Graduiertentagung Graduate Symposium November 2010



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 November 2010

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Vorwort / Preface

In diesem Jahr stellen unsere Doktorandinnen und Doktoranden zum dritten Mal im Rahmen der Graduiertentagung ihre wissenschaftlichen Arbeiten aus den verschiedenen Fachdisziplinen vor. Unser internes Doktorandennetzwerk ist mittlerweile ein fester Bestandteil der Forschungslandschaft unserer Hochschule. Nach dem gelungenen Start mit der ersten Graduiertentagung im September 2008 und einer viel beachteten Tagung im letzten Jahr möchten wird an diesen Erfolg mit der diesjährigen Veranstaltung anknüpfen. Die Resonanz der Teilnehmer, der externen Referenten und der Zuhörer hat uns gezeigt, wie befruchtend die Diskussion über die Fachgrenzen hinaus für alle Beteiligten ist.

Die Arbeit des Graduiertenkollegs hat im vergangenen Jahr weiter an "Fahrt gewonnen". Unsere Graduierten erfahren in der Hochschule eine zunehmende Wahrnehmung, sie vertreten ihre Belange in den forschungsrelevanten Gremien der Hochschule und erhalten durch Bereitstellung von Rektoratsmitteln eine finanzielle Unterstützung. Für das kommende Jahr ist ein Doktoranden-Training geplant, in dem wir ihnen neben dem fachlichen Rüstzeug auch weitergehende Qualifikationen vermitteln wollen, die für einen Start in eine hoffentlich erfolgreiche berufliche Karriere wichtig sind.

Die Zusammenarbeit über die Standortgrenzen hinweg entwickelt sich weiterhin positiv, so dass die FH Aachen mit der Graduiertenschaft eine wichtige Plattform besitzt, durch die die einzelnen Hochschulstandorte näher zusammenrücken.

Die diesjährige Graduiertentagung bietet Ihnen wiederum die Möglichkeit, Ihre wissenschaftlichen Arbeitsergebnisse im intensiven Dialog mit Ihren Kolleginnen und Kollegen sowie den geladenen Gästen zu diskutieren. Auch in diesem Jahr haben wir wiederum zwei bedeutende Gastredner gewinnen können, Prof. Dr. Claus-Dieter Kohl von der Justus-Liebig Universität Gießen und Dr. Oliver Funke vom Deutschen Zentrum für Luftund Raumfahrt.

Wir freuen uns auf einen interessanten Tag gemeinsam mit Ihnen und sind sicher, dass Sie mit Ihrem Beitrag auch in diesem Jahr die wissenschaftliche Landschaft der FH Aachen bereichern werden.

September 2010

Prof. Dr. Christiane Vaeßen Prorektorin für Forschung, Entwicklung und Technologietransfe Prof. Dr. Michael J. Schöning Institut für Nano- und Biotechnologien (INB)

Prof. Dr. Claus-Dieter Kohl



Studium und wissenschaftlicher Werdegang

1964 bis 1968 Oktober 1968	Physikstudium an der RWTH Aachen Diplomarbeit im 2. Physikalischem Institut der RWTH Aachen unter Leitung von Prof. Dr. G. Heiland, Thema "Feldeffekt am ZnO" Studienabschluss Diplom-Physiker
Ab 1968	Assistententätigkeit im 2. Physikalischem Institut der RWTH Aachen, gleichzeitig Anfertigung der Doktorarbeit, Disserta- tionsthema "Über den Zusammenhang zwischen elektrischen und strukturellen Eigenschaften polarer ZnO-Oberflächen"
12.12.1972	Promotion
Oktober 1974	Akademischer Rat
1974	Gastaufenthalt im Philip Morris Research Center in Richmond (USA), Messungen an elektrochemischen O2-Sensoren
1979	Gastaufenthalt im Racah-Institute in Jerusalem (Israel), Mes- sungen in der AG Prof. Many an Halbleiter-Randschichten
1990	Gastaufenthalt im Lawrence Berkeley Laboratory 1990, AG Prof. G. Somorjai Halbleiter-Metall-Wechselwirkung
1981	Habilitation an der RWTH Aachen für das Fach Physik
am 27.6.1991	Berufung auf C3-Professur an der Universität Gießen ins Insti- tut für Angewandte Physik
1998	Berufung auf C4-Professur, Vorgezogene Nachfolge Prof. Hei- den in Gießen

Aktuell bearbeitete Themen

- > Entwicklung mesoskopischer Sensormaterialien
- > Perkolation
- > Sensorik für Holztrocknung (Spanplattenherstellung)
- > Lecksuche (urbaner Bereich)

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1985 -1987 1987 -1993	Studium der Physik an der Universität Bremen Studium der Physik an der Universität Bonn; Schwerpunkte des
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1994 - 1999	Wissenschaftlicher Mitarbeiter Universität Bonn,
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2001 - 2004	DLR Institut für Raumsimulation
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2004 - 2006	DLR Microgravity User Support Center MUSC
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	Untersuchung zur Eignung von Einschmelzsonden zur Suche
	nach Leben in den Eiskappen des Mars und auf dem Jupiter-
	mond Europa
	Betreuung der Kometen-Simulationsanlage des DLR School-Lab
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seit Oktober 2006	DLR Raumfahrt-Agentur
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EGE 25/17

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Betreuender Professor an der Universität | Professor attending to the University Metabolic pathway design: transfer of a butyrate-forming module from Clostridium difficile to Escherichia coli

Prof. Dr. Thorsten Selmer

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Metabolic pathway design transfer of a butyrateforming module from Clostridium difficile to Escherichia coli

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Whole genome sequencing rapidly increases our knowledge on the genetic constitution of life on earth. The enormous number of new genes encoding previously unknown biocatalysts arising from every genome project offers novel routes in the development of carefully designed organisms for technical applications.

At present, however, synthetic biological use of genome information is hampered by insufficient characterisation of most of these genes. Thus, novel strategies are needed which allow i) rapid recombinant production of these novel enzymes in a functional state for individual testing, ii) systematic assembly of individually characterized enzymeencoding genes to yield functional metabolic pathway modules and iii) the tailor-made design of technical microbes for different applications from these metabolic modules. In order to test the capability of a recently developed novel combinatorial cloning system for these applications, we decided to transfer the capability to form butyrate from *Clostridium difficile* to *Escherichia coli*, which naturally lacks the ability to convert glucose to butyric acid.

E. coli naturally converts glucose under anoxic conditions via pyruvate to a complex mixture of lactate, acetate, formate, succinate, glycerol and ethanol. In contrast, C. difficile converts pyruvate to acetate and butyrate. In both pathways acetyl-CoA is a central intermediate, which was supposed to be redirected to butyrate formation by the introduction of 8 clostridial genes into *E. coli*, encoding 6 individual enzymes First, two molecules of acetyl-CoA are condensed by thiolase to acetoacetyl-CoA which is reduced to 3-hydroxybutyryl-CoA by a dedicated dehydrogenase. Then, water is eliminated by crotonase and the resulting crotonyl-CoA is reduced to butyryl-CoA by the butyryl-CoA dehydrogenase complex composed of three individual polypeptides. Butyryl-CoA is further converted by phosphate butyryltransferase and the butyrylphosphate thus formed is subsequently used for substrate phosphorylation of ADP mediated by butyrate kinase.

In a systematic approach, all these enzymes were first produced in *E. coli* and functionally tested in vitro. Substrate specificity, stability and kinetic parameters were established for these enzymes in order to address their capability for the synthesis of various metabolic intermediates in volatile fatty acid biosynthetic pathways. Then, the individual genes were combined in order to yield a synthetic metabolic pathway module, which was introduced into the host cells. Expressed in the host, these genes allowed significant production of butyric acid in *E. coli*. In the future, the butyrate-forming module or parts thereof can be combined with suitable dehydrogenases in order to afford commercially interesting solvent production in *E. coli*.

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Field-effect based electrolyteinsulator-semiconductor sensors

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Label-free DNA detection by means of nanoplate capacitive sensor array based on SOI structure

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Label-free detection of charged macromolecules utilising semiconductor field-effect devices is one of the most attractive approaches for a new generation of biochips (e.g., DNA arrays, protein chips) with direct electrical readout for a fast, simple and in-expensive analysis. In this work, we present a novel platform for a label-free electrical detection of DNA-hybridisation and denaturation using field-effect electrolyte-insulator-silicon-on-insulator (EISOI) nanoplate capacitors functionalised with gold nanoparticles. The proposed device detects the charge changes of the Au-nanoparticle/DNA hybrids induced by the hybridisation or denaturation event.

An array of electrically isolated individually addressable nanoplate capacitive sensors was fabricated from an SOI wafer with a 360 nm thick top p-Si layer on a 400 nm thick buried SiO2 layer. An isolation of the individual capacitors was achieved by forming a trench in the top Si layer. Thus, the realised sensor array allows addressable biasing and electrical readout of multiple nanoplate EISOI capacitive biosensors on the same SOI chip as well as differential-mode measurements between the spots. The Au nanoparticles (5-8 nm) have been deposited on a (3-mercaptopropyl trimethoxysilane)-modified sensing surface from a stabilised gold colloid solution. Then, the thiol-modified 20 base pair single-strand DNA molecules (ssDNA), perfectly matched or fully mismatched to the target ssDNA sequence, have been immobilised on the sensing area of the sensors. One of the sensors with fully mismatched ssDNA was used as reference.

The potential change of ~110 mV has been registered after the DNA hybridisation for the sensor immobilised with perfectly matched ssDNA, while practically no signal changes have been observed for the sensors with fully mismatched ssDNA. The denaturation signal was ~70 mV. Details of the experiments as well as a theoretical model describing the functioning mechanism of nanoplate EISOI capacitors functionalised with Au-nanoparticle/DNA hybrids taking into account direct electrostatic charge effects will be presented and discussed at the conference.





Fig. 1 | Schematics of an EISOI sensor functionalised with Au-nanoparticle/DNA hybrids (a) and 4-channel EISOI sensor chip (b).

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Modulares Sensorsystem für die Zellkultur-

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Electrochemical sensor array for bioprocess monitoring

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Due to their complex chemical structure pharmaceuticals such as antibodies or glycoproteins are usually biotechnologically synthesised. These pharmaceuticals are obtained from various microorganisms, for instance mammalian cells such as Chinese hamster ovary (CHO) cells, which have to be cultivated under optimal conditions since their metabolism strongly depends on external physical and chemical parameters. Thus, monitoring and control of these parameters during the cultivation is crucial for process optimisation in terms of a high-quality product and an increased yield.

In this contribution, a Si-based solid-state sensor array for multi-parameter monitoring of fermentation processes is presented⁽¹⁾. The developed sensor array consists of two chips (see Fig. 1) allowing continuous monitoring and quantification of five (bio-)chemical and physical parameters, namely pH value, electrolyte conductivity, temperature, and glucose and glutamine concentration by applying different transducer principles and/or different operation modes.

A semiconductor field-effect platform, using a capacitive electrolyte-insulator-semiconductor (EIS) sensor consisting of a p-Si-SiO₂-Ta₂O₅ structure was utilised to develop a pH sensor. Thin-film interdigitated electrodes served as impedance sensor. The geometry of these electrodes has been optimised to measure the conductivity of the electrolyte in relatively high ionic-strength solutions. Temperature measurements were performed with a resistance temperature detector made of a platinum thin-film electrode. An integrated Ag/AgCl thick-film chip electrode is intended to be used as (quasi-)reference.

The biosensor chip comprises three enzyme-based amperometric sensors for glucose and glutamine detection. Glucose oxidase, glutamate oxidase and a two enzymesystem made up of glutaminase and glutamate oxidase have been immobilised onto platinum working electrodes. The different enzymes specifically react with their target molecule and produce electroactive species that can be recognized at the platinum electrodes. An additional platinum electrode is left without any enzyme for differential measurements.



Fig. 1 | Silicon-based electrochemical sensor array Chemical sensor chip comprising the conductivity, temperature and pH sensor (left) and biosensor chip consisting of a glucose, a glutamine and a glutamate sensor (right).

¹ M. Bäcker, S. Beging, M. Biselli, A. Poghossian, J. Wang, W. Zang, P. Wagner, Michael J. Schöning; Electrochim. Acta 54 (2009) 6107-6112.

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01E11 / 01E20/21

Influence of ATP on Thermal Aggregation of Proteins

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Influence of ATP on Thermal Aggregation of Proteins

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In the post-genomic era, protein conformation and structure determination has become of paramount significance in order to understand protein function. Results lead to a three-dimensional picture of each gene product and, in many cases, reveal hints on the function of a protein. Evidences that proteins change their conformation during functioning are numerous. As for example, the change of solvent temperature combined with the addition of certain co-solvents can cause quantitative alterations of the -helical and β -sheet content of proteins. Small molecules like CO, ATP, NO etc. can interact with proteins, influencing their conformational, thermodynamic, and consequently, functional characteristics.

In our study, hemoglobin (Hb) as well as bovine serum albumin (BSA) was subjected to thermal denaturation at temperatures ranging from 25 to 80 °C in the presence and absence, respectively, of various low-molecular co-solvents. Proteins with and without co-solvents were prepared either in phosphate buffer saline (PBS, sodium based) or in its potassium- based analog buffer (CD-buffer) in order to distinguish the contribution of cations. Main techniques employed to study and characterize structural and dynamical properties of proteins were quasi-elastic light scattering (dynamic light scattering, DLS) and circular dichroism spectroscopy.

A series of more than 60 experiments was performed so far. The obtained results suggest that protein thermal denaturation in vitro is strongly affected by the NO, ATP and different ions types. For instance, nitric oxide and ATP generally facilitate protein denaturation, whereas the influence of the cations is controversial. Results will contribute to a more complex understanding of the interplay of proteins and small molecules on a nano-structural level and to better understanding of protein function.



Fig. 1 | Influence of nitric oxide, ATP and cation composition on the denaturation onset of Hb samples prepared in PBS buffer (a, b) and its potassiumbased analog buffer (c, d). Samples treated with NO denaturate earlier than those without NO.

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HiX for AGWS - XML-based History tracing in an Actor-driven Grid-enabled Workflow

18 | 3RD GRADUATE SYMPOSIUM

HiX4AGWS – XML-based Provenance Framework for WfMS

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During the last few years, operational procedures are abstracted and digitalized in form of workflows in more and more application domains. Thereby, a workflow mostly consists of multiple work items that have to be executed in a well-defined order. The modeling, execution, and monitoring of such workflows is usually done by proper workflow management systems. Once a workflow is modeled and started the workflow management system takes care of the individual work items, so that they are correctly executed within the expected order by delegating them to capable resources.

In particular, for distributed environments like Grid- or Cloud infrastructures the identification of suitable resources is quite cumbersome. Accordingly, we established an approach that inverts the distribution of work items within the scope of the project "Hi-X4AGWS". This means that the workflow management system does not look for suitable resources, but the resources actively apply for available work items by an intermediary that mediates between the management system and the resources. Such a resource driven workflow execution breaks with the established resource allocation strategies, which in general deals with trusted domains, where the workflow systems delegate work items to well-known, trusted resources. This workflow execution has the advantage that the workflow management system defines and therefore knows which resource has executed a work item. In contrast, the intermediary solution lacks of this knowledge because of the dynamic, resource driven binding of work items to resources. Hence, a framework has to be implemented that closes this gap by documenting in detail which resource has executed a work item under which constraints.

Within the scope of "HiX4AGWS" we developed such a provenance framework that is intended to close this gap. The framework has a web service layer that allows the integration in various existing workflow management systems. Apart from the identification of the data to document, the major task was to transfer all valid workflow patterns into a unique XML structure that allows the workflow's reconstruction either from process or data perspective. Especially, this was problematic because a workflow definition allows various kinds of execution graphs but a valid XML document supports only tree graphs. To solve this problem we established a shell-model whereby each predecessor is surrounded by its successor. Critical execution patterns like parallel sections or multi choices are handled by complex XML elements that can deal with several execution threads by mapping them to parallel tree branches linked with unique identifiers. Another important aspect, the provenance framework has to consider is the data integrity. This means that the resources have to be empowered to sign their execution of a work item under the documented constraints. Here, the shell-model proved to be a good solution, too, because of the included predecessors, which allow signing the current workflow's state. In combination with the input and output parameters, a resource is able to sign which work item was executed under which constraints.

In conclusion, using the developed provenance framework it is possible to document actor-driven workflow executions in a legally binding way. The resulting schema based XML document represents the concrete workflow execution path and data genesis. So the XML document allows to reproduce a concrete workflow execution and furthermore to repeat it anytime.

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Comparison of adherent mammalian cells for their application as cell-sensors for gas detection

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Eukaryotic cells are well known for their application as toxicity measurement entities in aquatic systems. Although some groups have done research in this area, very less is known of the cellular behaviour during the direct exposure of eukaryotic cells towards toxic gases. This study was done to compare the ability of several mammalian cell lines to react towards the exposure of toxic gases. Mammalian cells were used to get results which are closest related to the effects in the human body. The chosen cell lines were V79 (Chinese hamster lung fibroblasts), A549 (Human lung carcinoma) and RPMI 2650 (Human nasal septum squamous cell carcinoma). Their characteristics are described in Table 1.

Cell line	Name	Origin	Carcinoma	Doubling time
Fibroblasts	V79	Hamster	Yes	~16 h
Epithelial	A549	Human	Yes	40-50 h
Epithelial	RPMI 2650	Human	Yes	~ 40 h

Table 1 | Adherent mammalian cells used for gas measurements

The cells are directly exposed to wet synthetic air (80% N_2 , 20% O_2 ; ~65% relative humidity), enriched with different toxic gases. Cellular reaction is detected by a metabolic chip which acts as a culture vessel for the mammalian cells [Fig. 1A]. Short time toxic gas exposure leads to a loss off adhesion forces which can be determined by changes in their impedance in real-time. Toxic gases like carbon monoxide are able to inhibit the cellular respiration chain and therefore reduce the respiration rate of the cells.

B

A





Fig. 1 | (A) V79 cells on the surface of a metabolic chip, (B) A549 cells in a culture flask

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Development and Testing a Low NO_x Hydrogen-Fuelled Gas Turbine

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Control system modifications for the operation of a hydrogen-fuelled auxiliary power unit

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The control of pollutant emissions has become more and more important in the development of new gas turbines. The use of hydrogen produced by renewable energy sources could be an alternative. Besides the reduction of NOx-emissions emerged during the combustion process another major question is how a hydrogen fuelled gas turbine including the metering unit can be controlled and operated. In order to demonstrate safe engine control and low pollution combustion in a hydrogen fuelled gas turbine an Auxiliary Power Unit GTCP 36-300 is used. The modification is based on the main idea to feed the requested amount on energy in order to archive the same turbine operation characteristics. Within this scope the control system and the metering unit are modified and improved.

The gas turbine and the metering unit are controlled and operated by the VECB. The control of the engine proceeds in two different parts. During the starting sequence an acceleration from zero to 95 % speed including the ignition is controlled by the first controller. Then the second closed loop engine control takes over for all operating conditions of the APU. Its function is to keep the gas turbine's speed constant, between 99% and 101% rotational speed, for each load condition.

Besides several software modifications for the hydrogen operation such as an additional Dry Crank also the acceleration control of the hydrogen fuelled gas turbine was modified. The function of the controller of the kerosene fuelled gas turbine during the acceleration process is to assume the required acceleration based on a reference acceleration map. The mode of operation for the controller of the hydrogen fuelled gas turbine during the acceleration is different. Instead to control the fuel mass flow through an acceleration of the engine from zero to 95% a defined hydrogen mass flow is attributed to seven decided speed levels. Each speed step is attributed a valve opening position and therewith a hydrogen mass flow. Between the speed levels the hydrogen mass flow is interpolated. The controller's behaviour after 95% speed is the same as the kerosene ones.

For setting the hydrogen fuel steps several investigations are done. First the kerosene mass flow during the acceleration process was measured. The measured mass flow is the reference value for the setting of the hydrogen fuel steps but there are some critical moments, such as the off-peak starter moment and the changeover of the controller, which have to be improved for the hydrogen operation. For getting an impression on which amount the fuel steps can be decreased a simplified performance model based on the Brayton Cycle for gas turbines is prepared. The model comprehends all known engine data. Figure 1 shows the calculated energy amount as well as the measured kerosene energy amount in percent against the speed of the gas turbine. The calculated energy amount at 99% rotational speed is the 100 % reference. In addition Fig. 1 contains the applied hydrogen energy amount based on the hydrogen fuel steps.

For additional improvement of the security laws also a malfunction of the IGV movement and the resultant influence on the acceleration process is investigated.

The hydrogen fuelled gas turbine shows with the set fuel steps a gently acceleration from zero to operation state. The critical moments during the acceleration process can be avoided by adopting the injected hydrogen amount to the simplified calculation model. The controller changeover at 95% rotational speed appears without any problems.





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N109

Development of a high temperature air-sand heat exchanger for use in solar thermal power plants

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Projektpartner | Project Partner

24 | 3RD GRADUATE SYMPOSIUM

Development of a high temperature air-sand heat exchanger for use in solar thermal power plants

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In view of rising energy prices and an increasing share of power generated by renewable energy sources, the importance of energy storage is growing. In the framework of this project, which is conducted in cooperation of Solar-Institut Jülich (SIJ) of the FH-Aachen, the German Aerospace Centre (DLR) and several industry partners, a thermal energy storage concept for solar power towers is being developed, in which quartz sand serves as storage medium. Sand is suitable due to its advantageous high thermal stability and specific heat capacity properties as well as its low-cost availability. In comparison to storage systems with ceramic bodies as storage medium, the utilisation of sand has a potential to reduce costs of energy storage and thus the electricity generation costs. Alongside the usage in solar thermal power plants, the storage concept could also be applicable in the steel industry. The storage concept is shown in Fig. 1. The sand, which is heated in the air-sand heat exchanger up to approx. 800 °C, flows to the hot storage through a down pipe and from there to the fluid bed cooler. The fluid bed cooler, which is a standard component of fluidized bed combustion units, is the driving element of the steam cycle. The generated steam is finally fed to the steam turbine for power generation. The cooled sand exits the fluid bed cooler at a temperature of approximately 150 °C and is returned either to the air-sand heat exchanger or is stored in a cold storage tank.

The main advantages of this storage concept are:

- > low-cost storage medium
- > storage at atmospheric pressure
- > height-temperature storage
- > 100% of the hot storage volume can be used
- > the heat exchanger pressure losses are independent of the storage capacity

For implementation of the concept a suitable heat exchanger is required, which is being developed and analysed at SIJ. The heat exchanger should show the following properties:

- > good heat transfer: heat losses < 20 %, temperature difference between sand outlet and air inlet temperature < 10%</p>
- > low pressure loss: Δp_{air} < 5000 Pa
- > compact design

To meet these requirements a concept had been chosen with a

- > cross flow arrangement of the heat transfer media air and sand
- > low width design for reduction of pressure drop in the moving packed bed

The hot air enters through a porous wall, passes through the moving bed of sand, and flows out at lower temperature through another porous wall. The principle design is shown in Fig. 2.

The SIJ has created a first numerical model in 2D (Fig. 3) and has built a heat exchanger prototype. This allows a comparison of the produced simulation results with measured data from practical prototype tests. The next steps are to create a numerical 3D-model which includes the heat interaction with the material construction and analyses in detail the sand flow behaviour as well as the influence of variations of porous walls for an up-scaled prototype. First material stress simulations are shown in Fig. 4.



Fig. 1 | Sand storage concept for solar power towers



Fig. 2 | Design of air-sand heat exchanger



Fig. 3 | Numerical 2D-model of heat exchanger



Fig. 4 | Deformation analyses

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Partneruniversität Partner University	Technische Universität Darmstadt
Betreuender Professor an der Universität Professor attending to the University	Prof. DrIng. Charalampos Tsakmakis
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A versatile non-linear material model of biological soft tissues in medical simulation environment

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The system RASim (Regional Anesthesia Simulator) has been developed in a DFG-project at RWTH Aachen, ^{III}. It represents a virtual reality simulator for the training of students in regional anesthetic techniques. An X-FEM approach has been implemented for the effective Finite Element simulation of a needle cutting through tissue ^{III}. The future development will be based on the Open Source Program SOFA ^{III} which uses a simplifying corotational implementation of linear materials laws.

Soft biological tissue shows strongly nonlinear material behavior which may also be anisotropic, such as arteries, or be transversely isotropic, such as muscle, or be isotropic, such as brain. This is a judicious combination of the Fung model ^[4] with the neo-Hookean model [5]^[5]. As an exponential function of strains, Fung's model is suitable for fitting the elastic behavior of collagen fibres. Meanwhile, neo-Hookean model is suitable for simulation of matrix and elastine. By applying simple constraints on the material parameters of Fung's model, we receive an expected tissue behavior. The strain energy function of the presented model has the form

$$W(E) = W_{Eupa} + W_{pea} + U(J)$$
 (1)

where W_{Fung} , W_{neo} and U(J) stands for Fung strain energy, neo-Hookean strain energy and volumetric strain energy, respectively.

So far, there are only very few medical FEM programs, which can provide real time simulation with non-linear material models. We implement the non-linear model (1) of biological soft tissue in medical simulation environment. Therefore, SOFA simulations are significantly more universal so that students can feel better the "real forces" when cutting or deforming any kinds of biological soft tissues in the virtual reality simulator. Results of numerical examples ensure that our work can enhance the modeling of biological soft tissues modeled in SOFA, promising to feasible applications implemented in medical training programs. Nonlinear real time simulation remains to be a challenge.



Fig. 1 | Liver in SOFA: visual model, mechanical model, collision model, respectively, [3].

O. Grottke, A. Ntouba, S. Ullrich, W. Liao, E. Fried, A. Prescher, T.M. Deserno, T. Kuhlen, R. Rossaint: Virtual realitybased simulator for training in regional anaesthesia. Br J Anaesth 2009 103(4):594-600. http://dx.doi.org/10.1093/ bja/aep224

² L. Jeřábková: Interactive cutting of finite elements based deformable objects in virtual environments. Dissertation, RWTH Aachen (2007). http://darwin.bth.rwth-aachen.de/opus3/volltexte/2007/2094/

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 Y.C. Fung: Biomechanics: Mechanical Properties of Living Tissues. - 2nd ed., Springer, New York 1993.

⁵ A.F. Bower: Applied mechanics of solids. CRC Press, 2010.

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Einstellbares alloplastisches Schlingensystem zur minimalinvasiven Therapie der Belastungs-Inkontinenz bei Frauen

01A54

N.N.

N.N.

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Prof. Dr.-Ing. Manfred Staat

 FEG Textiltechnik Forschungs- und Entwicklungsgesellschaft mbH Aachen

Adjustable alloplastic sling system for the minimally invasive therapy of stress urinary incontinence in women

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Since their introduction during the 1990 textile alloplastic slings have revolutionised the chirurgical therapy of stress urinary incontinence in women. The slings augment degenerated ligaments and enable the repositioning of the organs in their anatomical correct position. In this way continence is restored. The slings are fixed in the tissue of the pelvic floor by small anchors. Presently available anchors causing either unnecessarily large wounds when applied or fail at low traction forces.

An improved anchoring system will be developed in a cooperation between the Aachen University of Applied Sciences, the FEG GmbH Aachen and the Continence Clinic Aachen.

The task of the Biomechanics Laboratory is to simulate the anchoring systems with the aid of finite element(s) method (FEM). This problem is very complicated because it is a contact problem and the deformations and displacements of some types of anchors are large. Thus nonlinearities arise in the material behaviour. The results of the simulation will be used to develop anchors of different shapes that allow bigger traction and decrease the risk of ruptures. In the FEM-Simulation the muscle and the anchoring are modelled. The possibility to simulate many different traction forces allows the calculation of the stresses and the deformations in the muscle in different cases. Finally animations will be created to visualize the exposure of the muscle and the anchors while increasing traction is applied.

The pictures below show an anchor that undergoes large displacements. If a traction force pulls the anchor at the lower end the hooks will spread and if the forces become too large the hooks will fold over.

Acknowledgement: The first author has been partially funded by the Federal Ministry of Economics and Technology (BMWi) through the ZIM cooperative project "SchlingenSystem" KF 254 560 1AJ9







Figure 2 | A discretized model of the anchor.

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Measurement of the Contractile Force of Autonomously Beating Cardiomyocytes in 3D Collagen Matrices

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Almost one in two deaths in Germany is due to a disease of the cardiovascular system like hypertonia, cardiac infarction and others. For in-vitro studies of the mechanical properties of cardiovascular cells, organ explants from animal donors are still the best available technology. Regarding the problems of limited reproducibility, costly application and not least the ethical concerns, a cell based in-vitro model for the evaluation of mechanical data from beating cardiomyocytes is established.

The CellDrum[™] System developed in the Laboratory for Cellbiophysics at the University of Applied Sciences Aachen provides a sophisticated environment for the measurement of the mechanical properties of cellular monolayers and thin tissue constructs based on collagen matrices. In previous studies, multiple cell types were examined with this system, such as vascular endothelial cells, human dermal fibroblasts, intestinal epithelial cells and rat heart myoblasts (H9c2). Additionally, first preliminary experiments were executed with beating cardiomyocytes in monolayers (chick and rat embryo isolates, Cor. At[®] atrial cardiomyocytes). In order to approach preferably physiological conditions, in a next step the cardiomyocytes will be embedded into a 3D collagen matrix.

Cell-seeded collagen gels are very weak and only grow stronger slowly in culture. For this reason, a simple but highly effective way of plastically compressing seeded collagen gels (external mechanical loading and capillary fluid flow) was developed at the Tissue Regeneration & Engineering Centre at the University College London.

The combination of the CellDrum[™] System and the plastic collagen compression method applied to Cor.At[®] atrial cardiomyocytes will provide a comprehensive model for studying:

- 1. Comparative estimation of pharmaceuticals with equal indications
- 2. Individual potency of pharmaceuticals
- 3. Toxicological tests (adverse reactions)
- 4. Screening of new substances
- 5. Test of new active principles



Fig. 2 | The CellDrum Principle



Fig. 2 | Cyclic Contraction of Cardionyocytes monitored with the CellDrum system

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EGE 22/EGE 26

Name des Projektes | Name of the project

"Bio-LAPS"-Optimierung des Betriebs eines Biogasfermenters mit Hilfe eines Feldeffekt Biosensors auf der Basis eines lichtadressierbaren potentiometrischen Sensors (LAPS)

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Optimization of a biogas fermenter by detecting the metabolism of immobilized anaerobic microorganisms based on a LAPS

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The conversion of biomass to the high-energy gas methane (CH_4 , biogas) is performed by syntrophic microbial consortia, which require strictly anoxic conditions and tolerate only small changes in environmental conditions. The initial degradation of complex polymers (carbohydrates, proteins and lipids) to monomers (sugars, amino and fatty acids) and subsequential conversion of these monomers to acetate, carbon dioxide and hydrogen is mediated by hydrolyzing and fermenting bacteria. Finally, acetoclastic methanogenes convert acetate to CH_4 . Likewise, CO_2 and H_2 are consumed by hydrogenotropic methanogenes to yield methane.

The formation of crucial methanogenic intermediates like acetate, CO_2 and H_2 proceeds by the action of bacteria and the concentration of these intermediates is also affected by the consumption by metanogenic archea. In particular acetate (acetic acid) formation is accompanied by acidification of the medium, while its consumption has detrimental effects. At disturbances of the methanogens, the acid concentration in the fermenter increases due continuing action of fermenting bacteria and the pH declines. Selective damage of the bacterial communities has the opposite effect.

The shifts in the pH caused by either production or consumption of acid might be detectable by light-addressable potentiometric sensors (LAPS). Given that microbes are located on the sensor surface, formation or consumption of acid might be readily measured. In prove of principle, we first immobilized *Escherichia coli* cells as model organism on the chip surface by inclusion in thin poly-acrylamide layers. In glucose containing medium, this organism forms acetate and acidification of the sensor surface was readily measured.

In order to sense acetate levels in biogas fermenters directly, the immobilization of an acetoclastic methanogen (*Methansaeta concilii*) is planned. The cleavage of acetate to yield methane and carbondioxid is predicted to cause pH up-shift (alkalization) of the sensor as compared to a reference surface and it might be possible to sense actual acetate levels *in situ*.



Fig. 1 | Immobilized bacteria detect the metabolic activity in the form of protons (red balls) with a pH sensitive LAPS to control the biogas building process.

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OG A 41

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Exfoliation of polyvinyl acetate-layered silicate nanocomposites by using low-molecular plasticizers

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Polymer nanocomposites have attracted great interest in recent years since they exhibit an enhancement of physical and chemical properties compared to the neat polymer matrix. In polymer-layered silicate nanocomposites, the layers are dispersed at nanoscale level in the matrix. They are used as nanofillers with the result that the nanocomposites show improved properties compared to those of composites filled with macro- or microscopic fillers, e.g. reduced gas permeability. The layered silicates are phyllosilicates whose negatively charged layers are counterbalanced by cations residing in the gallery between the layers. The cations can be replaced by organic cations such as alkyl ammonium ions changing the normally hydrophilic silicate surface hydrophobic. The organic cations improve the compatibility between polymer and silicate particles as well as they increase the distance between the layers. In order to achieve an improvement of the properties, the silicate layers have to be exfoliated, i.e. the polymer chains intercalate into the gallery and delaminate the silicate particles. Consequently, they are dispersed homogeneously as individual layers in the matrix. A good exfoliation corresponds to strong interactions between polymer and organic cation. Exfoliation polymer-layered silicate nanocomposites can be prepared by three main methods: the intercalation of the polymers from solution, the polymerisation of the polymer between the layers, and the melt-intercalation.

In order to obtain exfoliated polyvinyl acetate-layered silicate nanocomposites, we develop a new method of the melt intercalation, called masterbatch-method. First, the layered silicates were melt-mixed with low molecular polymers such as polyvinyl acetate or polyvinyl stearate which were synthesized by transfer reactions. These polymers improve the exfoliation since they diffuse easily into the gallery of the layers caused by their low molecular weight and melt viscosity. Moreover, the interactions between the short polymer chains and the alkyl chains grafted on the layered silicates are better than with high molecular polymers. In the second step, the masterbatch consisting of layered silicate and low molecular polymer was melt-mixed with the polymer matrix polyvinyl acetate to give the nanocomposite. The TEM (Transmission Electron Microscopy) microphotograph on the left-hand side indicates that an exfoliated polyvinyl acetate-layered silicate nanocomposite can be achieved using the masterbatch-method because the micrograph shows a small stack of only two silicate layers. In contrast, the micrograph presenting on the right-hand side illustrates a non exfoliated nanocomposite which is made up by mixing the silicates directly with the polymer matrix. Additionally, the use of the low molecular polymer effects a plasticization of the brittle polyvinyl acetate. Hence, it should be possible to create a flexible polyvinyl acetate film featuring low gas permeability and transparent appearance which will be the aim of the work for the next years.



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Investigation of a dissolved H₂ sensor for applications in anaerobic biogas monitoring

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Climate change concerns and high oil prices are the driving force for renewable energy sources such as biogas. In general, the natural process of anaerobic digestion is a relatively stable system that occurs in nature without the need for precise process control. However, under high loading conditions process failures are known to occur. The stability and efficiency of anaerobic digestion relies upon the balance between the degradation of organic waste to hydrogen, formate, acetate and volatile fatty acids and the conversion of these fermentation products to methane and carbon dioxide. Digester stress conditions can cause an imbalance between volatile fatty acids production and consumption resulting in the accumulation of volatile fatty acids. The digester breakdown involves tedious production losses and considerable financial expenses, which foil the intended advantages of energy generation. Therefore, a reliable monitoring of the anaerobic biogas production is important for the optimisation and controlling of the process. One relevant parameter for process monitoring is the concentration of dissolved hydrogen, because hydrogen build-up is a serious sign of imbalance in the net activities of the most important microbial groups in anaerobic digestion.

In this work, several transducer principles for the detection of dissolved hydrogen are presented - a hydrogen-sensitive metal-insulator-semiconductor (MIS) device in combination with a liquid-to-gas membrane and an amperometric sensor in combination with an electrolyte-insulator-semiconductor (EIS) structure. These sensors are evaluated in an anaerobic environment with known concentrations of dissolved hydrogen in distilled water. Simultaneous hydrogen measurements are performed with a commercially available hydrogen sensor and compared to the self-fabricated sensors.

Acknowledgements: The authors gratefully thank the Federal Ministry of Education and Research (BMBF) for financial support of this work, project "EMSiG".





Fig. 1 | Design of the proposed sensor (A) layout of the H₂ sensor consisting of an amperometric sensor in combination with a pH-sensitive EIS structure $[H_2 \rightarrow 2H^* + 2e]$; (B) expected response curve for the amperometric and field-effect sensor.

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A Reconfigurable Vector Signal Generator with Two Phase controlled $\Sigma\Delta$ -Synthesizers

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The emerging wireless communication trend in mobile phones demands a seamless connectivity to multi-service networks and communication standards such as GSM, WLAN, GPS, etc.. These multi-band radios require a transmitter architecture able to change between different operating bands and to adapt its features to available standards and requirements. At the same time the emphasis is to shrink the size and power consumption of the hand held mobile devices. A majority of the mobile RF transmitters employ in-phase and quadrature (IQ) vector signal modulator and benefits from their capability to implement linear and non-linear modulation standards. The drawback of IQ-transmitters is the non-linearity introduced by the components constituting the transmitter i.e. digital to analog converters, mixers, phase shifters, and power amplifiers. Dealing with this often leads to a complex transmitter architecture composed of linearisation techniques and dedicated front ends optimized to specific communication standards.

This thesis addresses the complexities associated with the classical IQ-modulators and presents an architecture for a new generation of a sigma delta vector signal generator ($\Sigma\Delta$ -VSG). In contrast to a classical IQ-VSG the $\Sigma\Delta$ -VSG is free of digital to analog converters and mixers and is composed of two phase controlled RF $\Sigma\Delta$ --frequency synthesizers. This concept is based on adding two phase modulated RF signals, which gives an architecture of a reconfigurable VSG for constant envelope and variable envelope modulation schemes. Furthermore, wideband PLLs can tune the VSG to the different operating bands of the required communication standard. In this thesis work classical and novel VSGs are discussed and their performance is compared by means of system level simulations. Prototype VSG hardware is realized and QAM modulations are performed to demonstrate the modulation accuracy and reconfigurable nature of the proposed VSG. The prototype $\Sigma\Delta$ -VSG with the reference frequency of 32MHz and loop bandwidth of 1.2MHz performed the 16-QAM with the symbol rate of 200kSym/s and with EVM values as low as 0.36%.

The thesis also includes the design concepts of low phase noise VCOs. The first design is of a 1.8GHz dual-mode oscillator with the phase noise of -143dBc/Hz at 1MHz offset as compared to a classical LC-oscillator which has -136dBc/Hz. It achieved the figure of merit (FOM) of -187dBc/Hz. The second design aimed at investigating the 1/f-noise up conversion in oscillator designs. The flicker noise reduction technique implemented resulted in an improvement of 7dB in an oscillator phase noise performance.

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EGA69

RFID-basiertes Sensorsystem zur Realisierung intelligenter Verpackungen, "Intellipack"

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Thin-film gas sensor with flexible polyimide foil for the detection of gaseous H₂O₂

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In aseptic filling systems for foods, the sterilisation of packages is the essential process for achieving a long shelf life of filled products and avoiding the transmission of pathogenic microorganisms, especially for perishable foods, like milk and fruit juice. Among the variety of physical, thermal and chemical methods, gaseous H_2O_2 has become the most significant sterilisation agent for carton packages in the last decades. For sufficient sterilisation efficiency at low exposure time, the packages have to be treated by H_2O_2 in combination with heat. Therein, the sterilisation efficiency primarily depends on the present H_2O_2 concentration on the inner surface of the packages.

For monitoring the sterilisation process with gaseous H_2O_2 inline, a thin-film gas sensor has been realised (s. Fig. 1). The calorimetric sensor was built up on polyimide instead of conventional silicon in order to optimise the sensor response behaviour. Thus, a flexible polyimide foil with a thickness of about 25 µm is used as substrate for temperature-sensitive thin-film resistances due to its expedient thermal properties (low thermal conductivity and thermal endurance up to 400 °C). The thin-film resistances were covered by spin-coated SU-8 photo resist, which is temperature-stable up to 350 °C and inert in H_2O_2 atmosphere, and catalytically activated by a dispersion of manganese(IV) oxide. The exothermic reaction mechanism of the H_2O_2 decomposition on the catalyst involves two pathways i) a redox reaction with electron exchange with the catalyst creating free radicals, and ii) a chain reaction in which the final products, namely water and oxygen, are formed. The calorimetric gas sensor possesses a linear response behaviour with a sensitivity of 7.15 °C/(% v/v) in a H_2O_2 concentration range from 0 to 8% v/v.

In a following step, the novel flexible gas sensor will be directly placed on the inner surface of a test package – on a critical location, like folding edge – and connected to a wireless electronic board for monitoring the sterilisation process of aseptic carton packages inline.





Fig. 1 | Thin-film gas sensor with flexible polyimide foil for H_2O_2 monitoring in aseptic carton packages (chip size 10 x 10 mm²).

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Relevance of the respiratory quotient in mammalian cell culture fermentation

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Relevance of the respiratory quotient in mammalian cell culture fermentation

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The production of biopharmaceuticals like recombinant proteins and monoclonal antibodies take place in cell culture fermentations. Only human and animal cells are able to synthesize complex substances with complicate structures like EPO (Erythropoietin, Roche) or Factor VIII (Bayer Healthcare).

To get high production yields with high quantity and accurate quality, which is relevant for the pharmaceutical function, the monitoring of the fermentation is very important.

In microbial fermentations, the respiratory quotient (RQ; ratio of carbon dioxide evolution rate (CER) and oxygen uptake rate (OUR)) is principally used to observe an industrial production process. Because of the difficulties with measuring the CER to evaluate the RQ in cell culture media that contains Sodium Bicarbonat (NaHCO₂), the RQ was not a parameter of interest in cell culture fermentations up to now. In presence of a cell produced acid (e.g. lactic acid), chemical carbon dioxide (CO₂) gets in addition to the biological CO₂ into the headspace of the fermenter. The CER can therefore not be detected directly [Frahm et. al. 2002]. Not only NaHCO₃-buffered media has certain effects on the examination of the RQ, but also antifoam agents that are used in fermentations interfere in the determination, however, in this case in a positive manner. Figure 1 shows a hybridoma cell fermentation, which includes no antifoam agent. The signals of the the CTR and the OTR proceed very calm whereas the CER and the RO go on very noisy. In contrast to this, figure 2 shows another hybridoma cell fermentation, that contains 0.1% of the antifoam agent Pluronic F68. During this fermentation process, the curves of all parameters indicate, in comparison to the other cultivation, very calm signals. Only at the beginning, where the cell density is low, the measurement of the RO is a bit agitated. In the further run the signal becomes more stable. This is caused by the addition of Pluronic F68. Although there is no foam development in the fermentation as a result of bubble-free gassing, the exclusive presence of an antifoam agent causes different chemical effects on the gas solubility in the fermentation broth [Morao et. al. 1999].





Fig. 1 | Fermentation without antifoam agent

Fig. 2 | Fermentation with 0.1% antifoam agent

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Biochemical structure of fetal membranes linked with premature birth

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While a normal pregnancy lasts 40 weeks, preterm birth is defined as the childbirth before reaching the end of the 37th week of gestation. One of the main reasons for preterm birth is the premature rupture of the fetal membranes (PROM = rupture of amniotic sac at least one hour before onset of labor) which leads in 30 - 40% of all cases to a premature birth. This is critical because the neonatal death rate is substantially due to the mortality of premature infants. Furthermore a preterm birth always requires immense expenses. Depending on age and birth weight the costs for a premature infant can amount to $12000 \in$. Gynecologists still do not have any diagnostic instrument that reliably indicates the probability of preterm birth or PROM.

The human amniotic sac tissue is a tough but thin (100 – 800 µm), transparent pair of membranes consisting of the two layers amnion and chorion. The membranes hold a developing embryo (after the twelfth week of gestation called fetus) until shortly before birth. When the membranes rupture they leak amniotic fluid and in most cases labor begins within 48 hours and the baby has to be born. To be able to comprehend why the membranes rupture, the understanding of the stability and the components of the amniotic sac tissue are of particular importance. As being a connective tissue, the fetal membranes consist of extracellular matrix (ECM). The ECM itself is made up of two main classes of extracellular macromolecules: glycosaminoglycans like Hyaluronan (HA) and fibrous proteins like collagen. The resilience of the fetal membranes is mainly due to its high collagen content which withstands overexpansion of the tissue.

In vitro examinations of fetal membrane samples shall show how this biochemical structure is linked to premature birth. Our previous studies have already shown that there is a positive correlation between maximal bursting pressure and collagen content of fetal membranes obtained after birth at term and after PROM. That means the higher the collagen content of the amniotic sac tissue, the more stable it is relating to bursting pressure.

It is assumed that towards term more HA is attached to the membranes or more water is absorbed by HA (theoretically up to 6 liters per gram HA possible). This could lead to a separation of amnion and chorion making the tissue considerably more unstable whereby a rupture of the membranes is promoted.

For this reason the next step is to show, if hyaluronic acid is also correlated to the maximal bursting pressure and collagen content and if it is also linked to premature birth.

The results are an important step towards finding biomarkers which allow a prediction of an upcoming premature birth.

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46 | 3RD GRADUATE SYMPOSIUM

HP Bioforce – The Final Phase

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To find and characterize new molecules in drug development for pharmaceutical industry, it is a necessary tool to perform mechanical (functional) measurements on isolated cells or thin 3D tissue equivalents, respectively. For cardiovascular systems contractility measurements of cardiomyocytes and vascular muscle cells play an important role. But how can such forces be examined in extremely thin cell layers or shown to be improved by drugs?

The answer to this was given by the project HPBioforce: Inside an incubator a fully automated system is measuring the forces excerted by cells growing in layers of only a few µm thickness. All steps - including all cell culture processes, drug application and measurements - can be controlled from the outside without opening the incubator. This is important, as slight environmental changes like variations in the temperature have a direct effect on the cell behaviour. The force measurement is based on the CellDrum™ technology, which is suitable to fulfil all the requirements for this fully automated system to work in high throughput. In the past the system was continuously optimized and it is now - due to the possibility to analyse a bigger number of samples in a relatively short time - ready to attract the interest of industial customers. In order to satisfy the needs of the industry, in this last phase of the project HP Bioforce the approval of all integrated processed has to be performed. This does not just include the validation of the measurements, but also the quality of the cell culture procedures. As the use of disposables is not practical in this closed environment cleaning procedures for the liquid handling components have to be optimized to avoid any cross-contamination with drugs between the different experimental groups. Additionally the results of the measurements were compared to those from manually performed experiments to prove the working principle and to show the advantages of this automated cell force measurements.



Figure 1 |: On the left hand the different components of HP Bioforce are shown. On the right hand some results from measurements of NHDF monolayers are presented (n=4): A is the control group, B samples were intrinsically damaged, C samples were damaged but recovered due to drug application

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Vismut: The knowledge-based design approach for car body construction

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Vismut: The knowledge-based design approach for car body construction for small sized vehicle production batches

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Due to high market demands for niche product cars and vehicle derivatives, small series production is recently gaining more importance in automotive industry (for example for electric vehicles). Compared to the mass productions, small series production faces number of problems. Quick to market, high productions costs, limited knowledge and resources are some to name. Project "Vismut" aims at developing a methodology to tackle these problems. It aims at constructing a vehicle body with simple to manufacture components and reduce development time by using a knowledge based design approach in the fields of CAD design, manufacturing techniques and structural design.

Following diagram illustrates the basic building blocks of the construction philosophy followed in project Vismut. Unlike the present unisized car bodies, which are constructed from joining thin sheet metal stampings, standard extruded closed sections (beams) are used. These beams are connected at junctions through joints (nodes) which are manufactured by special casting or milling processes. The philosophy takes into account predefined manufacturing restrictions in terms batch size, cost etc. Structural knowledge base is another key feature of this construction philosophy. It aims at developing a process with which the performance of such a car body, comprising of beams and joints, can be predicted by using simplified analytical calculation methods.



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A high-tech attempt to predict premature birth

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Premature birth is one of the main problems of modern obstetrics, which affects 6 % of the annual deliveries in Germany, causing parental suffering, increased perinatal morbidity and mortality of newborn children and extended costs for the German health care system. Biophysicists at the University of Applied Science Aachen and gynecologists at the University Hospital of Cologne developed new investigation methods and instruments to understand the structural integrity of the amniotic sac aimed at a future technology to predict premature birth.

In an extensive in-vitro-study carried out by both universities, amniotic sac tissue samples of 60 deliveries were collected and investigated with the "Advanced Device to Investigate the Mechanical Properties of Amniotic Sac Tissue" (DIMPAST). During th past month the DIMPAST has been improved technologically and methodologically (DIMPAST II). Additionally, amniotic sac tissue samples of 42 deliveries were collected and investigated with the new design.

DIMPAST II measures thickness, bursting pressure, deflection value under air flow, and Young's modulus of the amniotic sac tissues providing biomechanical data for amniotic sac membranes (and other type of soft tissue membranes). Using Spectral radar OCT, the membrane was measured at the relaxation state (no membrane pre-tension) and the stiff state (membrane at 2D tension, see oral presentation).

As one result, the rupture side of the membranes independently of the `kind` of birth was the weakest membrane area. There was a also a statistically significant difference between the `rupture-middle` and the `rupture-placenta` sides. At the relaxation state the chorion was thicker when compared to the thickness at the stiff state whereas the thickness of the amnion was unchanged. Thus, only the thickness of the chorion changed when the membrane was under tension.

Correlating the biomechanical data derived with optohistological imaging of fetal membranes and integrating it into a new diagnostic instrument called PROMPT (Premature Rupture Of Membranes Prediction Test) will provide a revolutionary step in obstetrics to safeguard the structural integrity of the amniotic sac by optical biopsy and mechanical testing.

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Limit and shakedown analysis of elasticplastic bounded linearly kinematic hardening structures.

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Upper bound finite element analysis of the influence of hardening on ratchetting

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This work develops a new FEM based algorithm to investigate the influence of hardening on ratchetting of structures made of elastic plastic bounded linearly kinematic hardening material. Mathematically, the issue is considered as a constraint nonlinear programming problem and solved by combined penalty function and Lagrange multiplier methods. Model of hardening is described in Fig. 1. The influence of hardening on ratchetting of structures is showed in Fig. 2.



Figure 1 | Stress-strain relationship for uniaxial tensile test



(a) Simple frame



Figure 2 | FE analysis for ratchetting of simple frame.

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Intelligente Hydrogele

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Intelligent Hydrogels and switchable pourous media

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Hydrogels are three-dimensional polymer networks which have the ability to absorb high amounts of water. Due to this behaviour they are used in baby diapers, cosmetic products, drug delivery systems, contact lenses or as ameliorant. In response to an external stimulus such as pH or ion concentration, the here investigated hydrogels can reversibly change their shape due to the change of number or kind of cations. Depending on their chemistry, they may swell or shrink.

The syntheses of intelligent hydrogels are based on acrylic acid, vinylphosphonic acid maleic acid and its anhydride to increase the charge density, different kinds of cross-linkers, co-monomers and cross-linker concentrations which influence the mechanical properties and the speed of swelling/shrinking behaviour such as poly(sodium acrylate-co-sodium maleate), which was crosslinked by a diole as shown in Figure 1. The new types of hydrogels bear potential for use as sensors, actuators, and switchable porous media.

The mobility change of sodium ions and possible exchange reactions between different ions have been investigated by ²³Na and ²⁷Al MRI during the individual stages of the collapse and regeneration of the gels. The different stages of collapse and regeneration were additionally characterized by determination of the actual self-diffusion coefficients and the NMR T_1 and T_2 relaxation times.



poly(acrylic acid-co-maleic acid)



poly(Na-acrylate-co-Na-maleate)

Figure 1 | Synthesis of poly (Na-acrylate-co-Na-maleate) hydrogels through condensation of prepolymers

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Multi-gas sensor system for electronic nose applications

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The sense of smell is one of the most interesting of the five human senses and yet is understood the least. The human nose is widely used as an analytical sensing tool to assess the quality of drinks, foodstuff, perfumes and many products in the food, cosmetic and chemical industries. However, practical use of the human nose is severely limited by the fact that the human sense of smell is subjective, often affected by physical and mental conditions and tires easily. Consequently, there is considerable need for a device that could mimic the human sense of smell and could provide an objective, quantitative estimation of smell.

Recently, there has been increasing interest in developing such devices, the socalled "electronic nose (e-nose)". This is an electronic instrument capable of reproducing human senses using sensor arrays and pattern recognition systems (see Fig. 1). The principle of an electronic nose is, however, not restricted to detecting and recognising gases and odours, but may beyond that also be adapted to various technical applications. Within this project a multi-sensor system by means of an electronic nose for the evaluation of aseptic processes will be developed.

Hydrogen peroxide vapour (HPV) is used as sterilising agent in aseptic processes. It has a high potential of bacterial and sporicidal inactivation and is at the same time friendly to the environment. The packaging industry demands high standards of product quality and sterility. To ensure process sterility, purposely contaminated test packages with spores of *Bacillus subtilis* are being exposed to the sterilisation process employing HPV. Afterwards, the test packages are being examined for viable spores. Thereby, the logarithmic reduction of viable spores (log-rate) is a measure for the process sterility. The described method is well established for testing aseptic sterilisation processes, but is on the other hand a time-consuming and costly procedure. The preparation and evaluation of the microbial reduction test may last up to five days.

To overcome this problem, a multi-gas sensor system for the real-time evaluation of aseptic sterilisation processes by means of an electronic nose shall be developed. Therefore, selected commercially available gas sensors have been investigated on their cross-sensitivity towards influencing factors of the sterilisation process by HPV, namely the hydrogen peroxide concentration, temperature and humidity. An MOX and a solidelectrolyte gas sensor (λ -probe) have shown good characteristics in terms of sensitivity towards HPV, considering also reproducibility, long-term drift and stability. Further, the sterilisation effect of the HPV has been investigated by means of the microbial reduction test. A correlation between the sensor data and microbial reduction was found. Subsequently, based on this correlation it was possible to predict the microbial reduction by means of the sensor output over a wide range of parameters. This early stage experiment has already shown satisfactory results; further investigations taking up the idea of an "electronic nose" will be pursued.



Fig. 1 | Conception of an electronic nose

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Development and Testing of Hydrogen-Fuelled Combustion Chambers for use in an Ultra-Micro Gas Turbine

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For more than a decade up to now there is an ongoing interest in small gas turbines downsized to micro-scale. With their high energy density they offer a great potential as a substitute for today's unwieldy accumulators, found in a variety of applications like laptops, small tools etc. But micro-scale gas turbines could not only be used for generating electricity, they could also produce thrust for powering small unmanned aerial vehicles (UAVs) or similar devices.

Beneath all the great design challenges with the rotating parts of the turbomachinery at this small scale, another crucial item is in fact the combustion chamber needed for a safe and reliable operation. With the so called regular micromix burning principle for hydrogen successfully downscaled in an initial combustion chamber prototype of 10 kW energy output, a new design attempt aimed at the integration possibilities in a μ -scale gas turbine was undertaken (Fig. 1). For manufacturing the combustion chamber completely out of stainless steel components, a recuperative wall cooling was introduced to keep the temperatures in an acceptable range. Also a new way of an integrated ignition was developed.

The experimental investigations comprise a set of mass flow variations, coupled with a variation of the equivalence ratio for each mass flow at different inlet temperatures and pressures. With the data obtained by an exhaust gas analysis, a full characterisation concerning combustion efficiency and stability of the prototype chamber was possible. Furthermore the data show a full compliance with the expected operating requirements of the designated μ -scale gas turbine.

The introduction of the recuperative cooling of the chamber walls proves the feasibility of an all stainless steel combustion chamber design in the 10 kW class. After a total burning time of 10.5 hrs, no sign of structural damage or signs of excessive wear could be found in a visual inspection of the chamber parts after the test campaigns. The use of stainless steel instead of the much more expensive and difficult to machine inconel alloys or ceramic materials allows a cost effective production of the combustion chamber, and thus helping to reduce the overall price of a possible µ-scale gas turbine.

Although many hurdles are still to be overcome until this burning principle can be seen working in a real μ -scale gas turbine, the presented prototype already fulfils all set design point criteria for a safe and reliable operation and introduced many new features regarding gas turbine integration at microscale.



Figure 1 | 3D cutaway of complete test rig installation for the micromix combustor prototype with recuperative cooled chamber walls

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EMSIG – Entwicklung eines Multisensorsystems in Siliziumtechnik zur Beurteilung der Gärbiologie eines Anaerobfermenters in der Flüssigphase

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Development of an enzymatic H₂ sensor for anaerobic fermentation processes

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The conversion of biomass to the high-energy gas methane (CH_4 , biogas) is performed by syntrophic interdependent microbial consortia, part of which require strictly anoxic conditions and tolerate only small changes in environmental conditions. The initial degradation of complex polymers (carbohydrates, proteins and lipids) to monomers (sugars, amino and fatty acids) and the subsequential conversion of the latter to mainly acetate, carbon dioxide and hydrogen is mediated by hydrolyzing and fermenting bacteria. Finally, acetoclastic methanogens convert acetate to CH_4 . Likewise, CO_2 and H_2 are consumed by hydrogenotrophic methanogens to yield methane.

The interdependence in methanogenic communities is reflected by tight associations of fermenting bacteria and methanogenic archaea. In particular the interspecieshydrogen-transfer from fermenting bacteria to hydrogenotrophic methanogens is of general importance since hydrogen producing bacteria essentially rely on the hydrogen consumption by the archaea for thermodynamical reasons, while the latter depend on the constant supply of hydrogen as source of reducing equivalents for methane production. Thus, the concentration of dissolved hydrogen is a crucial parameter for the description of biogas processes, and changes in this parameter will likely allow detection of process disturbances at an early stage of occurence.

While a quantitative detection of hydrogen in the gas phase by means of various chemical sensors is a state-of-the-art technology, at present no detector system is known, which can directly detect **dissolved** hydrogen. In biogas facilities, detection of dissolved hydrogen is a chellenging task due to the presence of a large number of reducing and interferring compounds, which give rise to cross reactivity with sensors lacking the required selectivity. Moreover, some compounds (e.g. H₂S) do not only disturbe hydrogen detection but also act as a contact poison for the sensor surfaces.

The aim of this project is to develop an enzyme-based sensor for the detection of dissolved hydrogen in complex anaerobic environments like biogas fermenters. Therefore, immobilization of a [NiFe] NAD⁺ reducing hydrogenase from the lithotrophic "Knallgas" bacterium *Cupriavidus necator* H16 (EC 1.12.1.2, Fig. 1) on the sensor surface is planned in order to create sensors specific for hydrogen which are insensitive to hydrogensulfide mediated inactivation. The chosen enzyme is unique in terms of its oxygen stability, which allows enzyme purification and immobilization on the chip under air, facilitating mass production of the sensor.



Fig. 1. | Scheme of the NAD⁺ reducing H_2 as from *Cupriavidus necator* H16. The enzyme consists of six subunits (hoxF, hoxU, hoxY, hoxH, hoxI.).

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Name des Projektes Name of the project	GPU Faser Vis – GPU based visualization of nerve fibers from polarized high-resolu- tion brain data
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GPU FaserVis – GPU based visualization of multi-volume data

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The aim of the BMBF aided project *GPUFaserVis* is real-time visualization of high resolution nerve fibers of the human brain in context to theirs anatomy. So the nerve fibers and their crossings can be better researched and it gives an improved insight into their functionality and the connections to each other. With these visualizations we expect new knowledge of neurodegenerative diseases.

Our aim is to develop suitable data structures and parallel algorithms to build the visualization. The algorithms are executed on the Graphics Processing Unit (GPU). The advantage of computing on the GPU instead of computing on the Central Processing Unit (CPU) is its high degree of parallelism, so the GPUs have more computing power. We use as programming language C++ and on the GPU C for CUDA from Nvidia.

In the first year of the project the visualization of multiple volumetric data was focused. Volume Rendering is subdivided into direct and indirect Volume Rendering.

Indirect rendering techniques determine a surface model from the volumetric data and render it as polygonal mesh. A common indirect technique is the Marching Cubes algorithm, where the 3D data set is subdivided into small cubes. The algorithm marches through these cubes and determines how the surface cuts the cubes and preserves the surface. Figure 1 shows an example.

Direct Volume Rendering is performed on the volumetric data immediately. Thereby every voxel is assigned to a color and opacity usually by a RGBA (red, green, blue, alpha) transfer function. After this assignment, the RGBA value is projected onto the corresponding pixel on the display. Very high image quality is provided by Ray Casting. Ray Casting approximates the emission-absorption optical model by integrating along the direction of light flow. An example is illustrated in figure 2.

The first step is to combine two volumetric data sets, where both volumes are rendered with the indirect technique of Marching Cubes. The fusion is trivial. The surfaces are extracted independently and then the geometric primitives are mixed and rendered with standard techniques. Figure 3 shows an example.

Combining two volumes with direct rendering techniques is more difficult. The fusion of the data sets can occur at several positions inside the rendering pipeline. Four common levels of intermixing are Classification Level Intermixing, Illumination Level Intermixing, Accumulation Level Intermixing and Image Level Intermixing. The first fuses the volumes before the assignment of color and opacity is done. The second mixes the volumes after the volumes are assigned to two separate transfer functions and before the illumination is done. Accumulation Intermixing merges the illuminated colors. And the last fuses the independent calculated display images. In our research results the Accumulation Level Intermixing techniques provides the best image quality (figure 4).

The third combining technique, indirect with direct Volume Rendering, is explored in the moment.

The proposed algorithms have been implemented and tested on a graphics workstation with Intel Core i7 920 processor with 2.67 GHz, a Nvidia Quadro FX 5800 graphics card with 4 GB video memory and with 12 GB RAM. We tested the methods with volumes of size 256x256x256 and observed 25-100 frames per seconds. That is real-time quality.



Figure 1

Figure 2

Figure 3

Figure 4

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Development of a LAPSbased biosensor system for water quality monitoring

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Water is one of the most important resources of mankind and providing clean water is a fundamental element of civil water supply. Continuously increasing industrialization jeopardizes the quality and increases the need of monitoring for potential harmful substances. Due to their diversity, today's water monitoring systems are not able to meet actual demands.

Measurement systems using living species, like daphnia, see shells or fish give a good opportunity to determine contaminations, but due to logistics, cost reasons and the need of trained staff, they are not applicable for a totally covered water monitoring. As a result, even in large, modern cities such as Zürich, online monitoring is limited to a small number of physical parameters such as temperature, pH, electrical conductivity, oxygen content and turbidity^[1].

Alternatively, vertebrate cells show a similar sensitivity to pollutants and toxins to that of higher life-forms, which makes them suitable for water monitoring, especially for chip-based sensors. Nevertheless, recent scientific base experiments show that multiple parameters of cell behaviour have to be determined in order to provide sufficiently sensitive and reasonable information for water monitoring.

As a part of the research cooperation "MultiCellSense" (MCS), this project concerns the development of a light-addressable potentiometric sensor (LAPS) to monitor the status of immobilized vertebrate cells. The sensor should include the determination of metabolic activity of the cells as well as impedance measurement of the cell layer, investigating changes of the cells' morphology.

The working principle of the LAPS system is based on a field-effect sensor consisting of an electrolyte-insulator-semiconductor (EIS) structure. Linked to the prevailing pH value of the sample or beneath the immobilized cell layer, the potential on the chip surface is modified, which influences the depletion region in the semiconductor layer (see Fig. 1a). Pointing a modulated light source on this layer induces a photo current, whose magnitude depends on the depletion region size. By illuminating the chip locally, multiple measurement spots can be defined on a single EIS structure (see Fig. 1b). This fact enables multiple spot evaluation strategies to reduce impacts of external influences (e.g., temperature, pH) and to enhance the signal stability.





a)

Fig. 1 | a) Distribution of potential for varying pH values at an EIS structure b) Multiple measurement spots with various cell types and blank spot for differential measurement on a single chip.

¹ M. Toman, "Wasserversorgung für Zürich," TU Wien, 2005.

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66 | 3RD GRADUATE SYMPOSIUM

Actor-driven Workflow Execution in Distributed Environments

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Distributed environments like Grid and Cloud computing have become very popular over the years. Whereas Grid computing links disparate computers to form one large infrastructure, harnessing unused computing resources that can be provisioned as a utility, Cloud computing goes one step further with on-demand resource provisioning. With the advent of these technologies scientists and engineers build more and more complex applications to manage and process large data sets, and execute scientific experiments on distributed heterogeneous resources. Such application scenarios require means for modeling and executing complex workflows that can be seen as a collection of tasks which are processed on distributed resources to achieve an overall goal. In order to support the definition, the coordination, and the execution of such workflows, various workflow management systems have been developed.

One central demanded quality criteria for such a workflow management system is the workflow execution time that highly depends on the used scheduling strategies, whose goals are to find dedicated available resources as actors for individual tasks in due course. A great and powerful amount of resources with different capabilities reduces the workloads and the size of the job queues of each individual resource resulting in minor execution times of tasks and workflows.

Because all workflow management systems use an approach where newly created workflow tasks are explicitly pushed to dedicated resources, the amount of resource candidates is often limited to the resources that provide a specific interface. This can for example be the computing resources of a particular Grid. Another consequence of this system-initiated resource allocation is that the resource providers have to give up some of their autonomy, making it difficult to enforce their local policies or to reject specific tasks. To increase the amount of available heterogeneous resources, we realize an alternative resource-initiated allocation, where the actors become the driving force of the execution of a workflow.

In such a scenario, the commitment to undertake a specific task is initiated by the resource itself rather than the workflow system's scheduler. This task distribution approach could effectively speed throughput by eliminating the notion of complex resource allocation by scheduling services. Indeed, this approach makes a centralized resource control by scheduling systems impractical. But, at the same time it opens new perspectives with respect to community approaches, where members delegate their resources to execute tasks as actors for the benefit of a community.

For the integration of an actor-driven approach, it is necessary to offer the tasks that need to be executed to the resources, e.g. by informing multiple suitable resources of the existence of a specific task. So the resources, to which a workflow task is offered, are free to choose whether they are interested in undertaking a specific task or not. Generally, this procedure results in the task being placed on an intermediary repository, the individual resources can access through well-defined interfaces to apply for the execution of the tasks.

This task repository has been implemented and integrated into the UNICORE Grid middleware, so that workflow management systems have been enabled to publish task in the repository, resources can apply for. In the future the actor-based concept should be extended to enable workflow execution in Cloud environments and take advantage of their provided elasticity.

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Pattern-driven engineering of SaaS applications for occasionally connected clients

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With Software as a service (SaaS) a new distribution model was established in the last few years. The basic idea behind the concept is the deployment of business (or personal) software via internet, typically consumed by a standard web browser. This software is customizable within fixed bounds. Usually external or own data sources can be integrated in a standardized way. The benefit for the consumer is, that he does not need to care about an own IT infrastructure and that he has a payment model based on an "on demand" way. Occasionally connected clients, like mobile devices, cannot consume this kind of applications continuously or in a constant quality. The deployment has to be done in a platform specific manner, serving the clients with efficient program code and strategies to work temporarily without a data connection to the service provider.

Composition, Customization and *Network independence* for mobile SaaS applications are the main target of the research project. Therefore so called "patterns" (proven solutions for common problems) are evaluated and developed. One of those patterns is called "Offline Strategy" and was recently published to the research community. By evaluating the current network status, it switches the strategy of the underlying service usage with consideration of the access transparency. In the current development phase, the pattern will be enhanced to work at a finer granularity level. Common known patterns are also used to build the underlying architecture. The design pattern "Model-View-Presenter" for example improves the composition/customization aspect. It allows a customer to select and easily switch the graphical interface component or create a new one. Furthermore, "Factory" patterns create the components at runtime, when they are needed and are crucial for the customer specific composition of the SaaS application.

Besides these patterns used for the underlying distributed architecture to establish mobile SaaS products, there are patterns under development, which encapsulate typical use cases for mobile service technicians. The "Identify Machine" pattern for instance, decomposes the problem of "identifying machines" for further information handling into common "solution portions". Methods like Barcode scan, QR Code photography, Radio frequency identification (RFID) or a simple Service Tag number are unified under a common (software) interface. Even yet unknown identification procedures are supported due to the underlying, pattern-based architecture. Another use case pattern is "Timesheet". It defines common data types in shape of domain entities. For the development of this pattern, multiple software solutions and form template were analyzed to factor out the common specifications, some typical details and the specific parts of timesheet use cases. This work affects the data being processed, the processes themselves, and best practices for the "user experience" (the behavior and structure of a good graphical interface).

Further research work has to be done, to find an adequate description style for the use case patterns and integrate them into modeling tools. One goal is to enable the "SaaS solutions" developer to easily select the right patterns in the software setup for one specific customer and its mobile context.

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Hydrostatic Propeller Drive How to transform an industrial heavyweight into a lightweight hydraulic system

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The development of a hydrostatic propeller drive for a self launching glider poses certain challenges which can mainly be summarized as maximizing the transmission's efficiency and minimizing its weight. Before discussing the details of how to realize such a system, it should be explained why a hydraulic power transfer can be advantageous for a glider with self-launch capability. Currently these gliders rely on a drive belt that directly couples the combustion engine's output shaft with the propeller. Therefore the engine cannot be started with the propeller still stored in the fuselage. In case the pilot wants to return to the airfield in the powered flight mode and the engine does not fire-up, or the belt fails, the glider's aerodynamic performance is significantly reduced due to the extended propeller. As the engine is usually started at an altitude as low as possible, this configuration leads to a significant chance for forced landing. The hydraulic system offers an easy to realize option to enable an engine start-up without extending the propeller beforehand, thus increasing the available altitude to select a landing field.

Apart from the flight safety aspect a hydrostatic transmission also offers additional flexibility in the overall aircraft configuration. Due to the fact, that the connection between the engine and the propeller is not rigid, both elements can be placed at their optimal position. This would allow propeller installations as shown in the figure below.

Returning to the challenges at hand, one must consider that the power to weight ratio of a single hydraulic motor is quite high. However, the total weight is significantly affected by the additionally required components. One of these is the fluid, which actually transfers the power. To minimize its weight, the volume needs to be reduced as much as possible. By proceeding in that direction, two effects occur. Firstly the system pressure needs to be increased and secondly the fluid's circulation time has to be reduced. While a system pressure of 400bar can be realized with off the shelf components, reducing the circulation time increases the thermal stress on the fluid and therefore requires careful control of the fluid temperature. To deal with these boundary conditions the current layout is essentially a closed loop system with an additional feed pump. To comply with the thermal requirements a heat exchanger is installed in the return line right after the hydro motor. To further drive down the weight, options to use lighter materials especially for the hydro pump's and motor's housings were discussed with the component manufacturer.

To increase the overall efficiency it is essential to design the system so the pump and the motor can be operated at their most efficient working point. The required analysis of the system's properties is based on simulation and experiments. The latter will be performed on a test stand that is currently under construction. The simulation tool in use is DSHplus, software especially developed for the calculation of fluid systems. The latest simulation results confirmed the principle system layout and the functionality of the test stand. Once the simulation and the test bench provide analogue results, the simulation will be used for parameter variation with the goal to optimize the system's operating conditions and properties. To conclude, the use of a hydraulic power transmission in a glider with self-launch capability provides a potential benefit for the aircraft designer due to greater integration flexibility of the drive train, and also offers enhanced flight safety by allowing engine start-up with propeller retracted. The key to a successful implementation is the reduction of the required number of components and the minimization of the weight of each component, including the oil volume. Experiments and simulation tools pave the way towards an optimal layout to run the system at its most efficient operating point.

Fig. 1 | Alternative aircraft configurations with the hydrostatic propeller drive





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On-line determination of the condition of microorganisms by a light-addressable potentiometric sensor

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The light-addressable potentiometric sensor (LAPS) is a semiconductor-based chemical sensor with the advantage to detect chemical species on the sensor surface in a spatially resolved manner (Fig. 1a). In this work, a LAPS platform has been established in order to determine the response of microbes to variable environmental conditions on the chip surface. Thereby, the extracellular acidification in consequence to the metabolic activity of the microbes has been detected. This sensor principle might be useful to analyse metabolic activities of microorganisms in biotechnical processes, e.g. for monitoring of the biogas process.

The easy to handle organism *Escherichia coli* was immobilised as a model organism on the sensor surface. The bacteria were immobilised by embedding them into polyacrylamide gel (Fig. 1b). During growth, *E. coli* produces organic acids, like acetic and lactic acid. The acid production results in local pH shifts, which change the local potential of the LAPS surface. Since the buffer capacity of the media influences the pH shift in response to the produced acid, this parameter has a strong effect on the sensitivity of the LAPS device. The surface potential shifts measured in bacterial cultures are very small. Thus, compensation for sensor drift and temperature effects is essential. In practice, this compensation was achieved by an "on chip" differential set-up.

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Fig. 1 | a) Principle of a LAPS, b) Layout of the "on chip" differential set-up.

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