OPTIMIZATION

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INTERACTIVE DECISION SUPPORT BASED ON MODELS AND DATA

The main activity of the division is to develop custom solutions for planning and decision problems, especially, in the logistic, engineering, and life sciences while working in close cooperation with our partners in research and industry.

The work takes a methodical approach by integrating simulation, optimization, and decision support systems. Simulation in this context refers to the construction of mathematical models while taking into account the design parameters, restrictions, and the variables to be optimized such as cost.

The division's core competencies include the development and implementation of application- and customer-specific optimization methods. These methods provide the best possible solutions for process and product design. The close integration of simulation and optimization algorithms that give special consideration to multi-criteria approaches is our unique selling point along with the development and implementation of interactive decision support tools.

Overall, optimization is viewed not so much as a mathematical problem to be solved, but rather as a continuous process to be supported by the department with the development of suitable tools. Particular attention is paid to the selection of an adequate model in terms of quantity and quality of available data. We use machine learning methods to process the data and to calibrate the models, as well as to supplement and explain phenomena that cannot be explicitly modeled.

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MAIN TOPICS

Operations Research

- Production planning and scheduling
- Layout and cutting problems
- Supply chain networks

Technical Processes

- Process engineering
- Medical planning
- Machine learning and hybrid models

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GAMOR – COLLABORATIVE DUTY SCHEDULING IN THE CARE SECTOR

1 *Digital wish book*

2 *Conflict resolution options*

The care sector suffers from a massive shortage of skilled workers. The nursing profession is perceived as unattractive: physical strain, shift work, comparatively low salary are the decisive factors. Negative effects of shift work can be reduced by increasing the autonomy of the employees. They no longer have the feeling that their private life is at their employer's disposal in addition to their professional life. Instead, they have the chance to create and shape the balance themselves.

The GamOR project addresses this creative scope: with the help of collaborative and digitally supported duty planning, the satisfaction of nursing staff is to be increased. The design of the duty planning process based on ergonomic and experience-oriented aspects ensures integration into everyday work life as well as sustainable motivation.

Minimal conflicts: recognition and resolution

From an employee's point of view, one of the main quality measures of a duty roster is compliance with desired days off. We call a set of such wishes, which can´t be fulfilled at the same time, conflicts. Conflicts that can be resolved by cancelling any involved wish are "minimal conflicts". These must be resolved independently of any wishes added later. In GamOR we develop algorithms for the efficient determination of minimal conflicts as well as game theoretical models for their (partially) automated resolution. In addition, we use constraint-based models to calculate optimized duty roster alternatives. In addition to wishes and staffing requirements, both legal and ergonomic rules are taken into account.

Implementation through a digital services platform

The concepts for collaborative duty scheduling and the algorithms for planning support are implemented prototypically by a service platform. The employees operate the platform via tablets, in perspective also from their own smartphone. Employees see the planning month with all wishes entered (Fig. 1). New wishes can be added, existing wishes can be withdrawn. Conflicts that involve the employee are presented clearly and possible solutions are shown (Fig. 2). Those responsible for planning can directly use a web interface for data maintenance.

This research and development project is funded by the Federal Ministry of Education and Research (BMBF) and the European Social Fund (ESF) as part of the "Future of Work" programme and supervised by the Karlsruhe Project Management Organisation (PTKA).

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

ESF Europäischer Sozialfonds für Deutschland

EUROPÄISCHE UNION

Zusammen. Zukunft. Gestalten.

ELIMINATING TRACE ELEMENTS WITH SUSTAINABLE ADSORBENTS

Water pollution from medications, biocides, and industrial chemicals is on the increase because sewage plants do not break down many of these substances, so they are released into the environment. BioSorb is a three-year joint project with Fraunhofer UMSICHT to develop new adsorbents that can eliminate such molecules from municipal wastewater.

The approach is based on renewable raw materials which are more resource-friendly and significantly more selective than conventional activated charcoal filtering. Especially promising are protein-based materials, called bioadsorbents, because these are cheap and a nearly infinitly available worldwide.

Step by step to cleaner water

We start by screening various protein-rich materials. We focus our detailed investigation on variants of renewable raw materials, test them initially in small-scale adsorption experiments. The most promising materials are then analyzed in the next step. Often, a chemical treatment – like a combination acid and heat treatment – improves the adsorption capacity.

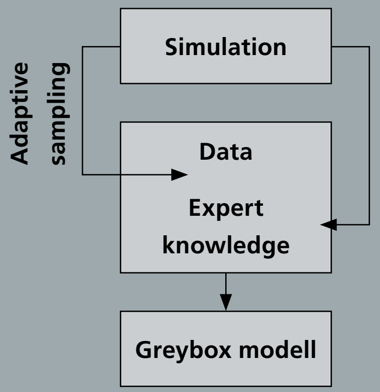
In a series of large-scale tests, selected bioadsorbents are characterized by their effectiveness to adsorb diclofenac (a pain killer) and metoprolol (a beta-blocker). These two molecules are suitable as test substances since they are often detected in ground and surface waters and, until now, are hardly degraded in sewage plants. From an economic perspective, a re-usable adsorptive material is the most promising. This is why we search for a renewable systems using different solvents and analyze and characterize the selected materials in great detail.

ITWM supplies simulation expertise

In parallel, a numerical adsorption model is being developed based on our institute's expertise with simulation tools for water supply and sanitation, which had already been proven in the EU's Nanopur project on drinking water preparation. BioSorb is now building on these findings. We use our high computing capacity and experience with simulation studies to provide the required expertise for multi-scale simulation, which evaluates the adsorbents.

The results are validated and verified in the final step. This step initially takes place using contaminated water, where we can test the effectiveness of the adsorbents without overlaying measurements. Subsequently, the adsorbents are introduced in practice-relevant waters, for example, the water from the sewage plant at Wuppertal-Buchenhofen.

1 *Protein-based bioadsorbents are being investigated to improve the adsorption of drugs from wastewater in order to reduce the burden on humans and the environment in sewage plants.*



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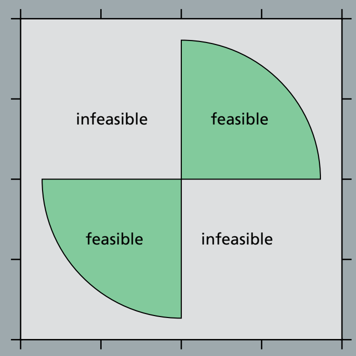

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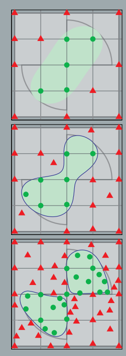

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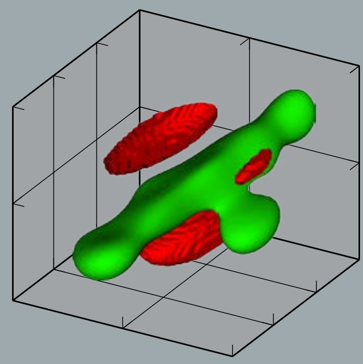

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MACHINE LEARNING WITH EXPERT KNOWLEDGE

1 *Workflow for the development of Greybox surrogate models from data and expert knowledge; adaptive sampling enables efficient data acquisition.*

2 *Two-dimensional parameter space of a toy example with a well-defined feasible range (green); this example demonstrates the efficiency of adaptive sampling for predicting operating windows.*

3 *The sequential development of the parameter space from Fig. 2 leads to feasible (green) and infeasible (red) simulation results and a corresponding model prediction for the operation window (blue), which improves with each iteration.*

4 *Visualization of the predicted operating window of a chemical plant*

In various research projects and in cooperation with industrial partners, we develop strategies to improve machine learning methods by including domain-specific expert knowledge. An important field of application is chemical process engineering.

Machine learning algorithms make it possible to derive patterns from data. The resulting models generalize the information contained in the data statistics in order to predict unknown results. However, it can be of decisive advantage to also consider the context of the data and to incorporate domain-specific expert knowledge in the models. This approach can take coherences into account which are insufficiently reflected by the pure data statistics.

The greybox approach

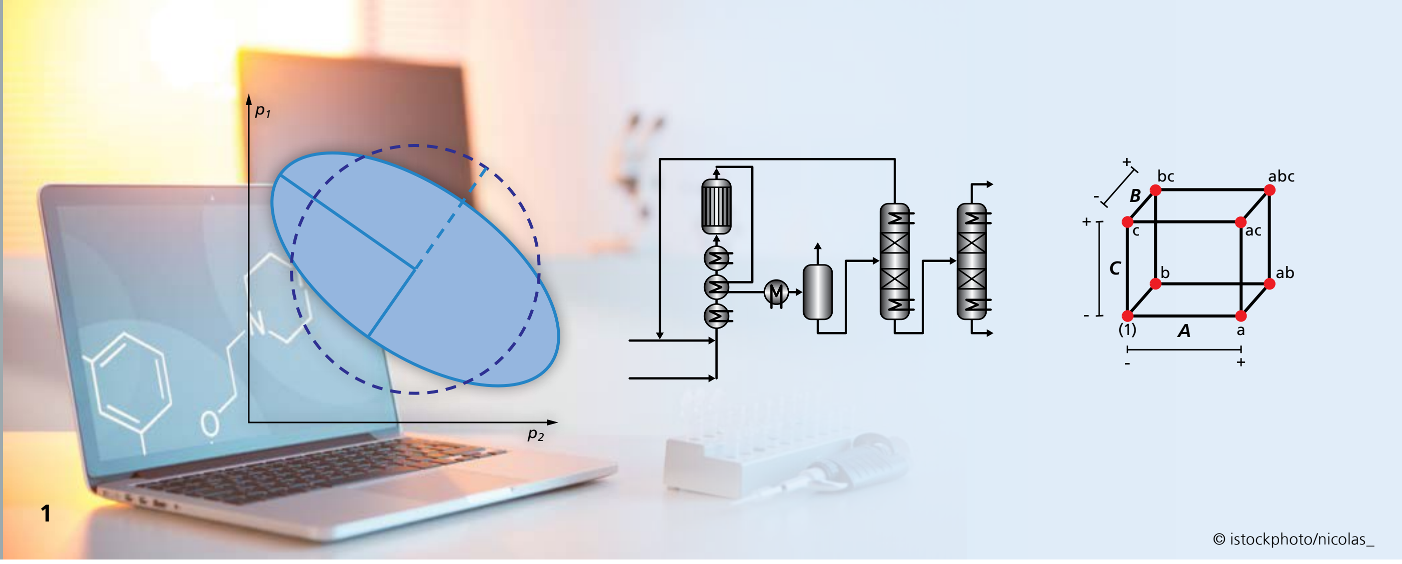
In industrial practice, data is often obtained from simulations since they are cheaper than experiments and free of measurement uncertainties. Solving optimization problems requires large amounts of such simulation data. Surrogate models, which can be evaluated faster than the original simulation, consequently bring a major speed advantage.

Since industrial simulations are based on physical laws, expert knowledge is already explicitly available. The challenge is to integrate it into a machine learning method in a suitable way. In this so-called "greybox" approach, knowledge-based models are combined with data-driven models to form a hybrid overall model.

Exploration of operating windows in chemical process engineering

Efficient data acquisition is crucial. Non-dynamic simulations of chemical plants can only be evaluated for process parameters for which the plant can be operated stationary. In a joint project with BASF SE, we are developing a method to determine these stationary operating windows with the aid of machine learning methods and greybox modelling.

With our novel strategy of adaptive sampling we are able to explore the parameter space sequentially in the most efficient way possible. For this purpose, a compromise must be found between the simulation effort and the expected information gain. The knowledge about the operating window then simplifies the optimization of process parameters by restricting the parameter space to be searched.



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MODEL-BASED EXPERIMENTAL DESIGN IN PROCESS ENGINEERING

In chemical process engineering, data are collected in experiments in order to calibrate physically motivated models. These experiments are always time- and cost-intensive. Therefore, their planning is about deriving as reliable models as possible from as few experiments as possible. In a cooperative project with BASF, we develop and implement methods that support this.

1 *Left: Scheme of a covariance ellipsoid to illustrate the confidence region of adjusted model paramaters*

Center: Scheme of a mini-plant with one tubular reactor and two distillation columns

Right: Statistical design of experiments for a linear model with three inputs

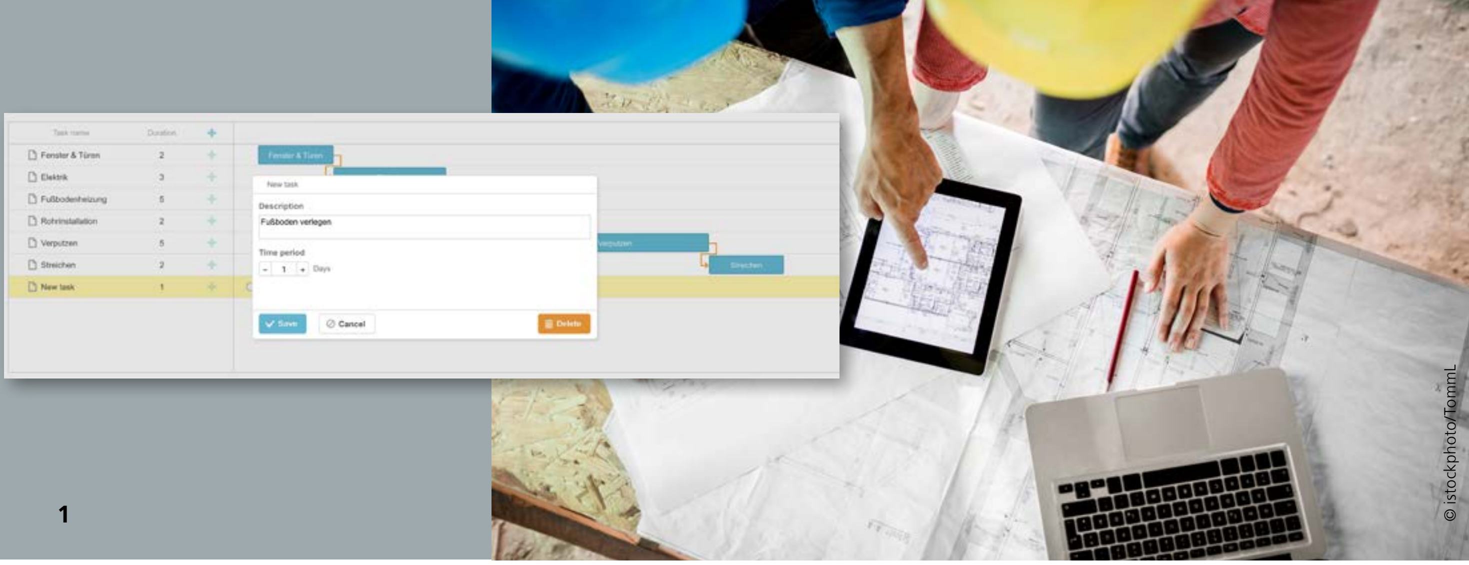
The reliability of model calibrations is influenced in two ways: On the one hand, the error bars of the estimated parameters, but also the prediction errors of the model are directly proportional to the measurement accuracy in the experiments. In other words, the more accurate the sensors, the more reliable the model prediction.

On the other hand, in order to calibrate successfully, it is crucial to consider correlations in the sensitivity of the models – especially with regard to the model parameters at the measurement points. This is illustrated in the following example.

Catalyst: Aging versus Temperature

Chemical reactions are generally faster at higher temperatures than at lower ones - this is why, for example, foods are cooled to prolong their shelf life. In chemical reactors, catalysts are often used to accelerate reactions. These catalysts age, so their effect decreases over time. Therefore, the reaction temperature is increased with increasing catalyst age in order to guarantee a constant quality of the reaction product. In this way, catalyst age and reaction temperature are closely related. It is not possible to calculate the separate effects of temperature and catalyst age on the end product. The experimental design proposes to run the reactor once at low temperatures and high catalyst age, and once at high temperatures and low catalyst age. With these two additional operating conditions, the effects can be separated and independently quantified.

The aim of the cooperation project with BASF is to transfer the concepts described above to complex models of pilot plants (Fig. 1). These are then calibrated to model parameters on the basis of their sensitivities, uncertainties are estimated (Fig. 2) and the corresponding experiments are planned. To this end, we solve large nonlinear optimization problems and make their results usable on interactive user interfaces.



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CONWEARDI
CONSTRUCTION WEARABLES DIGITIZATION

CONWEARDI – SMART PROCESSES IN CONSTRUCTION

1 *Planning assistance for construction sites*

In the project ConWearDi (Construction Wearables Digitization), we develop together with research partners and craftsmen a platform to enable the digitalization of services in the building industry with industry 4.0 technologies. The focus is on a tool for process planning.

The topic of digitalization is increasingly coming into focus. Construction companies in particular, which tend to be small or medium-sized enterprises, are still lagging far behind in the digital change. If you want to remain competitive in the future, you have to face digitalization and take advantage of opportunities that arise.

This is where ConWearDi comes in: The aim is to develop a web platform that enables the digital exchange of information between all those involved in construction. Building on this, services are developed to support the planning and implementation of construction site processes.

Web platform

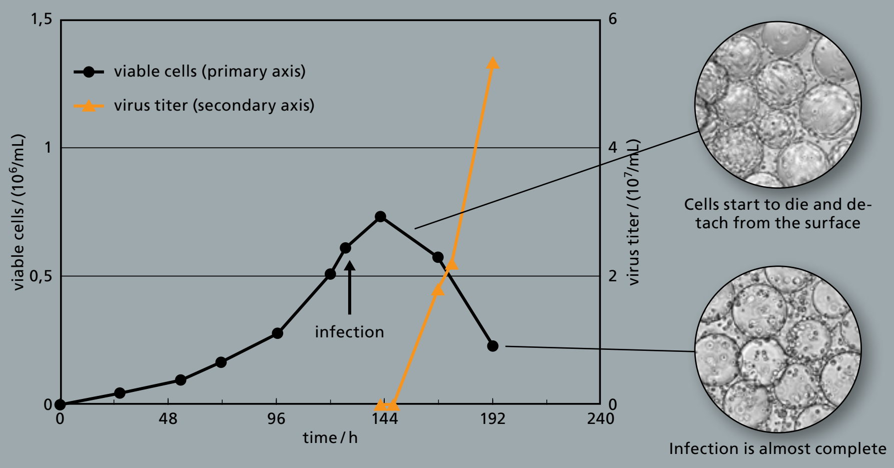
The platform connects (software) tools of different kinds. Examples are ERP systems, planning tools or machines and materials equipped with sensors. Wearables are also used, e.g. smart glasses, which record and process information in real time. As part of the project, we develop an application for process planning that is specially adapted to construction site processes and connected to the platform.

Construction site planning under uncertainty

The adherence to schedules across several construction projects is often only possible through a precise division of the work packages and an optimal use of the available resources. Changes in the course of the project (e.g. absence of employees) make it difficult for the planner to maintain an overview. In ConWearDi we develop models and algorithms that support the site planner in his tasks. An adequate consideration of the uncertainty of planning-relevant information plays an important role. For example, in many cases the feasibility of operations depends on the weather. In these cases, simulations help to develop suitable evasion strategies.

With the help of the resulting software, work packages can be automatically scheduled and optimized with regard to various goals. However, the final decision remains with the planner, who can interactively adapt the created plans (e. g. drag & drop) and is directly informed about the consequences of his decisions.

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung



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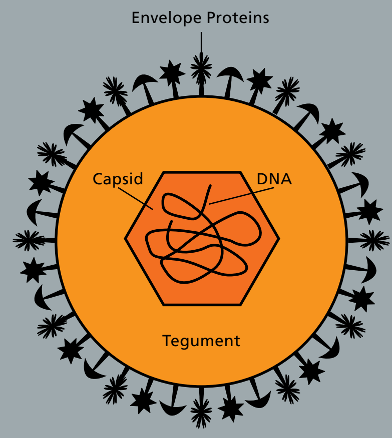

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VIRUSES IN TUMOR THERAPY: HOW TO GROW THERAPEUTIC VIRUSES

Clinical studies with first generation oncolytic (cancer destroying) viruses are very promising. To ensure this new approach is available to all patients, we develop scalable and robust production methods for these viruses. As part of the Fraunhofer-Gesellschaft, our experts are researching these issues using mathematical methods within the framework of project TheraVision.

When to infect and when to extract?

Preparation of the viruses consists of an upstream and a downstream process. Initially, special host cells are grown in the upstream process. At a certain time, these are infected with the virus. From this moment on, the viruses multiply in the host cells until the cells are destroyed and the viruses produced escape into the surrounding nutrient solution. After a certain period of time, the nutrient solution is extracted and fed into the downstream process where the virus is filtered out.

The aim of our project is a model-based optimization of the upstream process using experimental data. We have prepared a model that represents the cell and the growth of the virus as a function of controllable variables. The first variables to be optimized on the basis of the model are the infection and extraction points.

Parameter estimates and compromises

The model we use is a parameterized system of ordinary differential equations. Aided by the use of statistical methods (parameter estimation), we have identified the variables (growth and death rates) such that the model closely matches the experiments conducted at Fraunhofer ITEM.

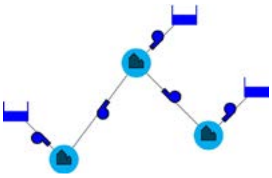
When the model is constructed in this way, the optimal time of infection and extraction is determined using a special optimization method (multiple shooting). The focus is on several target aspects: the maximal achievable number of viruses, and the effectiveness and purity of the extracted solution. These aspects are either individually optimized or an optimally balanced compromise is sought between the targets (multi-criteria optimization).

1 *Cell growth (black) and virus growth (orange). The images show the microcarriers the cells attach to, and the cells themselves.*

2 *Schematic representation of the herpes simplex virus*

NEWS

COpt2 – SAVING ENERGY IN THE DRINKING WATER INDUSTRY



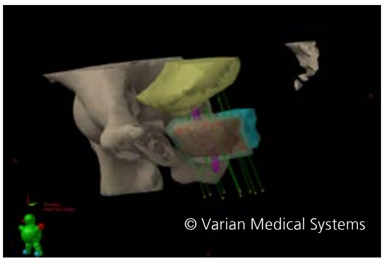
Complex networks in drinking water supply

The BMBF sponsored project, H2Opt, provides prototype software that supports energy efficient design and operation of drinking water plants. It results in energy and cost savings during planning and operations involving the drinking water supply. The software is in daily use at the energy company EWR, located in Worms, Germany. Launched in 2019, a follow-up project is to expand the prototype for the more complex water supply networks in Landau and Jockgrim. We simplify and improve workflows and develop new concepts to prevent water supply shortages. The project is funded by the European Fund for Regional Development (EFRE). Initially, the priority is the investigation of pumping operations because that is where an estimated 30 percent on average can be saved in energy costs.

COGNAC – ROBUST CAMPAIGN PLANNING FOR HARVESTS

The lighthouse project COGNitive AgriCulture (COGNAC) focuses on the design of an agricultural platform. The project is to deliver critical innovations in three areas: “Networked ecosystems”, “Sensor systems”, and “Autonomous field robots”. A variety of applications have been realized as demonstrators. One case study is about robust harvest campaign planning, in which we review continuously updated ripening data and weather forecasts for the fields to be harvested. This allows us to plan ahead in personnel and equipment scheduling, which gives agricultural contracting firms a higher likelihood of meeting their customer appointments. Our robust models and algorithms reduce drying and fuel costs, while at the same time increase food quality and customer satisfaction.

DECISION SUPPORT FOR BRACHYTHERAPY



In collaboration with Varian Medical Systems, our multi-criteria decision support system has been embedded in the world’s leading radiotherapy planning software for cancer patients. Our goal for next year is to make interactive planning available not only for external radiation therapies (IMRT, VMAT) but also for brachytherapy. This therapy directs the radiation source either on the immediate vicinity of the tumor or into the tumor itself, raising new questions that have to be solved, for example, regarding the optimal positioning of the catheter for directing the radiation.

Front, left to right: Johanna Schneider, Till Heller, Esther Bonacker, Dr. Katrin Teichert, Dr. Neele Leithäuser, Dr. Neil Jami, Dr.-Ing. Tino Fleuren, Dr. Cristina Collicott, Jasmin Kirchner, Dr. Sandy Heydrich, Dr. Elisabeth Finhold, Dr. Christian Weiß, Dr. Heiner Ackermann, Dr. Volker Maag, Dr. Michael Bortz, Prof. Dr. Karl-Heinz Küfer, Dr. Peter Klein, Dr. Gregor Foltin, Dr. Dimitri Nowak, Dr. Jan Schwientek, Dr. Tobias Fischer, Rasmus Schroeder, Dr. Dennis Heim, Dr. techn. Johannes Höller, Melanie Heidgen, Helene Krieg, Dr. Patricia Bickert, Dr. Martin von Kurnatowski, Dr. Raoul Heese, Andreas Dinges, Dr. Michal Walczak, Pascal Wortel, Dr. Sebastian Velten, Dr. Michael Helmling, Patrick Schwartz