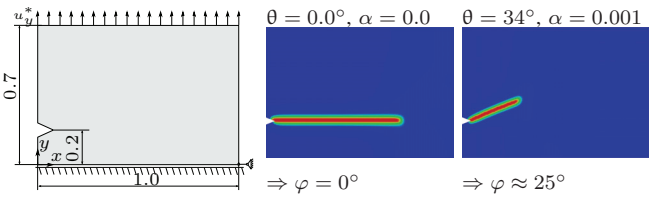

Fig. 2. Numerical example: load case and contour plots of the crack field.

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Development of a new self-sealing click-connection-system to transmit shear and normal forces

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Keywords—click-connection-system, Snap-Fit, joining force

I. ABSTRACT

Self-sealing click-connection-systems such as the so-called Snap-Fit-Connection [1] are used especially in mechanical engineering. A widespread form of usage of these Snap-Fit joints is the so-called Snap-fit beam connection. During the joining procedure of two components a cantilever as part of one component is deflected and snaps back into an opening or groove at the other component into its initial position. Following this principle a cylindrical version of the Snap-Fit-Connection, the so-called click-dowel has been developed as part of a cooperative research project. The objective was to introduce this self-sealing connection type to civil engineering.

The click-dowel consists of a steel dowel in the range of 12 to 20 millimeters in diameter. On one end the steel dowel has a groove and chamfered head as shown in Figure 1. The associated joining partner is a steel plate with cut out steel stripes (see Figure 1).

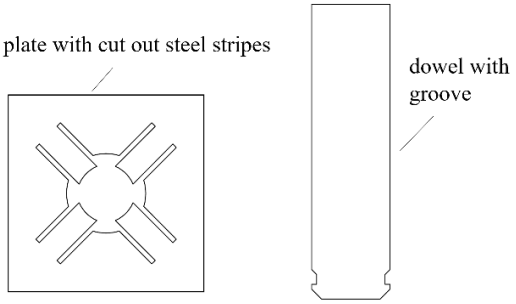

Fig. 1. Geometry of the click-dowel

During the joining procedure, plastic deformations in the steel stripes arise until the stripes flip back into the groove of the dowel. In the final state the steel stripes activate resistance against the pull out of the dowel, when lifting forces appear. Forces in transverse direction will be transferred as a shear-bearing connection between dowel and steel plate.

By means of FE-Simulations with the program Abaqus different geometries have been analyzed with regard to their mating force and the resistance against pull out and shearing loads of the dowel [2 and 3]. The geometry shown in Figure 1 offers a high resistance against the load of pull out and shearing with a low joining force. The following picture shows the results of the FE-Simulation with the above mentioned geometry.

In Figure 2 the Mises-stresses in the steel plate are shown with the corresponding force at the respective state. The joining force in state 1 with 0.2 kN is by a factor of 7 lower than the bearing capacity with 1.4 kN in state 3.

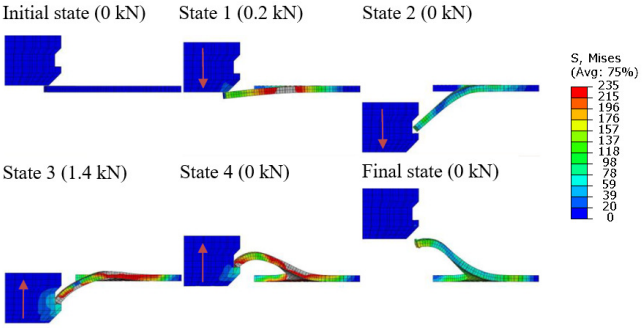

Fig. 2. Simulation results of the click-dowel geometry

In first tests these results could be verified. In a next step a cover plate was developed to embed the click-dowel connection into concrete as a possible application in civil engineering. Due to the set up of this cover plate the resistance against shearing and pull out could be improved [4]. Furthermore an additional load application construction at the cover plate was possible and the loads could be transferred into the surrounding concrete.

The tests and the comparative FE-simulations have shown that the self-sealing click-connection-system is also applicable with materials normally used in civil engineering.

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Adjustable droplet generation through a variable dispersion unit

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Keywords — separator, liquid-liquid, variable apertures, coalescence and break-up, measurement technique

Dispersions plays an important role in many areas of process technology, such as the chemical and pharmaceutical industries, but also in the petroleum industry. They are ususaly generated by mixing two immiscible liquids together in e.g. a stirred tank. Another possibility is the use of static mixers which can be integrated into a pipeline system.

There are different types of static mixers. These components are rather cheap and very effective and give no maintenance problems.

The alternative static dispersion unit used consists of two variable apertures with a variable number of holes (2 x 5, etc.). The 1.5 mm holes were made with a laser. The dispersion unit is a part of a phase separation test rig for the design and scale up of gravitational settlers.

The droplet size distribution in the tube after the dispersion unit is recorded and evaluated experimentally with the Sauter mean diameter (d_{32}) according to the transmitted light principle [1, 2]. The experiments are carried out with 50 mmol/L NaCl in deionized water as the continuous phase and paraffin oil (ρ = 823 kg/m³, μ = 12.9 mm²/s) as the dispersed phase.

In order to gain knowledge of the various influencing factors on the individual droplet processes, the experiments were carried out with different volume flows with a constant phase fraction of the disperse phase with 10 %. To monitor the volume flow and the density of the immiscible liquids a Coriolis meter is used.

The differential pressure at the dispersion unit is recorded parallel to the drop measurement. From the results of the drop measurements, a correlation based on the volumetric power relative to the volume between the differential pressure measurements could be obtained (P / Vol). This simple correlation has already been confirmed by several authors [3, 4].

The correlation results in $d_{32} = 160 \cdot \left(\frac{P}{Vol}\right)^{-0.4}$ and can reproduce the measured drop classes with increasing power density very well.

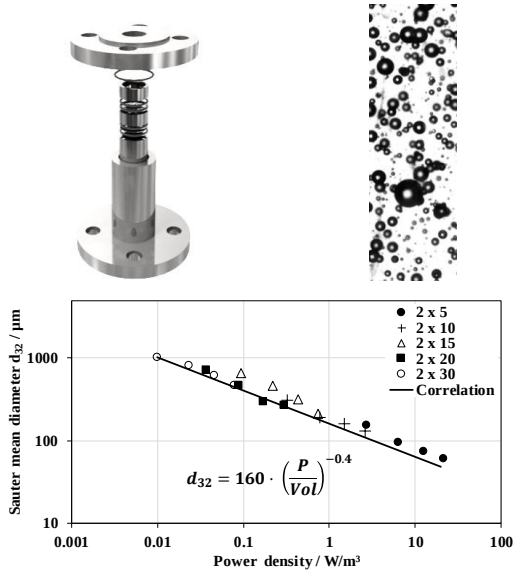

Fig.: Illustration of the dispersion unit, drop measurement and results

Based on the results of the Sauter mean diameter, CFD simulations can be validated for a detailed description of the dispersion unit.

CFD methods can be used to classify the flow field, the influence of the variable apertures and the dependency of the phase fraction. A prediction of the drop sizes of a dispersion unit is thus possible.

For the design of gravitational separators, the description and detection of the dispersion is an essential part. The droplet sizes are relevant to calculate the sedimentation velocity inside the separator.

Furthermore, the dispersion layer can be estimated in a liquid-liquid gravity separator. For small drops rather a dispersion band is form. Larger drops tend to form a dispersion wedge.

The obtained results of the contribution are used for the further development of models based on CFD simulations for the design of gravity separators. [5]

Further experiments with variable number of holes and phase fraction for the generation of the dispersion are carried out on a DN150 separator.

This contribution discusses the results of drop measurements. Validation of measurements and simulations is proposed and improvements of CFD modeling is presented.

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Arificial Neural Network Specific Memory Systems

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In recent years, a new range of smart applications like autonomous driving, speech recognition, voice assistant (e.g. Google Home), advanced gaming (Virtual Reality) etc. is emerging and showcasing an uprise trend. Due to the intense research and developments in the field of *Artificial Neural Network* (ANN) or *Machine Learning*, inspired from brain models, computers are capable making tremendous amount of intelligent decisions required by such applications. For this reason, ANNs are extensively used by tech giants like Google, Facebook, Microsoft, Amazon etc. for various background data processing, thus resulting in improved overall user experience. A simplest example of ANN application is, when an image is uploaded to Facebook, there is an automatic face detection and tag suggestion. All the above are only the stepping stone - in coming years, ANN will be an integral part of almost all application domains. As quoted by Google CEO Sundar Pichai *"Machine learning is a core, transformative way by which we're rethinking everything we're doing"*.

ANNs are implemented on various computing systems like general purpose systems (e.g. CPU) or Graphic Processing Units (GPUs) or custom Hardware (ASICs). One common requirement of any of these systems is very high main memory density and bandwidth. This is due to the fact that ANNs are highly parallel in nature and data intensive. One such ANN called *Bayesian Confidence Neural Network* (BCPNN) requires a storage of 30 TB and main memory bandwidth of 112 TB/s to emulate a human scale brain. On the other hand, Google built an ANN employing 16,000 computers designed to simulate human cognitive processes. These are the upper limits, when the whole computing system is partitioned into smaller units of computation to exploit the parallelism, ANNs require an average density of 4-7 GB and bandwidth of 100-200 GB/s. This high numbers are addressed by the new emerging 3D main memory devices like *Hybrid Memory Cube* (HMC) and *High Bandwidth Memory* (HBM) at the cost of power overhead. Irrespective of the type of memory (3D or traditional 2D DDR/GDDR DRAM), many recent study's have showcased the memory bottleneck, high energy consumption and extensive area utilization. Figure 1 shows the energy consumption comparison against other processing units [3]. The authors of [2] demonstrated that the main memory consumed the highest available area and power consumption (40% and 37% respectively). The work of [1] showed that 80% of total energy consumption was due to memory. Our internal implementation of BCPNN on a GPU (NVIDIA Tesla k80) system resulted in a DRAM energy consumption of 60% out of the total. The reasons for such high energy consumption by main memory are due to high operating frequency, non optimization for parallel applications (limited channels) and improper arrangement of data inside the memory that results in row-misses (closing of present DRAM row and opening other) causing DRAM power spike. Additionally, data movement in most cases are more expensive than the computation [3]. All these motivate to research on memory systems (Memory controller and architecture) customized for such parallel, data intensive applications in terms of energy and bandwidth.

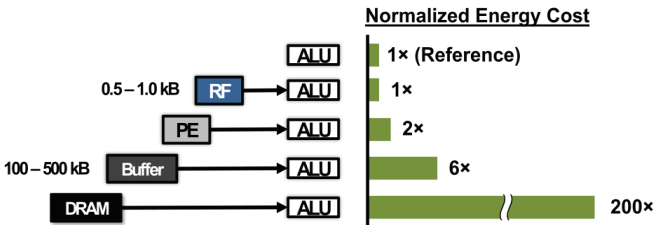

Fig. 1. Energy consumption of memory vs computation [3]

Researchers address the challenges imposed by the memory from the ANN algorithm or computational side like precision reduction, reducing the size of the data, exploiting the sparsity, changing the ANN algorithm etc.. All these solutions reduce the accuracy of the ANN model or are not effective for all cases. In this research, we focus on the design and implementation of memory systems applicable for data intensive applications. Our work[1] could be bifurcated into two parts. Firstly, exploring the huge DRAM design space and designing a 32 channel 3D DRAM optimized for BCPNN to address the energy vs bandwidth trade-off. Secondly, designing the memory controller that rearranges the data such that there are reduced row-misses, there by further improving bandwidth and energy consumption. Our goal is to extend this work to all ANNs. Our alternative solution to address the aforementioned issues are designing the *In-memory computing* systems, where the computational units are inside the DRAM to lower the data transfer cost and increase the data transfer rate.

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Building Planets in a Sandbox

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***Abstract*—In the formation process of planets, small grains of dust stick together to form large agglomerates with sizes up to metres. Other objects that can be formed are so called chondrites, meteorites consisting of glassy spheres (called chondrules) with sizes of millimetres and above, embedded in a "dough" of smaller grains of dust. In this work, simulations of collisions of chondrules with small rims of dust are performed. Bouncing probabilities are evaluated depending on velocity, chondrule size and rim thickness. This is essential to understand the physics of the formation of many kinds of objects in the early stages of the Solar System**

I. Introduction

The formation of chondrites is not yet sufficiently understood e.g. one open question is: Expected collision velocities in accretion disks are larger, than the maximum velocity that still allows sticking of chondrules (For detailed information about accretion disks, cf. [3] and [4]). Presumably, chondrules with dust layers are more prone to sticking. For discussion of dust rims, cf. [1]. In this work, chondrules with dust layers are constructed, boosted towards each other and statistical evaluation of many collisions is performed. Previous studies on this have been performed in [2].

II. Method

The 4 possible ways of relative motion for the grains are normal motion, rolling, sliding and twisting and are all associated with a frictional force or torque, cf. [5]; additionally, the normal force has elastic and adhesive components, cf. [5]. The forces and torques are implemented in LIGGGHTS, a Molecular Dynamics code for granular matter, cf. [5]. Based on the forces, trajectories for all particles can then be calculated numerically. The dust covered chondrules are described by positions, velocities and diameters of all the grains. To produce a starting conformation, we place the chondrule at the origin, then randomly attach grains to the chondrule. Two clusters can then be boosted towards each other.

Many collision velocities, rim thicknesses and chonrule radii are tested. Collision outcame is either bouncing or sticking. For any set of parameters, the bouncing probability is calculated.

Figure 1 shows a snapshot at $t = 14.5\,\mu s$.

III. Results

Example results are depicted in fig. 2, which shows: Lower rim thickness means higher bouncing probability. Overall one finds: Higher velocities, higher radii and smaller rims all lead to higher bouncing probabilities.

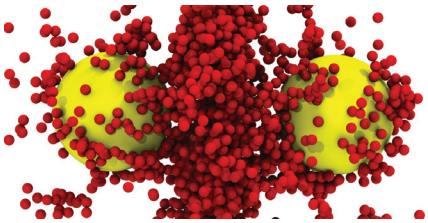

Fig. 1. Collision snapshot at $t = 14.5\,\mu s$. yellow: chondrules, red: dust grains

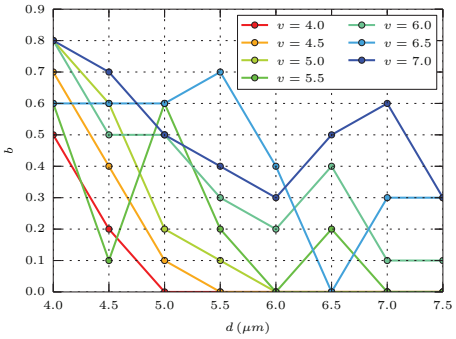

Fig. 2. Bouncing probability vs rim thickness for a set of collision velocities (m/s).

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Faster to the Goal: Ultrasonic Fatigue of Polymer Composites

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***Abstract*— To utilize the full mechanical potential of carbon fibre reinforced polymers for cyclically loaded lightweight applications, it is mandatory to understand the fatigue behavior and the corresponding failure mechanisms, even at very high numbers of cycles. Nevertheless, while fiber reinforced polymer composites (FRP) are increasingly used in very high cycle fatigue (VHCF) loaded primary structures, there is still a lack of knowledge on their fatigue behavior and the underlying damage mechanisms. Facing these issues, there is a limiting factor regarding conventional fatigue testing concepts, as these are not capable of performing very high cycles (N > 100 millions) in an economic reasonable period. Therefore, a novel ultrasonic fatigue testing facility for cyclic three-point bending of FRP was developed, which is schematically presented in Fig.1. (left). However, obtaining critical very high cycle fatigue data of polymer composites by using elevated testing frequencies of 20 kHz is especially challenging with respect to the viscoelastic nature of polymers. Overcritical heating due to viscoelastic damping and interfacial friction is therefore mitigated by resonant-based testing as well as pulse-pause control, resulting in an effective testing frequency of approx. 1 kHz. Furthermore, the monitoring of suitable fatigue testing conditions is realized by infrared thermography, high-resolution force measurements and cyclic displacement control via Laser Doppler vibrometry. Initially, the VHCF characteristics of two composite material systems with an aerospace background are analyzed. The induced VHCF damage of a carbon fiber 2/2 twill fabric reinforced polyphenylene sulfide with orthotropic layup, see Fig. 1. (middle), as well as a carbon fiber 4-H satin fabric reinforced epoxy resin with quasi-isotropic layup, see Fig.1. right, is characterized by light optical and scanning electron microscopy during interruptions of fatigue experiments at constant amplitudes. In summary of the lifetime-oriented results, a significant decrease of the bearable stress amplitudes of CF PPS and CF EP in the range between 10^6 to 10^9 loading cycles was observed. Hence, a fatigue shear strength at 10^9 cycles of $\tau_{a,\,13,\,PPS}$ = 4.2 MPa and $\tau_{a,\,13,\,EP}$ = 15.8 MPa was identified. Based on phenomenological investigations, different fatigue damage characteristics induced by composite-specific interface, matrix and layup properties could be determined. Frequency influence investigations are part of current research and will be addressed within the talk.**

Keywords*— *ultrasonic fatigue testing, very high cycle fatigue of composites, damage mechanisms and mechanics

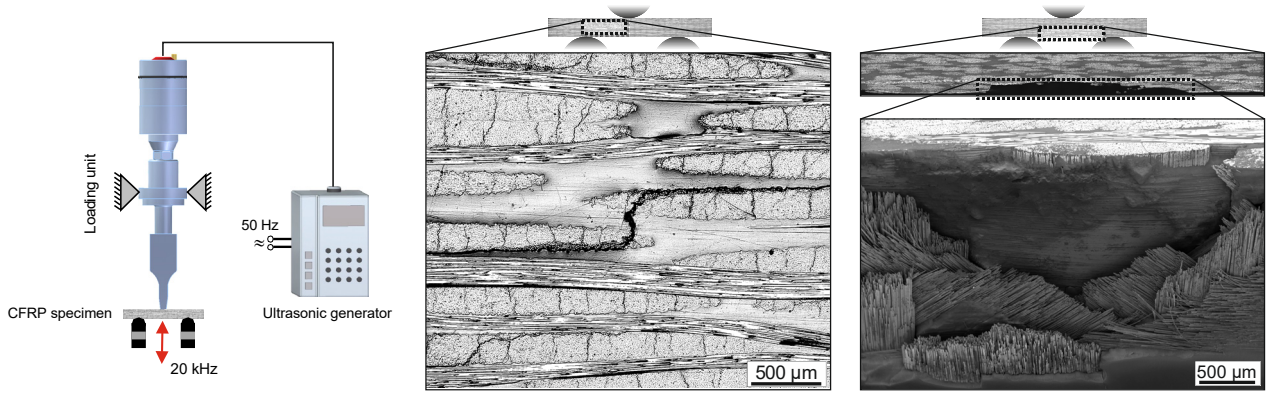

Fig. 1. Schematic experimental setup (left); microscopic VHCF damage of: CF-PPS (middle) and CF-EP (right)

An Optimization Tool for the Transformation of Wastewater Systems

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A software-based optimization and decision support system can enable the systematic analysis and multi-criteria evaluation of future scenarios and options for action. A problem-oriented visualisation with intuitive recording of results is particularly important for achieving a high transparency of results and a good understanding among the model application's target groups.

Keywords - Optimization, transformation processes, visualization, decentralized water technologies

I. INTRODUCTION

Future developments like demographic and climate change as well as changes in the energy sector have an impact on the long-established municipal infrastructures of water supply, urban drainage and wastewater disposal systems. Innovative sanitation systems in combination with source-based stormwater management measures enable the transformation of existing systems to new decentralized concepts of wastewater disposal. The challenge is to assess these new solutions and combinations of adaptation measures and to estimate the effects on the existing infrastructure.

II. MATERIAL AND METHODS

In the BMBF (German Federal Ministry of Education and Research) – research project SinOptiKom an innovative software-based optimization and decision support system for long-term transformations of wastewater infrastructure has been developed. The overall structure of the software based optimization system consists of and integrates three components. These components are mainly a pre-processing tool with a database and a scenario manager, a mathematical optimization model and an interpretation tool [1,2]. In order to determine an optimized transformation strategy of urban drainage systems, a mathematical model based on integer linear programming (ILP) is used. Input data and generated results (e.g., geodata, demographic data or adaptation measures) are stored in a knowledge and evaluation data base [3]. The developed scenario-manager enables the generation of comprehensive scenarios by combining different drivers. The system uses user-specific evaluation criteria and visualizes transformation processes including their effects and time-dependent costs.

III. RESULTS AND DISCUSSIONS

The optimization system has been applied to two individual municipalities for a time period of 50 years (Fig. 1). The model application demonstrates that "optimal decisions" are significantly influenced by the level of importance given to the single evaluation criteria. Decentralised measures for the separation of material flow with separated blackwater and grey water treatment and the establishment of decentralised wetlands are selected in cases in which both flexibility and the conservation of resources take on considerable weight. A standard level of importance given to cost, on the other hand, leads to the preservation of centralised systems. Decentralised measures for the separation of material flow with separated blackwater and grey water treatment and the establishment of decentralised wetlands are selected in cases in which both flexibility and the conservation of resources take on considerable weight. A standard level of importance given to cost, on the other hand, leads to the preservation of centralised systems.

Fig. 1. Display in demonstration model: Existing sewers in selected residential areas in the year 2060.

IV. CONCLUSIONS

The presented method and general adaptation strategies can be applied to settlement areas facing the same challenges. The demonstration and visualization of different solutions for an expedient future transformation of wastewater infrastructure is a great benefit for planners, engineers and political decision-makers.

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Model Based Inspection Planning for Complex Surfaces

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***Abstract*—Reliability of a system declines with a number of required human interactions. When it comes to planning of acquisition setups for visual inspection systems, the process heavily relies on the experience of the designer. Such an ad hoc approach gets more and more problematic, the more complex the surface becomes. The number of different ways to acquire images grows rapidly, and it is hard to confirm if the object was inspected completely, let alone optimally, making the image acquisition for inspection purposes a hard problem to solve. In order to solve it, we seek to automatize the planning step by using a CAD model of the inspected object and computing the acquisition setup based on this object.**

Keywords—surface inspection, inspection planning, complex surface, geometric modeling

I. Introduction

Quality of every single product around us was at some point inspected. Have you ever stopped to wander how it was done? What about the products which can make a difference between life and death, like car brakes, airplane blisks or pacemakers? You surely want to be sure the quality inspection process was done thoroughly. In a perfect world, each product is given an unlimited amount of undivided attention to make sure it meets all the standards. The given attention is always the same and the defect detection results are obtained based on constant, clearly defined criteria. Unfortunately, the world is far from perfect. Existing systems work well when custom developed for a given problem but often require a significant amount of human input. Hence, they are hard to modify or generalize, as each new inspection problem comes with a very specific set of parameters and restrictions, mostly based on the geometrical and material properties of the inspected object.

Reliability of a quality assurance system is greatly influenced by the number of manual interactions and human judgements it requires. This is not due to humans being incapable of making a decision, but because the human decision process is hard to quantify and is highly susceptible to both intrinsic and extrinsic influence. Our general work aims at setting up a visual inspection system development pipeline which will shift the human interaction to a higher abstraction level. We are developing a simulation framework used for quantification and optimization of the overall planning process. The framework will be capable of producing a valid inspection plan, based on inputted set of parameters and restrictions. This idea can be applied to various sensors and system configurations, here we focus on visual surface inspection.

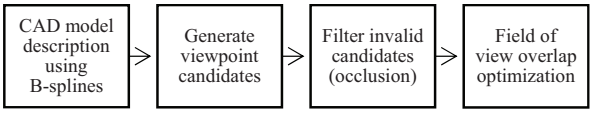

Figure 1 Selection of optimal viewpoints based on field of view overlap

II. Inspection Viewpoint Selection

Overall inspection system performance is influenced by four factors: object, acquisition equipment, algorithms, and timeframe. This contribution focuses on the visual coverage of the object's geometry regardless of illumination. The method shown in Figure 1 approximates the CAD model analytically in order to suggest appropriate viewpoints - points on the surface of the model, at which the camera should be pointing at. A B-spline model is created by subdividing the object into patches with disk-like topology and approximating them with B-spline surfaces via least squares fitting. Once the B-spline model is obtained, for every patch of the model local curvature is estimated, and viewpoint candidates are created by a new scheme inspired by analysis-driven refinement [1] using curvature as refinement criterion. The result of our novel approach is a set of points being dense in high-curvature and sparse in low-curvature regions.

Figure 2 Viewpoint candidates

III. Conclusion

With this work a new inspection planning method is introduced, which uses analytical representation of the model for the identification of surface areas needing higher sampling density. The results confirm the possibility to automatize the acquisition setup design and to thus reduce the number of critical decisions an operator is required to make.

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Improved Channel Coding with Manipulated Matrices

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In today's world, being connected to the internet is an important part of everybody's life. Without noting it explicitly, the amount of data shared is constantly increasing. For example, according to [3], there are around 66,000 Google searches per second, around 2,700,000 emails are sent per second, and overall, around 55 TB of data are shared via the internet in one second. To deal with this large amount of data, communication needs to be fast and reliable. During wireless data transmission, e.g. while streaming a video on the smartphone, data can become perturbed due to weather conditions, obstacles, or interfering signals. Therefore, it is important to make data robust to disturbances by adding redundancy to the sent information. The redundancy is appended by an encoder at the transmitter in such a way, that small disturbances which occur during transmission lead to an invalid message at the receiver. The decoder's task is to correct these errors by finding a valid message close to the received invalid one.

A typical communications system is depicted in Figure 1. To make the message u robust to noise during transmission, the encoder maps u to a codeword c by multiplying it with a so-called *Generator Matrix* G, so $u \cdot G = c$. The set of all codewords, called *Code*, can be computed from this generator matrix. Upon receiving the channel output $y = c + \eta$, where η is some noise vector, the task of the decoder is to reconstruct the sent message. The decoding is successful, if the decoder output $\hat{u}$ matches u.

The task of channel coding is twofold. On the one hand, a "good" code, defined by the generator matrix, has to be constructed. This task is referred to as code design. On the other hand, the redundant information has to be used in a clever way to detect and correct as many transmission errors as possible. This task is referred to as decoder design.

Standards like IEEE 802.11 for WLAN already determine the used code, but not the used decoding algorithm. Therefore, we decided to research for improvements in decoder design.

There are mathematical concepts like *Maximum-Likelihood (ML) Decoding* [2], which give an optimal result to the decoding problem. However, they are too complex to use them in practice. In fact, we want our decoder to neither slow down applications, nor to take too much space, or to require too much power, which would lower the battery lifetime. These are hard requirements on the decoder, namely throughput, area and power, so the goal is to maximize the error-correcting performance under these constraints.

Therefore, heuristic decoders are used in applications. They

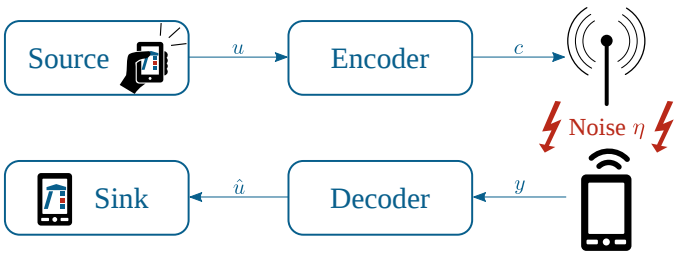

Figure 1: Model of a Communications System

fulfill the above mentioned requirements, but need improvements to be able to compete with the ML decoder regarding error-correcting performance. Many heuristic decoding algorithms use a so-called *Parity-Check Matrix* H for which $H \cdot c = 0$ for every valid codeword c, so the code equals the kernel of H. This matrix defines a bipartite graph, on which iterative message-passing algorithms work.

Changing the parity-check matrix in a way that preserves its kernel modifies the underlying bipartite graph, but does not change the code. Thus, we can improve or worsen the error-correcting performance of heuristic decoding algorithms by "manipulating" the parity-check matrix H in a kernel-preserving way [1], e.g. with elementary row operations, that are also used in Gaussian elimination. Unlike the ML decoder, that finds the most probable valid codeword from the received message, regardless of the code's matrix representation, the performance of heuristic iterative decoders heavily relies on the representation of the code's H matrix. Our goal is to find good parity-check matrices for different decoding algorithms, which is a challenging and truly interdisciplinary task, combining *linear algebra*, *graph theory* and *integer optimization* – always keeping in mind the physical requirements on throughput, area and power coming from the application in *electrical engineering*.

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Disproportionation of Saturated Hydrocarbons over Heterogeneous Bifunctional Catalysts

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Fossil resources are the foundation of the familiar modern society and the associated standards of living that seem natural to us. While coal and natural gases are primarily used for the production of electricity, oil is the main feedstock for the production of fuels for vehicles and aircrafts in the petroleum industry. At the same time, certain crude oil fractions are used as raw materials for fine chemicals such as plastics, paints, fertilizers and hygiene articles.

Accompanied by competitive market pressure and country-specific availability of certain raw materials, a large variety of different conversion technologies have been developed within the last century. The development of the "disproportionation of alkanes" at the beginning of the 1970s enabled to control the chain length of light hydrocarbons and hence increase the economic value of less demanded alkanes [1]. The "molecular redistribution" can be seen as one of the most promising processes in this perspective [2]. In chemical industry this application is known as "Chevron process". Within this process, saturated hydrocarbons are varied in their chain length in a three-step reaction (dehydration - metathesis - hydration) at 63 - 138 bar and 340 – 430 °C (see figure 1). The catalyst consists of platinum sites located on Al_2O_3 and tungsten sites located on SiO_2.

One conceivable application for this conversion process is the issue of gas flaring and venting of natural gases which, despite intensive international efforts, is still an enormous unwanted side effect of crude oil production. Beside the pure economical loss by wasting valuable hydrocarbons, the critical effect on the environment and on human health is a matter, which counts even more. In order to deal with this challenge it could be envisaged to convert parts of the otherwise flared gas into longer chained hydrocarbons which could be, due to their higher boiling points, reintroduced into the fluid crude oil stream.

In this lecture, we will give an overview over the introduced conversion process. Further, we will present some pertinent results of our own research on catalyst optimization and the possible reaction mechanism, which were obtained in a recently completed bench-type apparatus with a fixed-bed flow-type reactor working at pressures up to 10 MPa (100 bar).

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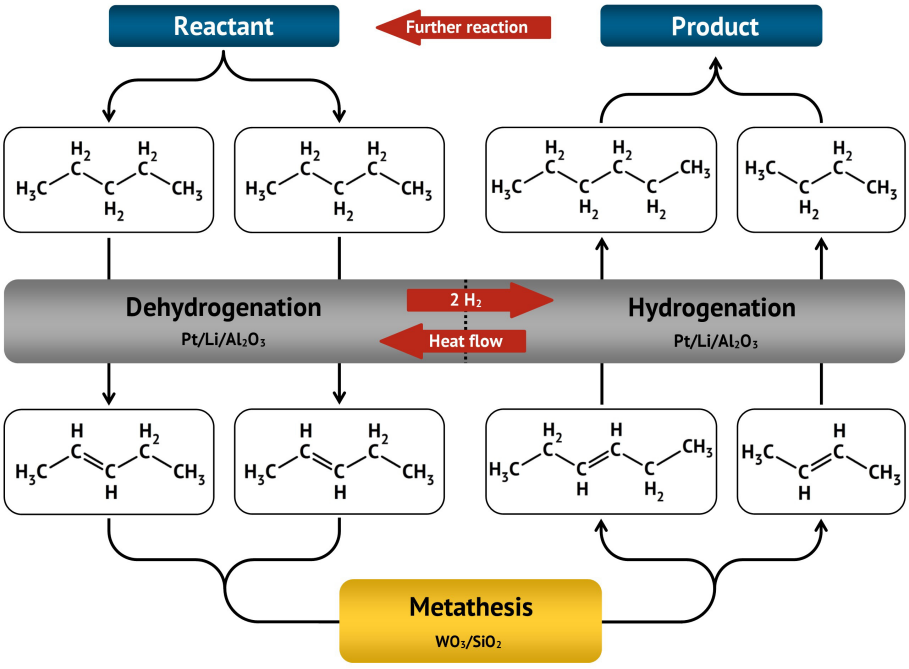

Fig. 1. Reaction scheme of the molecular redistribution of n-pentane.

Numerical Analysis of a Metal-Free Pedicle Screw System for the Use in Human Lumbar Spine

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***Abstract*—**Since life expectancy steadily increases, surgeries become more and more important to insure quality of life. Due to the aging population, the number of surgeries steadily increases. Spinal and back disorders are common problems of older people. But also the younger population suffers from back pain. Reasons can be natural bone aging which is difficult to prevent but also just office work or bad attitude.

Fig. 1. Metallic pedicle screw system

Surgery is mostly the last option to prevent patients from pain and to correct spine misalignments. Pedicle screw systems are widely used in spinal fusion surgery to fix certain parts of the human spine. The motion of two vertebrae can be restricted so that bone fusion occurs and pain is eased. The standard material for pedicle screw systems is titanium. There are several advantages concerning this material in comparison to ordinary steel implants. Titanium pedicle screw systems can be characterized by a good biocompatibility and lower stiffness and strength values. Due to their lower mechanical properties, the implant behavior fits to the mechanical characteristics of human bone in a better way. However, stress shielding is still a common problem of metallic pedicle screws. This phenomenon describes the degeneration of surrounding bone since most of the stresses are absorbed by the stiff implant. Another well-known disadvantage of metallic implants refers to radiotherapy. Due to the presence of the metallic implant, X-rays are attenuated and do not reach their aim. Furthermore, medical images show artefacts which contribute to complicated patient follow-up. Because of these artefacts, there is a lack of information. Thus, during surgery as well as during post-operative patient follow-up uncertainties arise. Additionally, heavy metal implants contribute to discomfort and restrictions in the daily activities of patients. Another disadvantage of the use of titanium implants are allergic reactions which can occur after the implantation.

These disadvantages will be eliminated when metal-free pedicle screw systems are used. Typically, carbon fiber reinforced plastics (CFRP) are commonly used as structural materials in the aircraft and meanwhile in the automotive sector. Engineers benefit from their high specific stiffness and strength values. Here, the term “specific” accounts for physical properties related to the volumetric mass density of the material. Especially for lightweight application, high specific stiffness and strength values are required to save material and weight. CFRP is not only used in the aircraft and automotive sector but also in other industries such as for medical applications. Carbon fiber reinforced polyether ether ketone (CF-PEEK) is biomedically approved and can be used as an implant material nowadays. A CF-PEEK pedicle screw shows no artefacts in medical imaging technologies, such as in a computer tomography (CT) scan or in magnetic resonance imaging (MRI). Due to this fact, patient follow-up is easier and uncertainties as well as risks of post-operative procedures are reduced. The problem of stress shielding is alleviated since the mechanical properties of CF-PEEK implants are closer to bone than with a metal implant out of titanium or even steel. Thus, bone degradation is reduced and its strength preserved. Since the volumetric mass density of CF-PEEK is close to bone, the comfort of patients is addressed.

In this study, a metal-free pedicle screw system out of CF-PEEK is developed. When designing an already existing metal product in plastic, a simple substitution is possible but usually does not account for the advantages of plastic material. Thus, profound design studies are established and the design of the CFRP pedicle screw system is adapted. One focus is laid on the screw. To ensure freedom in the thread design on the one hand and to achieve high mechanical properties on the other hand, a new hybrid concept of CF-PEEK pedicle screws is developed. By this concept, the mechanical screw properties are maximized and the freedom in its design is ensured.

For the development of the pedicle screw system, calculations have to be performed. A parametric finite element model is built up with the commonly used programming language Python to conduct simulations in the finite element solver Abaqus (SIMULIA, Dassault Systèmes). Due to the parametric structure, there is the possibility to conduct various studies for the evaluation of the screw.

Keywords—CFRP, metal-free design, optimization, parametric modelling, pedicle screw

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Run-Time Adaptation in Cyber-Physical Systems

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I. Abstract

The constant pressure to create machines that are more reliable motivates manufacturers to make optimization throughout the whole life-cycle of their products. In order to increase availability and at the same time reduce the service costs, more efficient maintenance approaches are applied.

One approach towards these goals includes monitoring of the machine health and operation in the field as well as the environmental impact. Abilities like over-the-air update and upgrade, or remote monitoring and diagnostics during operation are the main drivers, and constitute big selling points and enables new business models additionally. This increases the number of intelligent sensors and actuators needed in a machine and implies enormous amount of data that must be exchanged and evaluated. Moreover, cyber-physical systems, like autonomous agricultural machines, have to deal with limited resources in changing environments during operation, e. g. degrading computational power and bad connectivity. To solve these and other related problems adaption at run-time in cyber-physical systems needs to be enabled. Existing approaches often focus on the adaptation logic only or miss to address necessary requirements of adaptive systems.

Therefore, we design a reference architecture for run-time adaption based on identified scenarios for bandwidth optimization in the context of predictive maintenance.

Maintenance is done traditionally in a reactive or a preventive way. Reactive maintenance, a. k. a. corrective, is a strategy where the maintenance is carried out after failure detection and is aimed at restoring an intended function of a machine [1]. There are no high demands for IT, measuring availability, etc. However, the unpredictable down-time reduces efficiency and increases the overall costs. Preventive maintenance means in practice time/calendar based maintenance. Even though it is in many cases an improvement to reactive maintenance it is not an ideal approach, as it can easily lead to over maintaining, i. e. such equipment are also repaired or maintained that actually do not need maintenance. [2]

Making monitoring, analysis, adaptation and control at run-time possible, enables predictive maintenance. Cyber-physical systems, like modern trucks, buses, and forklifts, tractors, etc. are equipped with many different sensors that monitors parameters like oil pressure, different temperatures, status of subsystems and much more. The environment is also observed and evaluated continuously. The resulting massive amounts of data is used to characterize the usage history, operational condition, location, movement and other physical properties of the system and its context. Different types of diagnostic algorithms are used to analyze the behavior, to estimate the health status, perform root-cause analysis, and estimate remaining useful life. Furthermore, the optimal time for maintenance can be scheduled to maximize the up-time and reduce maintenance costs. The innovation potential of predictive maintenance creates additional value in the business. Although driven by the context of cyber-physical systems the proposed solution can be applied in several different domains. Cyber-security, driver assistance systems and development operations can benefit from the ability of a system to adapt at run-time.

Since run-time adaptability is one strong enabler for predictive maintenance, the reference architecture should support it in a way that increases reliability and availability. The solution should fulfill all the necessary requirements for the structure of the adaptation logic as well as the executing system and its components in order to realize the necessary adaptation mechanisms. A reference implementation is proposed to validate the solution and to give guidelines for applying it in real-world systems. Our approach is being validated in a prototype system realizing adaptation scenarios in the context of a smart farming. As a first result, we learned some key lessons about the architectural requirements to support run-time adaptation:

1) Separate adaptation logic from application logic.
2) Monitoring, analyzing, planning, and execution activities become first-class entities.
3) Components need a clear representation at development- and run-time.
4) Component dependencies must be resolved at run-time.
5) Components need a life-cycle that is subject to external adaptation.
6) Components and their dependencies need a semantic versioning schema and a strategy for version mismatch.
7) Communication between components requires a dedicated decoupling technology.

While the execution of adaptation is possible for different adaptation scenarios, most real-world systems require not only suitable execution mechanisms but also new methods for monitoring, analysis and planning. Many critical quality properties can only be maintained by combining approaches from all these activities, which is also our future work.

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Ultrafast Scattering of Electrons and Relativistic Spin Mixing in Ferromagnets

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Keywords—ultrafast; electronic dynamics; spin-orbit interaction;

I. INTRODUCTION

Conventional electronics based on the charge of electrons will soon reach its physical limits, because the circuits cannot be made any smaller. Different systems are candidates to replace silicon-based electronics but it is not clear what will come next. One possibility is to use the electronic spin, which is an additional quantum-mechanical effect, which causes electrons to behave like a small magnet. These small electronic magnets can themselves be used to store information and in a ferromagnet, their contributions, called magnetic moments, add up to yield the macroscopic magnetization of a ferromagnet.

While the manipulation of single electron spins is also a current research topic, we will focus here on electrons in metallic ferromagnets, which also form the basis of conventional magnetic hard drives. A breakthrough experiment of Beaurepaire and coworkers showed [1], that one can induce a change in magnetization with an ultrashort laser pulse on a timescale of less than a picosecond (=10^{-12} s). This time scale is much faster than what can be achieved by electronic charge currents, and this result has created a lot of excitement that it may be possible to control electronic spins in ferromagnets as information carriers by optical pulses at speeds that far exceed what is presently possible. One of the reasons that electronic spins are promising is that less energy is needed to influence them as compared to moving a charge. Another important property of the electronic spin is, that it is, unlike the charge, not conserved. This is due to a relativistic effect, the so-called spin-orbit interaction, that couples the electronic spin to the electronic motion. In a solid, this effect can sometimes be visualized as an effective magnetic field that the electronic spin experiences. It is still an active area of research how this spin-orbit interaction affects the ultrafast dynamics of the electron spin in ferromagnets [2].

II. ABSTRACT

We use an idealized model to describe electrons in a ferromagnetic metal that experience spin-orbit interaction. It constitutes a rather drastic abstraction of a real metal but we have chosen this model to achieve basic insight into the electronic dynamics that occur after excitation by an ultrashort optical pulse as they interact with the crystal lattice. This interaction can be viewed quantum-mechanically as the scattering of electrons with the quanta of lattice vibration, the so-called phonons. It has long been known that this electron-phonon scattering together with the spin-orbit coupling can lead to a change in the electronic spin. There are two basic ideas how this can happen that were developed in the 1960s: either by a collision of an electron with a phonon that directly changes the electronic spin, the so-called Elliott-Yafet mechanism [3], or by a precession of the electronic spin around different effective magnetic field combined with a lot of scattering events, the so-called Dyakonov-Perel [4] mechanism.

We show that these two cases are limiting cases of what happens in ferromagnets. The electrons often behave like there were spin-flips, but this actually results from the precessional dynamics that is only occasionally disturbed by a scattering event. This picture is valid for low scattering rates (blue lines in Fig. 1). For increasing scattering rates (red lines in Fig. 1) we find a new regime of electronic dynamics that had not been identified before.

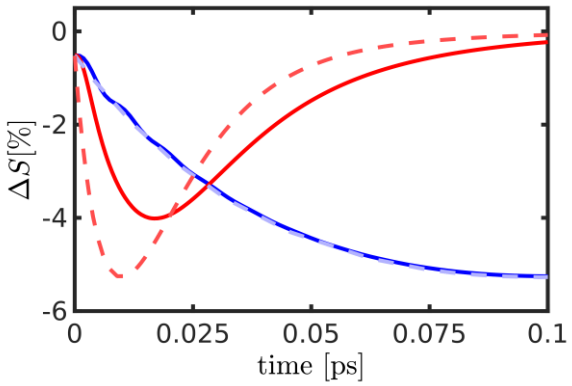

Fig. 1. Electronic magnetization change ΔS due to electron-phonon scattering due to precessional (solid lines) and spin-flip scattering (dashed lines). For different electron-phonon scattering rates (red 10 times higher than blue).

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Self-regulating Hybrid Materials for Application in Tribological Systems

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I. Introduction

Tribology, the science of friction, wear and lubrication, is an integral part of almost all industry sectors. In transportation for example, around 28% of the fuel energy is needed just to overcome frictional processes [1]. Low density, corrosion resistance, and self-lubrication make plastics the number one choice for maintenance free tribological systems like sliding bearings. Plastics are, however, not known for their temperature resistance, which is why the friction induced heat remains a huge challenge in material design processes. High temperatures have a negative impact on the mechanical properties so that the possible loads are strictly limited. In the event of an overload, even complete system failure cannot be excluded. To ensure safety and reliability it is therefore necessary to investigate and eventually control the tribological behavior of plastic based materials.

The study introduces magnesium hydroxide $Mg(OH)_2$ as a new filler for tribological applications. $Mg(OH)_2$ is capable of dampening the heat generation and keeping the system in a normal operational state [2]. On reaching a certain temperature threshold, the filler undergoes the chemical transformation

$$Mg(OH)_2 \rightarrow MgO + H_2O \ (\Delta H \approx 1450 \text{ J/g}) \qquad (1)$$

which acts as a heat sink. In addition, a metal oxide layer is formed on the surface and steam is released, further influencing the contact interface and hence the tribological behavior, Fig. 1.

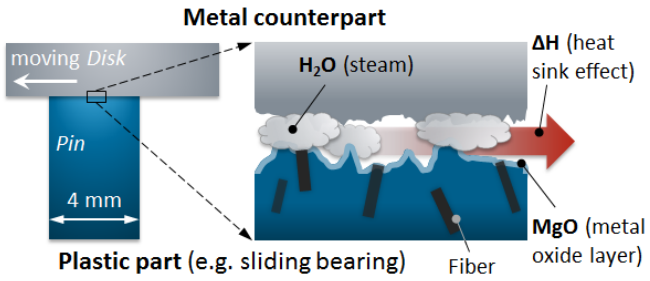

Fig. 1. Effects of $Mg(OH)_2$ on the contact interface.

II. Experimental

Using a twin-screw extruder, two carbon fiber reinforced plastics (CFRP) were manufactured. One version contained $Mg(OH)_2$, provided by TER Chemicals (Germany), the other one acted as a reference. After extrusion, plates were injection molded and samples (Pins) were cut out mechanically. The tribological performance of the materials was put to the test on a self-constructed Pin-on-Disk(PoD)-Machine. During the tests, the external load was increased incrementally. Wear, coefficient of friction (i.e. energy loss), and sample temperature were monitored continuously.

III. Results and Discussion

Compared to the reference, the relative performance of the $Mg(OH)_2$ filled material averages out at 415%, meaning a performance increase by a factor of 4. Values of up to 750%, depending on external load, unmistakably prove the capabilities of the filler to greatly improve the efficiency of tribologically stressed components. But not only does the filler effectively reduce friction and wear in general, it also makes the performance load independent: Controlled by the friction induced heat in the contact interface the chemical conversion rate of (1) changes and thus, the release rate of the reaction products actively regulates itself to match the external load. Established passive additives in contrast only work in certain isolated load regimes which greatly impairs their usability.

IV. Conclusions

Without doubt, the results illustrate the potential of this new type of filler for tribologically stressed CFRP. Further study of the effects will evidently lead to a systematic use and, as a result, to the development of reliable, energy efficient plastics with a higher life expectancy, lower ecological impact, and greater range of application than any other material currently available.

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Idealized switchable thermal insulation for summerly overheating protection

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Keywords—switchable insulation; thermal building simulation; summer overheating protection

From the first thermal insulation ordinance taking effect in 1977 [1] the requirements regarding the thermal insulation of buildings have been continuously intensified. As a result of this development the insulation layers are continuously getting thicker. Thick insulation layers lead to energy savings during the heating period. During the heating period this is desired but in summer times the low losses can lead to overheating of the building. Solar energy entering the building through the windows heats up the building. While longwave radiation (solar energy) will pass through a window without great losses, shortwave radiation like thermal radiation is largely blocked. Due to the high insulation of the building the conductivity through the boundary surfaces of the buildings is low. Therefore, the building overheats. Especially during the cooler night time it could be helpful to reduce or ideally fully switch off the insulation of the wall so that surplus energy could leave the building.

While there exist different ways to realize a switching system [2–4], in this paper an idealized switching system is examined and compared to night ventilation. This idealized system combines all the advantages of the existing systems and represents the best possible setting. Simulations with TRNSYS [5] were carried out. The object of observation is a room with 25 m² floor space, representing a typical room in a multiple story residential building. Chosen location for this study is Potsdam as normative reference site for Germany [6].

The results show that by using a switchable insulation during the night time the peak temperature during the following day can be reduced significantly. A reduction of hours with unacceptable high room temperatures up to 37% is possible with the system. This value is equal to the result of a night ventilation with an air change rate of 1/h [7]. Switchable insulation can be an addition to classic summer overheating protection (like external shading) to create a more user friendly building environment.

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Redox regulation of cellular time-keeping: a novel role for peroxiredoxins and hydrogen peroxide

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***Abstract*—** The circadian clock is an internal biochemical oscillator, which enables organisms to synchronize their biological processes with daily environmental changes, especially day-night cycles. This clock (with 24-hour period) is conserved across all domains of life, from bacteria and archaea to humans. Disruption in mammalian circadian timing has been linked to several metabolic diseases such as diabetes, obesity and cancer, as well as neurodegenerative disorders. In yeast, the 'circadian' clock is ultradian (shorter-period) in nature – ranging from 40 minutes to 5 hours – and known as the yeast metabolic cycle (YMC, Fig. 1). It shares features that are conserved with the mammalian circadian clock, and thereby serves as a convenient model to understand cellular time-keeping and circadian rhythms. The YMC was first identified as a reduction-oxidation (redox) cycle, during which cells switch between low and high oxygen consumption modes of metabolism. Cyclical changes in the expression of more than 50% of cellular genes also occur during the YMC. Additionally, the YMC appears to regulate entry and exit into the cell division cycle [1,2]. Genetic or chemical perturbation of cellular redox processes can strongly disrupt the YMC; however, the mechanistic underpinnings remain unexplored. To understand how redox processes impact upon the YMC, we treated YMC-synchronized cultures with oxidants (e.g. diamide) and reductants (e.g. DTT). Addition of diamide to a low oxygen consumption phase of the YMC resulted in delayed switch to high oxygen consumption in a concentration dependent manner. On the contrary, DTT addition results in a rapid and sustained switch to high oxygen consumption. This indicates that cellular respiratory rate is responsive to, and perhaps regulated by, changes in cellular redox conditions.

Hydrogen peroxide (H_2O_2) is an important cellular oxidant, which acts as a signal molecule in a variety of cell signaling pathways and can elicit large-scale changes in gene expression. H_2O_2 has also been suggested as a key regulatory signal that may regulate the YMC and gate cell cycle entry. However, how H_2O_2 signals are transmitted within the cell is not completely understood. Peroxiredoxins are a highly conserved family of proteins with high reactivity towards H_2O_2 and serve as relays passing oxidation from H_2O_2 to proteins. Circadian peroxiredoxin redox cycles have been observed across all domains of life [3], although a functional role for peroxiredoxins remains to be demonstrated. We hypothesized that H_2O_2 and peroxiredoxins play important regulatory roles during the YMC and in controlling cellular time-keeping in general.

In order to monitor changes in endogenous H_2O_2 levels during the YMC, we developed a genetically-encoded fluorescent reporter and integrated it into the genome of yeast [4]. With these engineered yeast strains, we observed cyclical changes in endogenous H_2O_2 levels during the YMC. To determine if H_2O_2 changes can influence YMC progression we added boli of H_2O_2 to YMC-synchronized cultures. We observed a rapid switch from low to high oxygen consumption upon addition of peroxide, which thus paradoxically appears to behave as a reductant, like DTT. The explanation appears to be that high levels of H_2O_2 inactivate endogenous peroxiredoxins, which normally transmit oxidation from H_2O_2 to other proteins. Consequently, this leads to peroxiredoxin-target protein reduction. We therefore propose that peroxiredoxins couple cyclical changes in H_2O_2 to changes in respiratory rate via a yet unidentified mediator protein(s). We speculate that this constitutes a metabolic feedback loop that, at least in part, is required to establish the synchronized metabolic cycles observed in the YMC.

Keywords— redox, signaling, metabolism, circadian rhythms

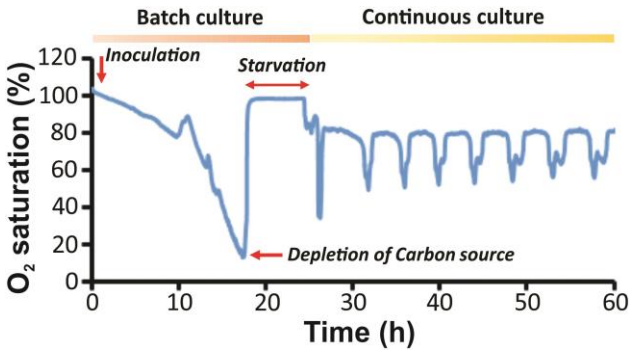

Fig. 1. The Yeast Metabolic Cycle (YMC). The YMC consists of highly robust, periodic oscillations representing alternation between fermentative and respiratory metabolism.

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