OPTIMIZATION

Multi-criteria optimization and interactive decision support for process planning based on models and data as well as support for Design of Experiments (DoE) to accelerate and improve products are core activities in research and development assignments of BASF under the umbrella of the High Performance Center Simulation- and Software-Based Innovation in cooperation with the University of Kaiserslautern and led by Fraunhofer ITWM.

PROF. DR. KARL-HEINZ KÜFER
HEAD OF DEPARTMENT

MODEL- AND DATA-BASED DECISION SUPPORT

The core competence of the department of Optimization is to develop individual solutions for planning and decision problems in logistics, engineering sciences and life sciences in close co-operation with customers.

Methodologically, our work is characterized by the interrelationship of simulation, optimization and decision support. Simulation in this context refers to the creation of mathematical models while taking into account the design parameters, restrictions and optimization of the quality and cost.

The division´s core competencies include the development and implementation of application and customer-specific optimization methods to calculate the best possible processes and products. Unique selling points are the integration of simulation and optimization algorithms, the special consideration of multi-criteria approaches as well as the development and implementation of interactive decision support tools.

Overall, optimization is viewed not as a mathematical problem to be solved, but rather as a continuous process, which we support by developing suitable tools. We particularly focus on the adequate choice of the model in terms of quantity and quality of the available data. Methods of machine learning are not only used for data processing and calibrating models, but also to represent physically non-explicitly modeled phenomena.

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MAIN TOPICS

- Process Engineering
- Medical Therapy Planning
- Model Learning and Smart Data
- Production Planning and Resource Efficiency
- Arrangement and Cutting Problems
- Supply Chain Networks

USEFUL DATA AND MODELS WITH MACHINE LEARNING

1 *Planar glass plate before the bending process*

2 *Elevated glass plate after the bending process*

Model-based optimization of production processes significantly reduces production costs while maintaining or even improving product quality. However, to get the best possible results, it is crucial that the underlying models are reliable. Oftentimes expertise is already available in practice, either through experience or through well-established scientific equations. From this knowledge one can derive a preliminary expert model. Most of the time though, this model contains too many gaps, so that an overall process optimization is not possible. This is where our optimization department with its proficiency in “machine learning” comes into play.

Supervised and unsupervised learning methods

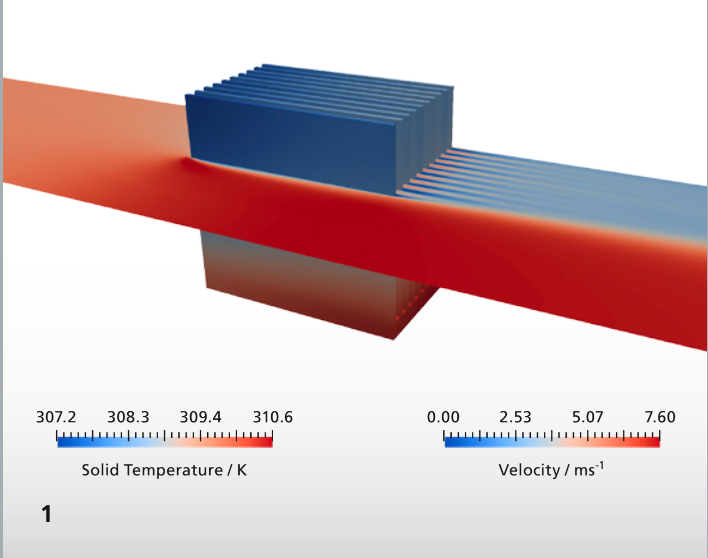
In addition to the expert knowledge, large sets of data are usually available for implemented production processes, where sensors monitor and log the operating state of the production system over time. In chemical production plants, for example, these sensors might monitor pressure, temperature or electrical power consumption. With a sufficient amount of data, statistical learning algorithms can be used to close the gaps left in the expert models.

There are many kinds of learning algorithms, broadly divided into unsupervised and supervised learning. Examples of unsupervised learning are pattern recognition and time series clustering. The supervised learning algorithms include, for example, classification methods or approaches via mathematical regression. It is often not trivial to find which algorithm to use in which situation.

Statistical learning algorithms create coherence and reliability

One difficulty with the expert models is that a production process usually consists of many individual, interconnected production units. Gaps in the expert models can result from a lack of data on these individual units or from insufficient knowledge of how they interact.

Through statistical learning algorithms the overarching interactions within the production system can be explored. More detailed models can then be developed and their reliability evaluated with confidence intervals. If physical knowledge is used not only in areas where data exists, but also for extrapolation to areas where no data has been collected. Using strategies for the optimal design of experiments, we can even make suggestions for further data acquisition in order to further reduce uncertainties.



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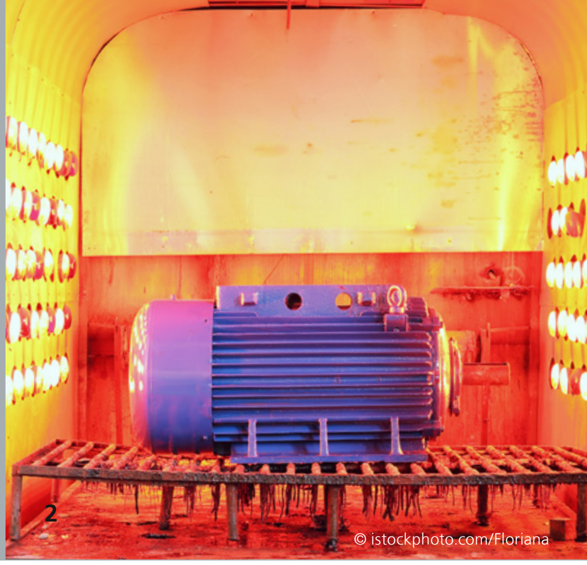

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OPTIMIZING HEAT TRANSFER AND COOLING OF ELECTRONIC COMPONENTS

During the operation of electronic components and computer processors, electrical resistance causes heat. Higher computational power increases the temperature. In the worst case, over-heated components malfunction or break. We improve heat-sink designs to provide sufficient cooling for industrial products.

1 *Simulation of air flow and heat transfer*

2 *Oven curing of an electric motor*

Our algorithms outperform the genetic algorithms

Commercial plate-fin heat-sinks transfer heat from the source along multiple fins to the cooling air. The number of fins, their thickness, the height and the distance between them define the heat transfer and fluid dynamics during the cooling process. Our algorithms for the computation of best geometries are efficient and precise. In comparison to commonly used evolutionary algorithms, they outperform by a factor of ten.

Ranging from electronics over paper making to oven curing, we can optimize any problem modeled by a CAD engine. Sandwiching algorithms perform best for convex problems. Hyperboxing algorithms are not as efficient, but, they can process nonconvex information. Sometimes model simplifications help us to reach the optimum faster. If necessary, algorithms are adjusted to adapt to new problems. We are constantly working to improve our algorithms.

Automotive industry, watch out – we optimize cooling processes

Our next goal is the optimization of oven curing processes in the automotive industry. Temperature, air flow and position of painted car parts change the oven curing process. We optimize this process in terms of heat distribution and energy consumption while quality shall not be lost.

Our cooperating partners, the Fraunhofer-Chalmers Research Centre for Industrial Mathematics FCC at Sweden, have developed an innovative simulation method. Due to IPS IBOFlow, we can implement many industrial processes and analyze them automatically. We use it to compute the heat transfer and fluid dynamics during the cooling process.

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DIGITAL PRODUCT DEVELOPMENT AT BASF

1 *Laboratory employee tests the wetting properties of a silicon wafer.*

One of the biggest challenges in the chemical industry for product developers is to spend the least possible effort to come up with a low-cost chemical compound that meets certain cost and quality properties.

Problem description, sample project, and software development

An example is the production of surface coatings. Various properties are desirable depending on the area of use of the coating. In addition to surface protection, for example, certain smoothness or optical properties may be required. Frequently, the objectives are competing, so that a suitable compromise must be found.

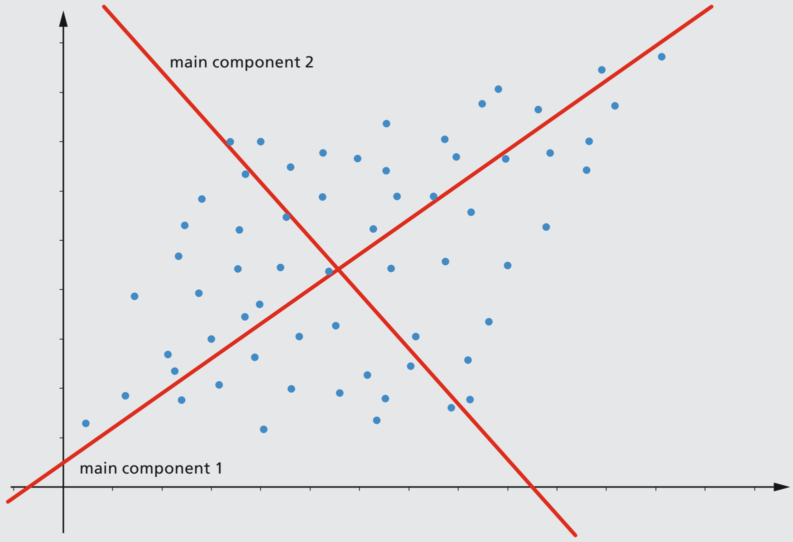
Below, we present a typical workflow for a new research project: First, one defines the objective functions and design variables before starting the first series of experiments. Based on the initial results, one then generates a mathematical model to predict the appropriate design specifications. These are used to start a new series of experiments and this process continues until a satisfactory compound is found.

Our department has developed a software tool to assist the chemists throughout this process. It starts with the analysis and visualization of the data, continues with the modeling of the individual target variables and supports in finding best compromises and in planning of a new experiment.

Machine learning and modeling

The mathematical model chosen to describe the desired functions depending on the design variables is of major significance. The processes in chemical manufacturing are often highly complicated and difficult to model. Together with BASF SE, we are developing a tool to address this issue using machine learning methods. A particularly complex challenge is selecting a suitable model, as this is essential for the quality of the optimized solution.

Various methods are used to measure the suitability of the model, such as cross-validation. This method uses part of the data for training and the remaining part for the validation of the model. For example, it is used in selecting the components for linear regression models in order to avoid over-adaptation of the data.



Specifically, it is about improving model quality by filtering out the low-impact components that are random in nature. However, in very few cases do purely data-driven models lead to the goal. That is why we include the user's expert knowledge in the modeling process.

2 *The figure shows a data set with two principal components in a two-dimensional space. Principal component analysis finds the directions which best explain the variance of the data.*

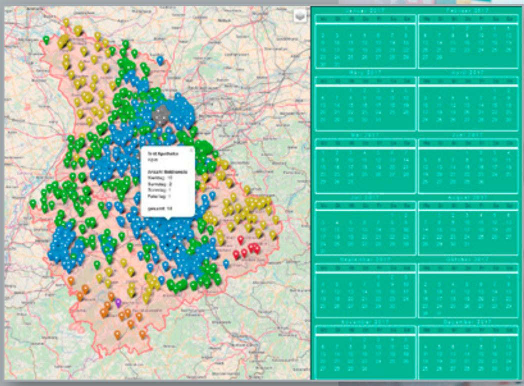
Optimization and experimental design

As mentioned above, a key element is the planning of new experiments. This activity is often time consuming and costly, which makes efficient design of experiments even more important. Our tool helps to reduce the number of attempts required and saves valuable resources for the user.

The problem is solved as follows: The user navigates within a range towards the most attractive target functions. This requires a multi-criteria optimization to be performed in advance. The new experiments are planned within the boundaries of this range. The tool also supports forward planning based on the model, which means the user can directly test particularly promising individual recipes. The user also receives information about the uncertainty of the prediction in the form of confidence intervals.

Web architecture in a big data system

The software is implemented as a web solution with a modern database, which is able to manage a large amount of data. By doing so, a simple and computer-independent use of the tool on mobile devices such as tablets is ensured. At the same time, team productivity is increased because all data are stored centrally and all users always have access to the latest version.



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HealthFaCT – OPTIMIZING OUTPATIENT MEDICAL CARE IN RURAL AREAS

1 *Interactive evaluation and exploration of optimised pharmacy emergency service plans*

2 *Pharmacies are an essential component of outpatient medical care.*

Our healthcare system faces major challenges in outpatient medical care. Despite the decline in population and rising costs, medical care must still be guaranteed in rural areas. The aim of HealthFaCT (Facility Location, Covering and Transport) is to find the optimal distribution of the scarce health care resources in rural areas.

The collaborative project HealthFaCT is developing an innovative software-based optimization and decision-making system to improve outpatient medical care. The software quickly identifies and evaluates the best possible option for strategic, tactical, and operational decisions. In addition, the user can interactively visualize, explore, analyze, and verify the results. We are developing a web-based simulation platform that integrates the optimization methods designed by our project partners.

Research alliance with focus on three pillars

The project is funded by the German Federal Ministry of Education and Research (BMBF) and focuses on three major pillars of outpatient care: Pharmacies, emergency doctors, and ambulance and rescue services. Together with our project partners RWTH Aachen University, Technical University of Kaiserslautern, and University of Erlangen-Nuremberg, we are optimizing the following three areas based on future requirements forecasting:

- Location structure and emergency service plan for pharmacies
- Location structure and resource distribution for emergency doctors
- Waiting times in the ambulance and rescue services

Software-based implementation of mathematical algorithms

The project primarily studies location, coverage, and route planning problems from a mathematical perspective. The main challenges are real time optimization and robustness against uncertainties. Moreover, in a complex use case with divergent target functions, it is not possible to determine a single optimal solution by means of a purely algorithmic approach.

Therefore, we develop a data-driven tool that focuses on the decision maker. The software objectively shows the user different options and provides opportunities to interactively evaluate the solutions. Discussions with the application partners prove the need and the enormous potential of such a software-based optimization and decision-making system.

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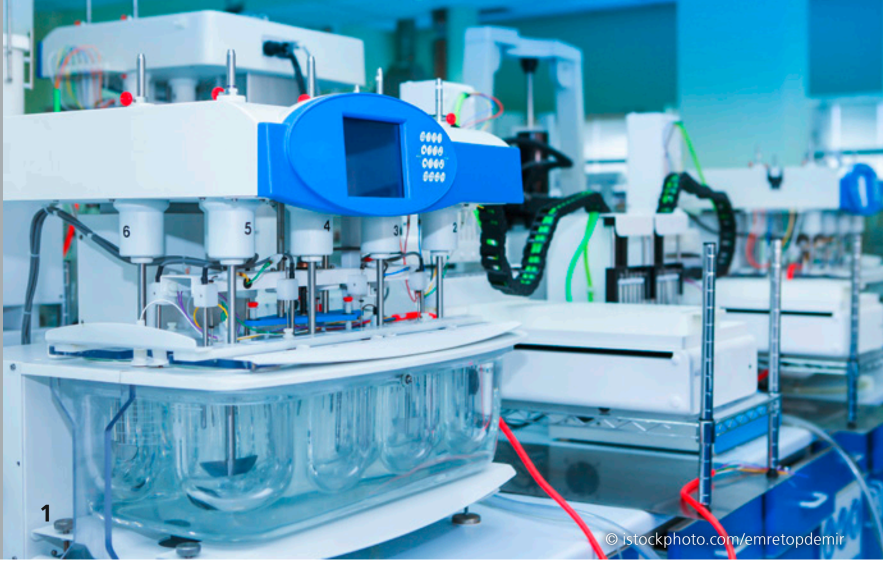

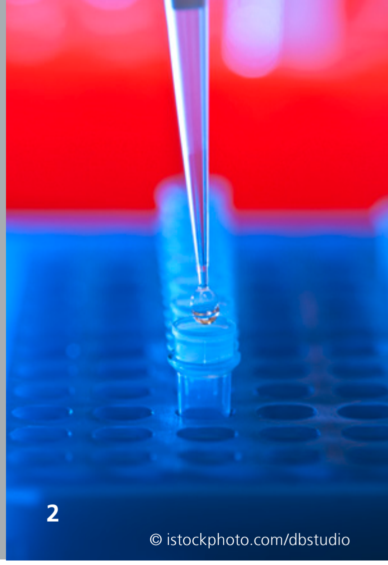

PERSONALIZED MEDICINE – METHODS FOR PRODUCTION PLANNING

Personalized therapies are new and promising trends for the treatment of many diseases. They have been proven exceptionally effective in low scale tests. However, in order to succeed economically, the production processes need to be scaled to an industrial level. They need to be secure, cost efficient and last, but not least, fast. After all, long waits will be unacceptable for patients – especially in life and death situations. Therefore, it is of the essence that the production is planned and executed optimally.

1 *Laboratory equipment*

2 *Pipetting a DNA solution*

Challenges of bio-processes

Bio-processes show characteristics that complicate the optimal design and efficient management of industrialized processes.

- High quality standards often call for re-executing process phases for individual patients.
- Heterogeneous processing times complicate the development of a periodic production flow.
- The probabilistic nature of processing times and error occurrence prevent a structured, predictable workflow.

Approaches for process optimization

First, we can get a better understanding of the processes by carefully studying the capacities of different process phases, especially those with high failure rates. For example: In which period should a patient ideally arrive so there are no long waiting times? Knowing this, we can align process phases and determine where to keep additional production capacities ready to compensate for workload spikes. Furthermore, the purchase of more or better devices can be evaluated.

In order to avoid frequent changes to the production plan, we can add puffer times between production steps. Thereby, we can limit the impact of delays to a small part of the process and it is possible to set up a periodic production schedules: For every process section, we determine when best to start and how many patients should roughly be processed at the same time. The resulting schedule is more stable, although errors and probabilistic processing times still cause some variance.

These are just two examples of how we analyze the individual challenges of bioprocesses and develop new methods to manage and optimize workflows. Using digital twins of the processes, we assess our strategies and simulate the interactions of different ideas.

NEWS

SOFTWARE-PLATFORM FOR COLLABORATIVE WORK-SHIFT SCHEDULING IN HEALTHCARE PROFESSIONS

In 2017, our department started the GamOR (GameOfRoster) research project with the aim of developing models and algorithms to assist nurses and others in the planning of their work schedules. The special focus is on the identification of incompatible planning requests and their resolution using methods from game theory. In cooperation with ergonomists, designers and application partners, we implement the models and algorithms in a prototype software to test and evaluate the services in daily operations.

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DIGITALIZATION OF CONSTRUCTION SERVICES AND PROCESSES WITH INDUSTRIE 4.0 TECHNOLOGIES

How can digitalization be used to improve and redesign services and processes in construction engineering? Answering this question is the aim of the collaborative project ConWearDi (Construction – Wearables – Digitization) launched in 2017. The main effort of the Optimization department, besides implementing a prototype of integrating software-platform, is the study of stochastic scheduling models that can be used for scheduling and control on construction sites.

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FLAGSHIP PROJECT – QUANTUM METHODS FOR ADVANCED IMAGING SOLUTIONS (QUILT)

In recent years, a second generation of quantum technologies has emerged. The flagship project QUILT bundles the expertise of six Fraunhofer Institutes and other quantum technology centers, such as the Institute for Quantum Optics and Quantum Information at the Austrian Academy of Sciences, and the Max Planck Institute for the Science of Light. We make contributions in the field of quantum imaging and play a key role in the modeling, simulation, and optimization of quantum-based non-contact methods. Launched in 2017, the project aim is to make rendering processes for material surfaces more reliable, faster, and less expensive.

Front, left to right: -Dr. Alexander Scherrer , Jasmin Kirchner, Pascal Wortel, Prof. Dr. Karl-Heinz Küfer, Dr. Christian Weiß, Dr. Michael Helmling, Dr. Tobias Fischer, Dr. Gregor Foltin, Dr. Michal Walczak, Dr. Sebastian Velten, Dr. Martin von Kurnatowski, Dr. Volker Maag, Dr.-Ing. Tino Fleuren, Dr. Heiner Ackermann, Dr. Patricia Bickert, Dr. Neil Jami, Julie Damay, Diana Ackermann, Andreas Dinges, Dr. Neele Leithäuser, Dr. Elisabeth Finhold, Felix Riexinger, Dr. Dimitri Nowak, Dr. Michael Bortz, Till Heller, Esther Bonacker, Dr. Johannes Höller, Melanie Heidgen, Johanna Schneider, Patrick Schwartz , Dr. Raoul Heese, Tobias Seidel, Dr. Jens Babutzka, Dr. Philipp Süss, Dr. Kai Plociennik, Dr. Jan Schwientek, Rasmus Schroeder