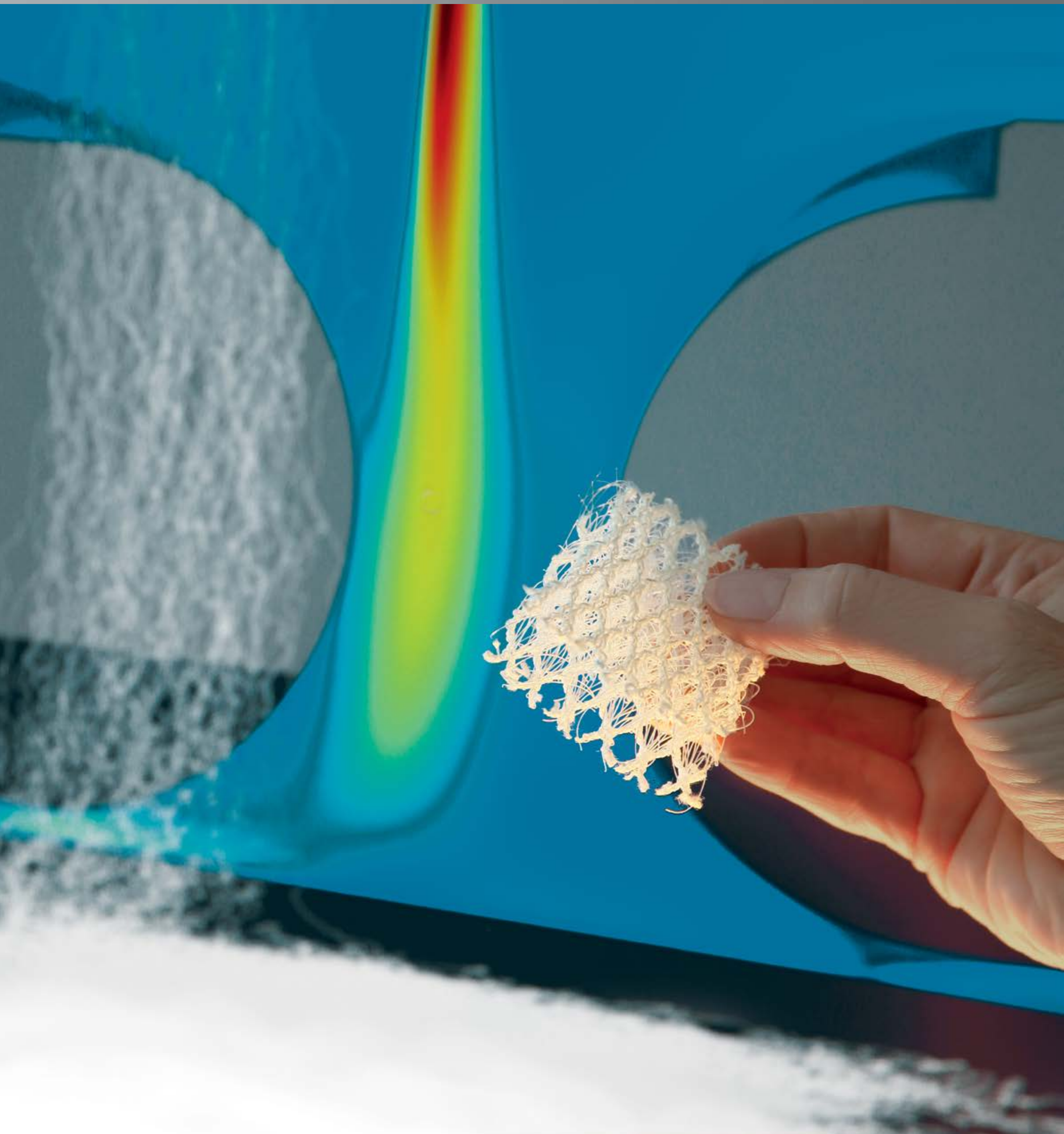
TRANSPORT PROCESSES



DR. DIETMAR HIETEL
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HEADS OF DEPARTMENT

MATHEMATICAL MODELING AND SIMULATION-BASED OPTIMIZATION OF TRANSPORT PROCESSES

The Transport Processes department models complex industrial challenges and develops efficient algorithms for their computer-based simulation and optimization. Our primary tasks occur in the context of the technical-natural sciences (fluid dynamics, radiative transport, optics, structural mechanics, etc.) which, when modeled, lead to differential equations that are mainly characterized as transport algorithms.

From the perspective of our industry customers, such tasks typically concern product optimization or the design of the production processes. The department's expertise includes collaborative research projects with engineering-oriented research and development departments at our partner companies, studies that include design and optimization recommendations, as well as software programming support of components or complete tools.

As in previous years, we balanced the budget and were economically successful again in the year 2018. As part of a scientific institution, our department further improved its position as documented by the increase in publication activity. Consequently, we were able to acquire new, longer-term, public funding for research projects.

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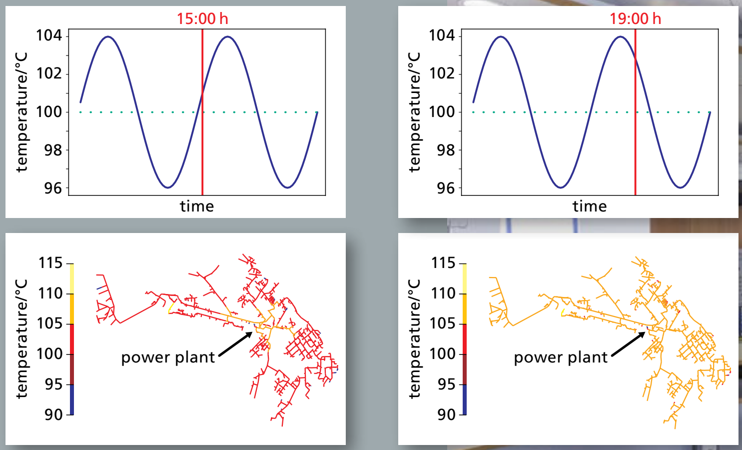
MAIN TOPICS

- Flexible structures
- Fluid dynamical process design
- Grid-free methods
- Energy transport networks and model reduction



1

DYNAMIC SIMULATION TO IMPROVE EFFICIENCY OF DISTRICT HEATING GRIDS

1 *Dynamic simulation of the sub-network in Ludwigshafen: feed-in temperature at the power plant (top), temperature in the district heating network (bottom)*

The project is sponsored by the Federal Ministry for Economic Affairs and Energy (BMWi) and implemented in cooperation with GEF (engineering company) and TWL (Technische Werke Ludwigshafen) with the aim of developing dynamic network simulations to improve the efficiency of district heating operations. The project has already developed and tested a software tool for network simulation, which TWL uses to optimize its operations.

District heating grids supply heat and warm water. The operators of district heating plants generate part of their revenues from the sale of electricity, generated in parallel at the combined heat and power (CHP) plants. The integration and dynamic control of the district heating grids as energy storage systems ensures efficient operation of the turbines and optimal use of the existing storage tanks.

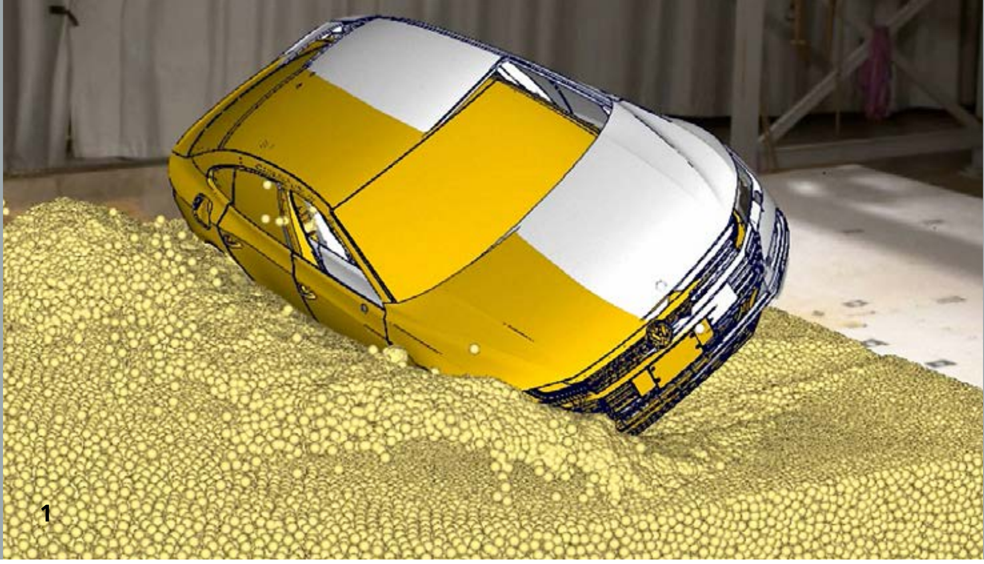
Software models optimize grid operations at district heating power stations

The current software to support the operation of CHP plants focuses on either the optimal use of local resources, where the district heating network is managed as an unstructured sink, or on detailed models of the power grid and locally triggered hydrothermal conditions to ensure supply to all customers. However, this usually happens without having an integrated simulation of the overall picture with fluctuating operating conditions.

The dynamic simulation of district heating grids has huge advantages: using the software, the grid operator can read both the temperature and the flow conditions at any point in the district heating grid at all times. In doing so, the inlet temperatures provided at the power plant and mass flow fed into the grid can be controlled, which implies that the costs of switching on gas turbines for heat generation can be avoided.

Mathematics creates a digital twin behind the software

The traditional methods of solving the fluctuating thermohydraulic equations are too inaccurate or too expensive for use in proposing operational controls for district heating grids. This is the reason the project developed a new numerical method that does not need to further subdivide the lines. The software creates a digital image of the real district heating grid and an automated control center, which is more necessary than ever before considering the ongoing decentralization of input points. The optimization horizons over a few days can be mastered using model-predictive control and automatic differentiation.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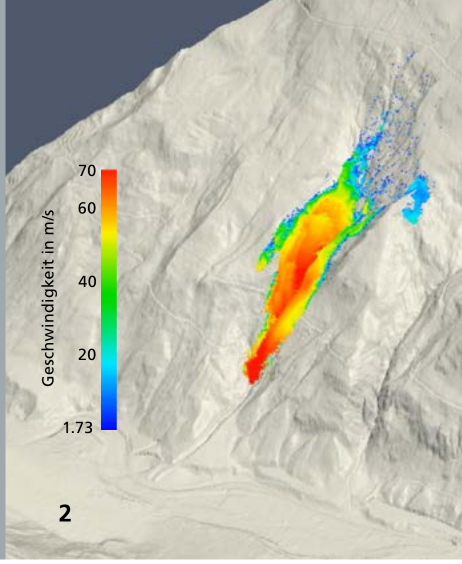


2

MODELING NON-NEWTONIAN FLUIDS WITH MESHFREE

In cooperation with Fraunhofer SCAI since 2018, we supply a software product for the mesh-free simulation of physical processes. The innovative software combines the expertise of both institutes in the area of meshfree scientific computing and satisfies a wide range of applications.

Our development of the Finite-Point-Method

Meshfree simulation expands the horizon of computational models, in particular, in the context of industrial applications. The Finite-Point-Method (FPM) was originally developed at ITWM and has been in use since the year 2000 in many projects with European partners. The method was first developed and used to model airbag deployment. Later, FPM evolved into an implicit, meshfree flow tool.

The absence of calculation grids saves preparation time for the simulations. How do you model the flow of rain water, the passage of water, the filling or sloshing from a passing auto? How do you emplace floating pontoon bridges? How do you optimize Pelton turbines in hydropower plants? The applications are plentiful and FPM has a clear advantage over mesh-based methods in the area of free surface flows and fluid structure interaction (FSI). This implies the need to solve large linear equation systems. Combining FPM with the algebraic multi-grid process (SAMG, Fraunhofer SCAI) enables efficient solving of linear systems. The resulting software is called MESHFREE.

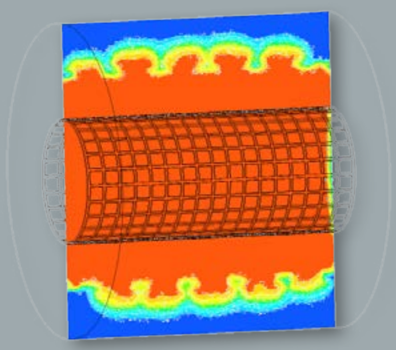
Meshfree simulation of granular media

We are significantly expanding the focus of meshfree simulation. Not only do we rely on completely new applications, for example, for process engineering or processes in the food industry. We are also exploring a much wider range of materials. In addition to traditional computational fluid dynamics (CFD), we also focus on non-Newtonian fluids – for example, foams, batters, or polymer melts. MESHFREE is also used to model the dynamics of granular media like sand, gravel, snow, grain, flour, etc. For example, this is part of a German Research Foundation (DFG) project at University of Innsbruck (Working Group for Geotechnical and Tunnel Engineering). In addition to the simple Drucker-Prager material model, we anchor hypoplastic and barodesy descriptions (complex, non-linear, constitutive frameworks to express very exact surface behavior) in MESHFREE. Together with automobile manufacturer VW we rely on VPS (Virtual Performance Solution), a software package from the ESI Group, for example, to simulate an overturning vehicle (rollover processes) on sandy surfaces.

1 *Lateral rollover of a vehicle in sand: comparison of experiment and simulation*

2 *Simulation of the Wolfsgruben avalanche (March 13. 1988), geo data: with kind support of BFW Austria.*

MESHFREE



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MACHINE LEARNING IN TEXTILE MANUFACTURING

1 *CFD simulation of a virtual bobbin in a dye bath*

2 *Colored bobbins in textile production*

Today, we see dramatic changes in the demands being made of the textile industry. The trend in many areas is towards customization, similar, for example, to buying a new car. Consumers increasingly demand tailor made products. This shift in consumer behavior is lucrative for European textile companies as production of customer-specific products in small lot sizes results in the return of manufacturing to Europe. However, this requires the digital transformation of production, which we support with our hybrid simulation-based machine learning (ML) methods.

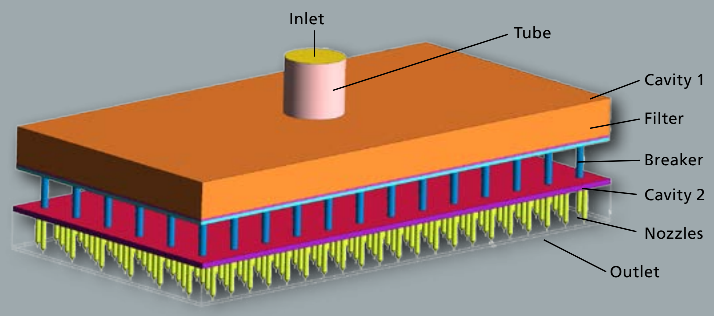
Data-based machine learning by itself is not sufficient

In data-based machine learning, we develop statistical learning algorithms that recognize patterns and laws in given data. The benefits of ML algorithms depend to a great extent on the quality and quantity of the available data. As a rule, enough measured data is collected for the purpose of quality assurance in the textile industry. However, only in the rarest of cases is sufficient data available to make a connection between the process parameters and the product quality. Consequently, we are not able to use pure, data-driven machine learning – especially for plant and process optimization for today's customized production processes.

Hybrid simulation-based machine learning

To design and optimize production processes in the textile branch with ML methods, we develop and apply a hybrid approach. Extensive experience is available for process and product design in textile industry. We formalize this expert know-how by building a physical model to describe the process and, subsequently, implement a computer based simulation. Models provide the missing data for the development of suitable ML algorithms and linking with available measurements. In this concept, ML closes the gap between physical based simulation of production processes and the level of quality of the end products – which, in many cases, is not accessible to physical models.

The optimization of winding machines with regard to a better dyeing of the wound bobbins illustrates this innovative hybrid ML process in AiF's DensiSpul project.



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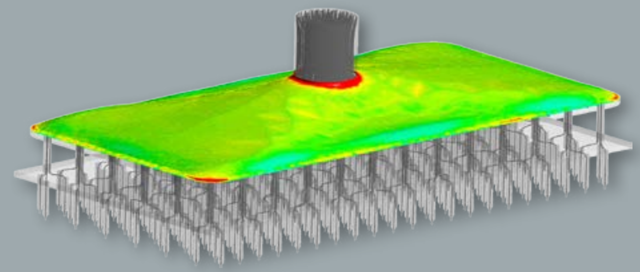

2

DYNAMIC FLOW DESIGN OF POLYMER SPIN PACKS

The melt spinning process is the most common way to produce synthetic fibers. We use simulation and optimization methods to help our clients with the development, design, and improvement of spin packs.

1 Geometry of a characteristic spin pack

2 Spin pack with improved distributing cavity

Spin packs are used in the manufacture of synthetic fibers and nonwoven fabric. The spin pack is a metal block, consisting of cavities and tiny channels through which the thick viscous liquid – the polymer melt – is forced to flow. The molten mass is fed through a tube into the spin pack. On entering the first cavity, the molten mass spreads across the entire width of the spin pack. The melt passes through several layers of filters that are held in place by a support plate before being extruded through the fine capillaries of the spinneret. The extruded filaments are either wound into yarn or formed into a nonwoven fabric.

Analysis and simulation provides a look inside the spin packs

Our work always begins with a fluid dynamics analysis of the actual state. We simulate the flow within the spin pack while taking the characteristic flow properties of the polymers into account. Using special tools, we then evaluate the residence times and pressure profiles.

The analysis provides specific information about which component of the spin pack needs to be improved. Frequently, we find significantly long residence times in the cavities. This is damaging to the polymers which decompose after some time under thermal stress. To prevent this, we use shape optimization to design components with very low and even residence times. The analysis also reveals strong pressure generators, which indicates the need to make appropriate adaptations to the corresponding components.

The simulation-based analysis enables us to look inside the spin pack, which otherwise remains hidden. This is a decisive design advantage, as now all fluid dynamic parameters become directly quantifiable. Problematic components are identified and modifications are directly validated. Another benefit is that the development times are faster and companies can avoid costly design errors.

NEWS

SEMINAR ON MACHINE LEARNING IN PROCESS ENGINEERING

In November 2018, the department organized a workshop titled "Introduction to machine learning (ML) in process engineering." The seminar gave participants a detailed introduction to the world of machine learning. The workshop focused on understanding the most important terms like supervised versus unsupervised learning, as well as an overview of ML algorithms typically used in regression or classification problems. An overview of Deep Learning completed the theoretical background portion. Dr. Simone Gramsch and Dr. Andre Schmeißer shared their expertise in lectures and a stimulating final discussion round of questions and answers. The event was jointly organized together with our long term partner, the non-profit association COMPETENCE NETWORK PROCESS ENGINEERING PRO3.

NEW WEBSITE "MESHFREE.EU"

The department has worked with the Fraunhofer Institute for Algorithms and Scientific Computing, SCAI since 2018 to develop MESHFREE, an innovative software product for meshfree simulations of physical processes. We combine the expertise of both mathematical institutes in the field of mesh-free systems computing on the English language website meshfree.eu. All developments surrounding the product are quickly and clearly visible on that media for industry and research purposes. The website is one leg in our support and promotion of the software as a major player in the market. More information is provided on page 25.

MESHFREE

TOOLS FOR FLEXIBLE AND EFFICIENT DISTRICT HEATING SUPPLY SYMPOSIUM

The March 2018 symposium highlighted the ongoing transformation in the district heating industry and showed participants how to optimize the operation of district heating networks and make them more flexible. AGFW, the energy efficiency association for heating, cooling, and co-generation organized the event and Fraunhofer Center Kaiserslautern provided the venue. The research project DYNEEF (see page 24) served as the incentive for the event. The project develops new methods for requirements-based operational control of district heating power plants.

Front, left to right: Dr. Andre Schmeißer, Dr. Tobias Seifarth, Dr. Almut Eisenträger, Dr. Isabel Michel, Sergey Antonov, Dominik Linn, Dr. Norbert Siedow, Dr. Pratik Suchde, Dr. Jaroslaw Wlazlo, Sebastian Blauth, Niklas Lehne, Dr. Raimund Wegener, Dr. Dietmar Hietel, Dr. Jörg Kuhnert, Johannes Schnebele, Markus Rein, Manuel Wieland, Jens Bender, Dr. Robert Feßler, Matthias Eimer, Dr. Jan Mohring, Dr. Christian Leithäuser